



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 01:47 PM EST

PDB ID : 2KR9
BMRB ID : 16632
Title : Kalirin DH1 NMR structure
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Deposited on : 2009-12-10

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

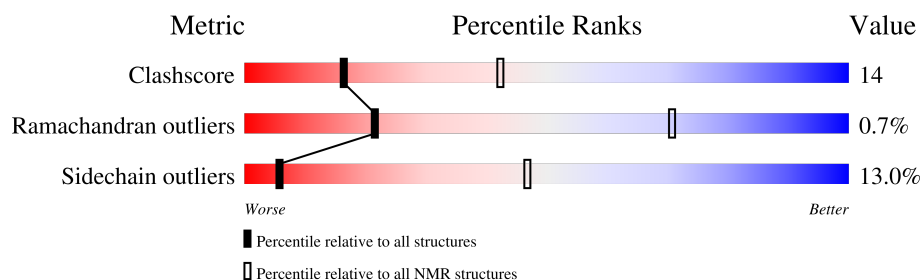
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	190	<div> <div>52%</div> <div>29%</div> <div>•</div> <div>15%</div> </div>

2 Ensemble composition and analysis

This entry contains 15 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest total energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:16-A:160, A:170-A:185 (161)	0.33	10

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	3, 4, 6, 7, 8, 9, 10, 11, 13, 14
2	1, 2, 12, 15
Single-model clusters	5

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3079 atoms, of which 1534 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kalirin.

Mol	Chain	Residues	Atoms						Trace
1	A	190	Total	C	H	N	O	S	0
			3079	993	1534	251	291	10	

There are 10 discrepancies between the modelled and reference sequences:

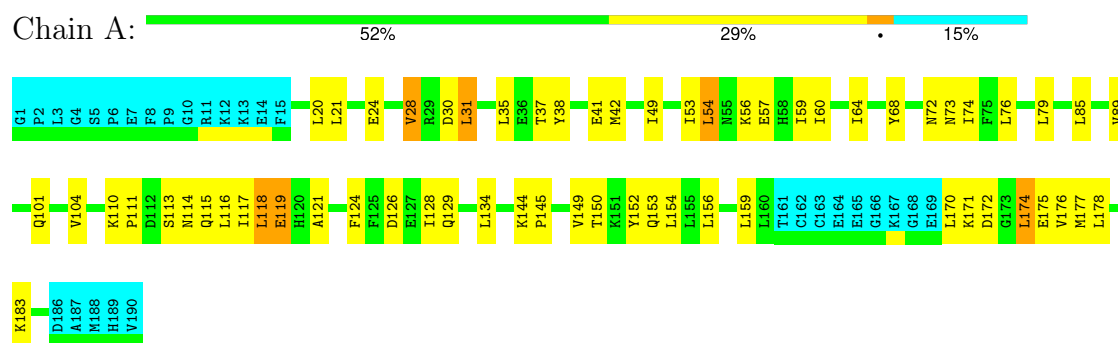
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P97924
A	2	PRO	-	expression tag	UNP P97924
A	3	LEU	-	expression tag	UNP P97924
A	4	GLY	-	expression tag	UNP P97924
A	5	SER	-	expression tag	UNP P97924
A	6	PRO	-	expression tag	UNP P97924
A	7	GLU	-	expression tag	UNP P97924
A	8	PHE	-	expression tag	UNP P97924
A	9	PRO	-	expression tag	UNP P97924
A	10	GLY	-	expression tag	UNP P97924

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: Kalirin

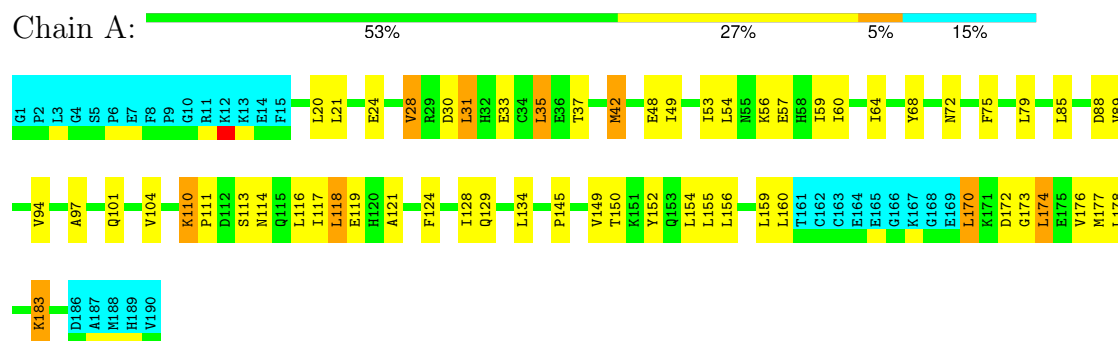


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

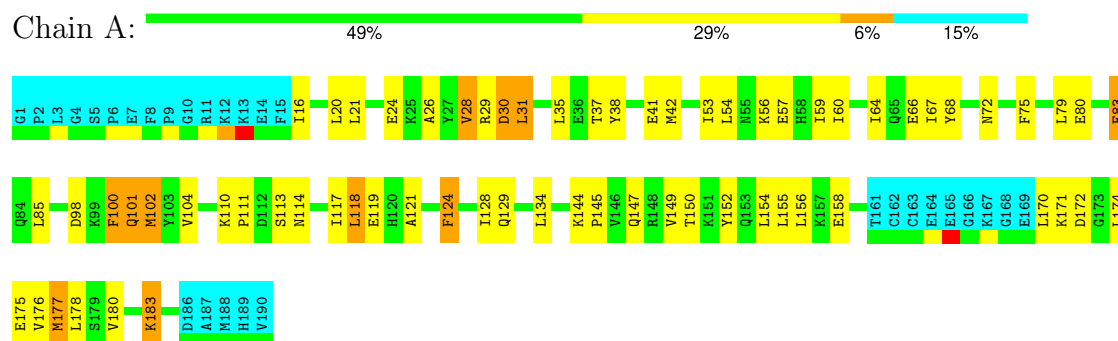
4.2.1 Score per residue for model 1

- Molecule 1: Kalirin



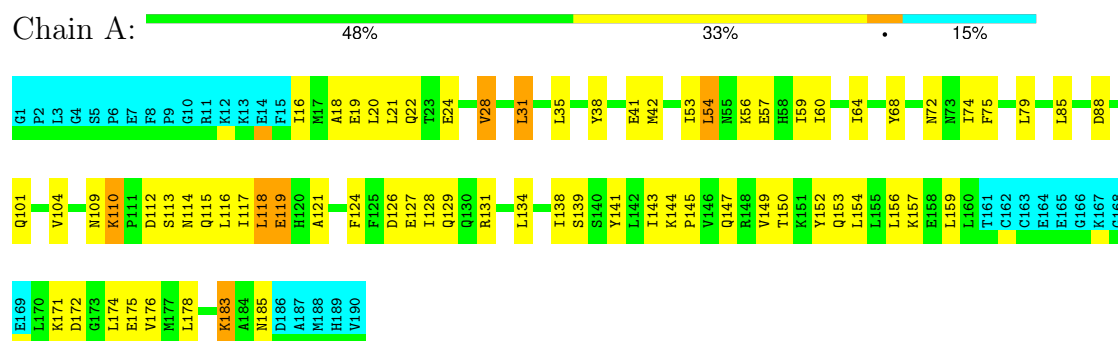
4.2.2 Score per residue for model 2

- Molecule 1: Kalirin



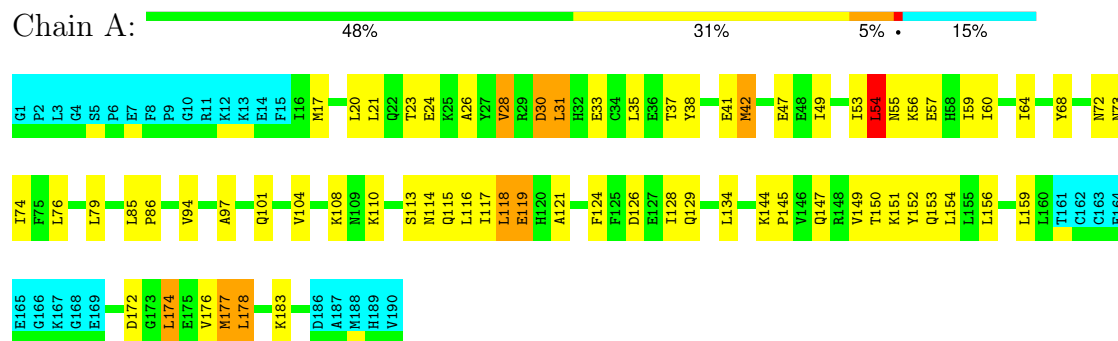
4.2.3 Score per residue for model 3

- Molecule 1: Kalirin



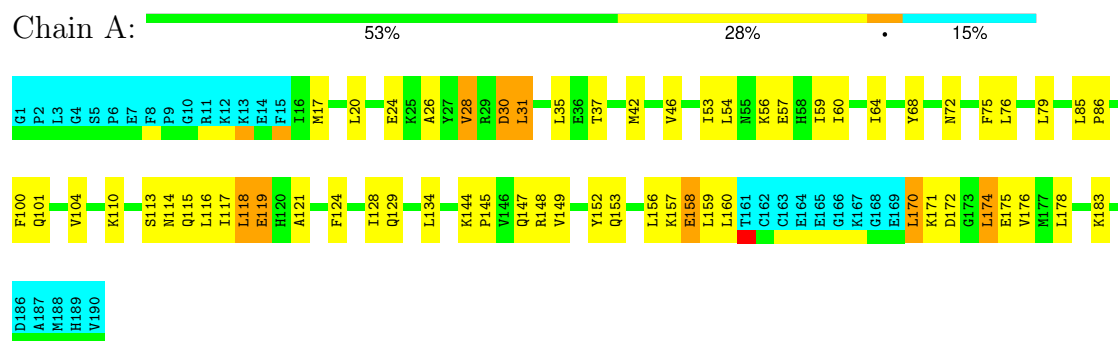
4.2.4 Score per residue for model 4

- Molecule 1: Kalirin



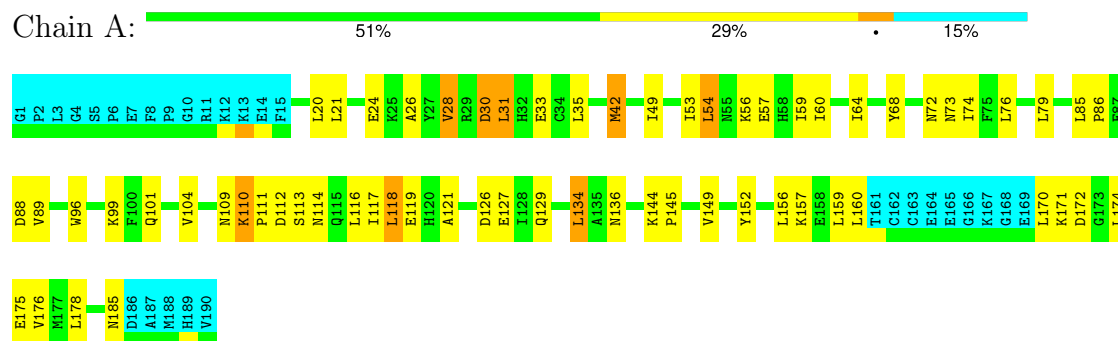
4.2.5 Score per residue for model 5

- Molecule 1: Kalirin



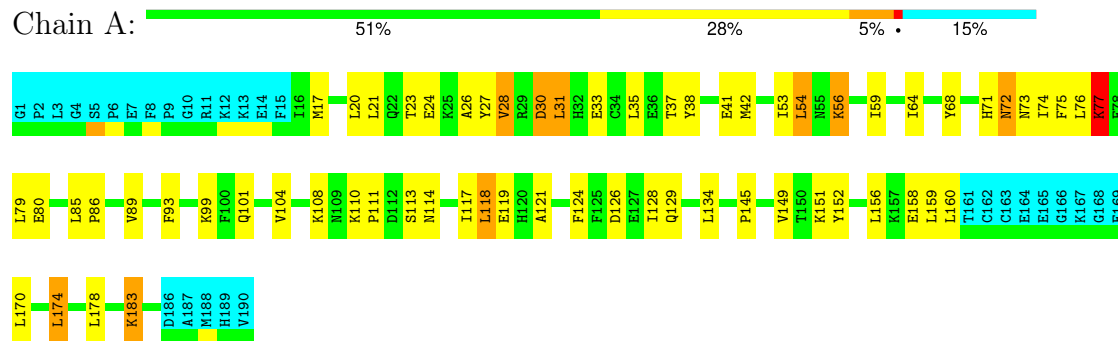
4.2.6 Score per residue for model 6

- Molecule 1: Kalirin



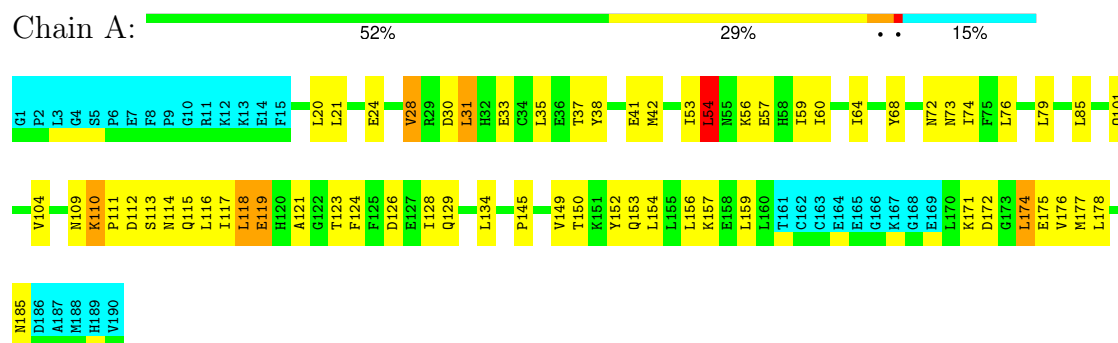
4.2.7 Score per residue for model 7

- Molecule 1: Kalirin



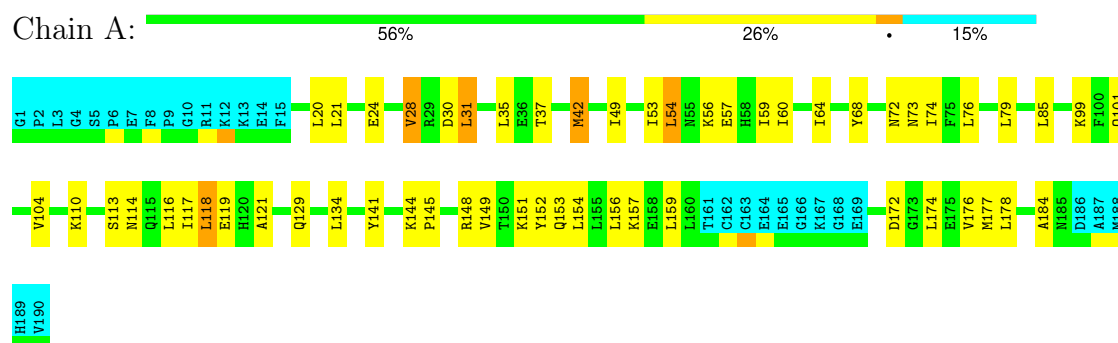
4.2.8 Score per residue for model 8

- Molecule 1: Kalirin



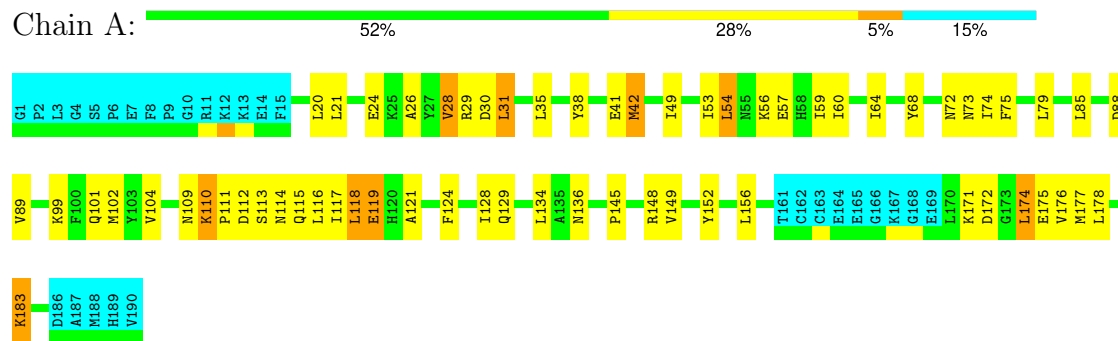
4.2.9 Score per residue for model 9

- Molecule 1: Kalirin



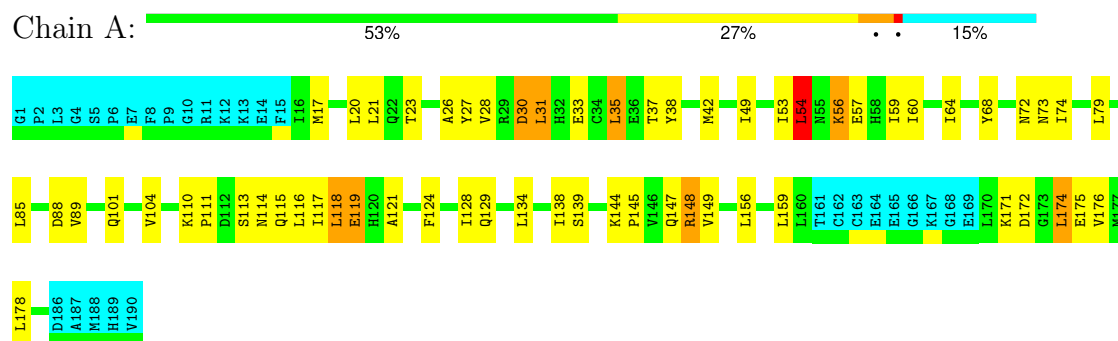
4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Kalirin



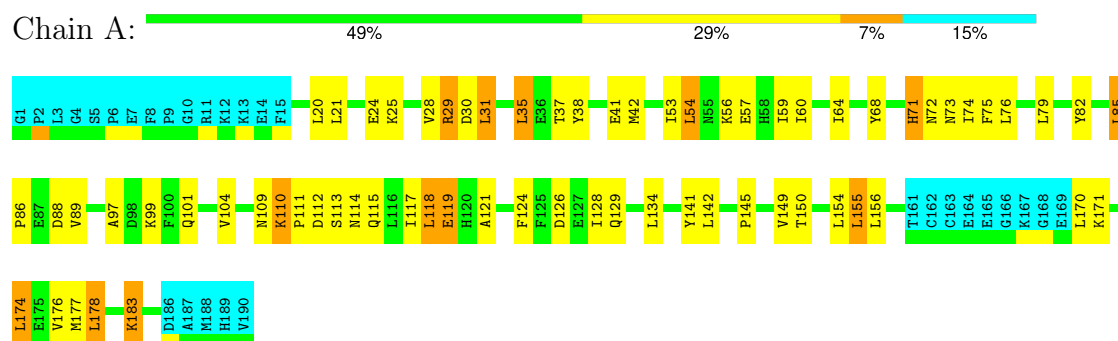
4.2.11 Score per residue for model 11

- Molecule 1: Kalirin



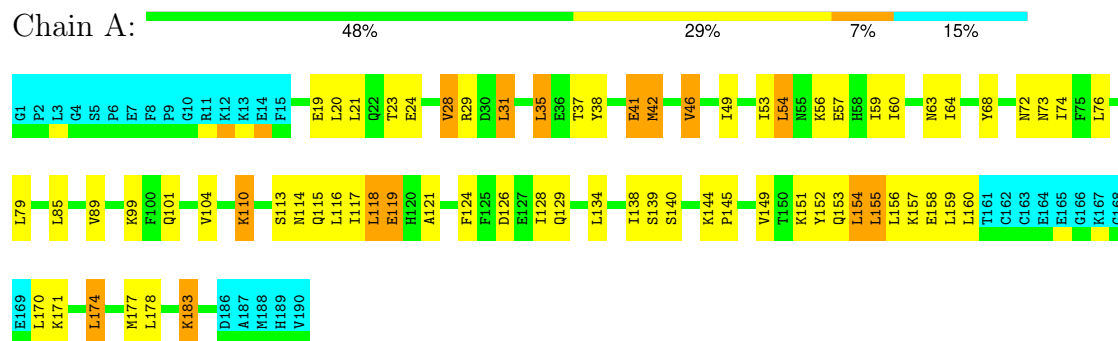
4.2.12 Score per residue for model 12

- Molecule 1: Kalirin



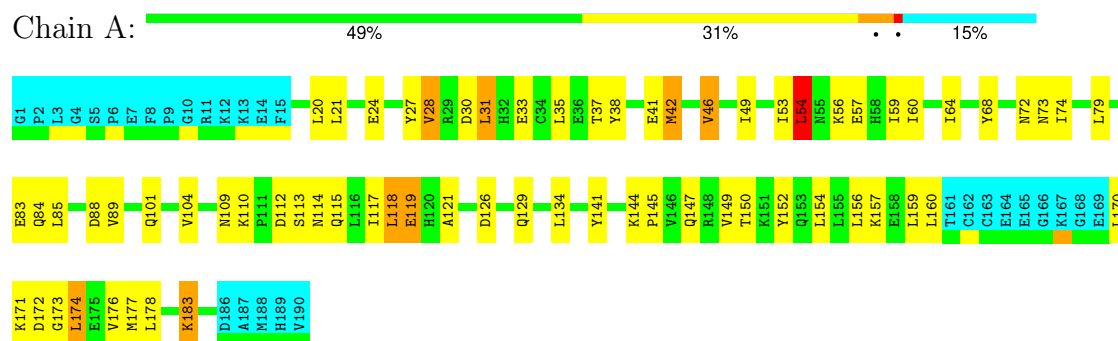
4.2.13 Score per residue for model 13

- Molecule 1: Kalirin



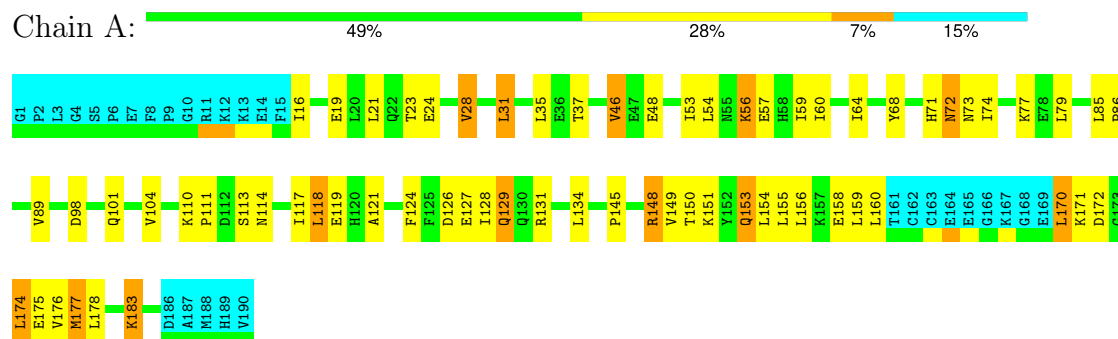
4.2.14 Score per residue for model 14

- Molecule 1: Kalirin



4.2.15 Score per residue for model 15

- Molecule 1: Kalirin



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *Total energy*.

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

Software name	Classification	Version
ARIA	structure solution	2.2
CYANA	geometry optimization	2.1
ARIA	refinement	2.2

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	2
Total number of shifts	4978
Number of shifts mapped to atoms	4978
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.34±0.01	0±0/1358 (0.0± 0.0%)	0.54±0.03	0±1/1838 (0.0± 0.0%)
All	All	0.34	0/20370 (0.0%)	0.54	4/27570 (0.0%)

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
1	A	0.0±0.0	0.1±0.2
All	All	0	1

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	77	LYS	N-CA-CB	-11.25	90.35	110.60	7	1
1	A	101	GLN	N-CA-CB	-9.66	93.22	110.60	2	1
1	A	101	GLN	CB-CA-C	-6.21	97.99	110.40	2	1
1	A	77	LYS	CA-CB-CG	-5.78	100.69	113.40	7	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	100	PHE	Peptide	1

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	1327	1328	1322	37±4
All	All	19905	19920	19830	551

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:100:PHE:HB3	1:A:180:VAL:HG21	0.86	1.48	2	1
1:A:129:GLN:HA	1:A:134:LEU:HD12	0.85	1.49	12	14
1:A:24:GLU:HB3	1:A:76:LEU:HG	0.76	1.58	4	7
1:A:148:ARG:HH11	1:A:148:ARG:HB3	0.75	1.41	11	1
1:A:101:GLN:O	1:A:104:VAL:HG12	0.74	1.82	13	15
1:A:151:LYS:HD3	1:A:154:LEU:HD12	0.73	1.59	9	2
1:A:37:THR:HG21	1:A:134:LEU:HD21	0.72	1.61	14	12
1:A:183:LYS:HA	1:A:183:LYS:HE3	0.71	1.60	12	5
1:A:145:PRO:O	1:A:149:VAL:HG23	0.70	1.86	9	15
1:A:152:TYR:O	1:A:156:LEU:HB3	0.69	1.87	4	10
1:A:156:LEU:HD21	1:A:174:LEU:HA	0.68	1.65	13	15
1:A:110:LYS:HA	1:A:110:LYS:HE2	0.66	1.65	1	1
1:A:74:ILE:O	1:A:77:LYS:HB2	0.66	1.90	7	1
1:A:53:ILE:HA	1:A:56:LYS:HB2	0.65	1.68	15	15
1:A:174:LEU:O	1:A:178:LEU:HG	0.64	1.92	3	15
1:A:104:VAL:O	1:A:108:LYS:HG3	0.63	1.93	4	1
1:A:126:ASP:O	1:A:129:GLN:HB3	0.63	1.93	13	9
1:A:42:MET:HA	1:A:49:ILE:HD11	0.63	1.71	14	7
1:A:56:LYS:HG3	1:A:59:ILE:HD13	0.63	1.71	12	15
1:A:176:VAL:HG13	1:A:177:MET:HE3	0.62	1.71	2	2
1:A:30:ASP:HB3	1:A:144:LYS:HE2	0.62	1.72	9	1
1:A:17:MET:HB2	1:A:86:PRO:HB3	0.62	1.72	5	3
1:A:21:LEU:HD23	1:A:79:LEU:HD23	0.61	1.71	15	13
1:A:18:ALA:O	1:A:22:GLN:HG2	0.60	1.97	3	1
1:A:156:LEU:HG	1:A:160:LEU:HD23	0.60	1.74	6	2
1:A:23:THR:HB	1:A:148:ARG:HD3	0.60	1.73	11	2
1:A:129:GLN:HG3	1:A:134:LEU:O	0.60	1.97	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:GLY:O	1:A:177:MET:HG2	0.59	1.97	1	2
1:A:27:TYR:HA	1:A:30:ASP:OD2	0.58	1.97	14	1
1:A:141:TYR:O	1:A:144:LYS:HB3	0.58	1.98	9	2
1:A:31:LEU:O	1:A:35:LEU:HG	0.58	1.98	3	15
1:A:171:LYS:O	1:A:175:GLU:HG3	0.58	1.98	5	7
1:A:153:GLN:OE1	1:A:177:MET:HG2	0.58	1.98	15	2
1:A:110:LYS:O	1:A:113:SER:HB3	0.57	1.99	1	4
1:A:110:LYS:HB3	1:A:111:PRO:HD3	0.56	1.75	10	9
1:A:104:VAL:HG21	1:A:183:LYS:HB3	0.56	1.76	10	4
1:A:144:LYS:HA	1:A:147:GLN:HG3	0.56	1.76	5	2
1:A:38:TYR:CE1	1:A:134:LEU:HD13	0.55	2.36	8	9
1:A:117:ILE:HA	1:A:121:ALA:CB	0.55	2.32	8	15
1:A:153:GLN:O	1:A:157:LYS:HG2	0.55	2.01	8	4
1:A:20:LEU:HG	1:A:79:LEU:HD21	0.55	1.78	10	12
1:A:31:LEU:HB3	1:A:68:TYR:HB2	0.55	1.78	15	15
1:A:101:GLN:HA	1:A:101:GLN:OE1	0.54	2.02	8	1
1:A:60:ILE:HD12	1:A:117:ILE:HG23	0.54	1.78	5	14
1:A:151:LYS:O	1:A:155:LEU:HG	0.54	2.02	13	1
1:A:171:LYS:O	1:A:175:GLU:HG2	0.54	2.02	2	1
1:A:114:ASN:O	1:A:118:LEU:HD22	0.54	2.03	4	15
1:A:148:ARG:HE	1:A:152:TYR:HE1	0.53	1.45	5	1
1:A:24:GLU:HG3	1:A:76:LEU:HA	0.53	1.80	4	3
1:A:59:ILE:HG21	1:A:116:LEU:HD22	0.53	1.80	1	10
1:A:98:ASP:O	1:A:101:GLN:HG2	0.53	2.04	2	1
1:A:144:LYS:HA	1:A:147:GLN:CG	0.53	2.34	4	4
1:A:24:GLU:O	1:A:28:VAL:HG13	0.53	2.02	7	13
1:A:73:ASN:OD1	1:A:74:ILE:HG13	0.52	2.04	6	10
1:A:172:ASP:O	1:A:176:VAL:HG12	0.52	2.05	3	12
1:A:157:LYS:HA	1:A:160:LEU:HG	0.52	1.79	6	1
1:A:22:GLN:HA	1:A:22:GLN:OE1	0.52	2.05	3	1
1:A:117:ILE:HA	1:A:121:ALA:HB3	0.52	1.80	7	11
1:A:100:PHE:CE2	1:A:152:TYR:HE2	0.52	2.22	5	1
1:A:72:ASN:O	1:A:77:LYS:HE2	0.51	2.05	7	2
1:A:30:ASP:HB2	1:A:141:TYR:CE1	0.51	2.40	14	2
1:A:16:ILE:O	1:A:19:GLU:HB3	0.51	2.06	15	2
1:A:67:ILE:CD1	1:A:102:MET:HG2	0.51	2.35	2	1
1:A:160:LEU:HB3	1:A:170:LEU:HB3	0.50	1.83	7	4
1:A:148:ARG:HB3	1:A:148:ARG:NH1	0.50	2.18	11	1
1:A:26:ALA:O	1:A:30:ASP:HB3	0.50	2.07	4	5
1:A:113:SER:O	1:A:117:ILE:HG12	0.50	2.07	12	14
1:A:156:LEU:HD21	1:A:174:LEU:CA	0.49	2.36	13	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:PHE:CZ	1:A:128:ILE:HD11	0.49	2.43	5	12
1:A:21:LEU:HD22	1:A:80:GLU:OE2	0.48	2.08	2	1
1:A:99:LYS:HG3	1:A:102:MET:SD	0.48	2.48	10	1
1:A:150:THR:O	1:A:154:LEU:HG	0.48	2.09	4	8
1:A:109:ASN:HA	1:A:112:ASP:OD1	0.48	2.08	8	4
1:A:129:GLN:OE1	1:A:134:LEU:HB2	0.48	2.07	13	2
1:A:183:LYS:O	1:A:183:LYS:HE3	0.48	2.09	2	1
1:A:23:THR:O	1:A:27:TYR:HB2	0.47	2.08	11	1
1:A:25:LYS:O	1:A:29:ARG:HB2	0.47	2.08	12	1
1:A:20:LEU:HB2	1:A:155:LEU:HD22	0.47	1.86	12	2
1:A:86:PRO:O	1:A:89:VAL:HG22	0.47	2.10	12	2
1:A:115:GLN:O	1:A:119:GLU:HG3	0.47	2.10	3	9
1:A:155:LEU:O	1:A:159:LEU:HG	0.47	2.09	1	2
1:A:144:LYS:HA	1:A:147:GLN:HG2	0.47	1.86	4	1
1:A:73:ASN:HA	1:A:77:LYS:HE3	0.47	1.85	7	1
1:A:17:MET:O	1:A:21:LEU:HG	0.46	2.09	11	1
1:A:71:HIS:CD2	1:A:75:PHE:HB3	0.46	2.46	12	1
1:A:151:LYS:O	1:A:154:LEU:HB2	0.46	2.10	13	1
1:A:155:LEU:O	1:A:158:GLU:HB3	0.46	2.10	2	2
1:A:73:ASN:C	1:A:77:LYS:HD2	0.46	2.31	7	1
1:A:19:GLU:O	1:A:23:THR:HG23	0.46	2.10	13	1
1:A:151:LYS:HA	1:A:154:LEU:HD12	0.46	1.87	15	2
1:A:85:LEU:CD1	1:A:88:ASP:HB2	0.46	2.40	12	1
1:A:85:LEU:HD12	1:A:88:ASP:HB2	0.46	1.88	12	1
1:A:67:ILE:HD11	1:A:102:MET:HG2	0.46	1.88	2	1
1:A:100:PHE:HB3	1:A:180:VAL:CG2	0.46	2.32	2	1
1:A:82:TYR:CD2	1:A:89:VAL:HG12	0.45	2.47	12	1
1:A:26:ALA:O	1:A:30:ASP:HB2	0.45	2.12	11	2
1:A:157:LYS:HD3	1:A:160:LEU:HD11	0.45	1.87	14	1
1:A:109:ASN:HA	1:A:112:ASP:OD2	0.45	2.12	14	2
1:A:99:LYS:HG3	1:A:99:LYS:O	0.44	2.11	9	2
1:A:157:LYS:HD2	1:A:160:LEU:HD21	0.44	1.89	13	1
1:A:183:LYS:HA	1:A:183:LYS:CE	0.44	2.42	1	2
1:A:171:LYS:HD2	1:A:174:LEU:HD23	0.44	1.89	11	2
1:A:110:LYS:HB3	1:A:110:LYS:NZ	0.44	2.27	13	1
1:A:27:TYR:O	1:A:31:LEU:HD22	0.44	2.12	7	1
1:A:59:ILE:HG22	1:A:113:SER:HA	0.43	1.89	3	1
1:A:183:LYS:HA	1:A:183:LYS:HE2	0.43	1.90	1	1
1:A:127:GLU:O	1:A:131:ARG:HG3	0.43	2.13	3	2
1:A:104:VAL:CG2	1:A:183:LYS:HB3	0.43	2.44	2	1
1:A:80:GLU:O	1:A:83:GLU:HG3	0.43	2.13	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:VAL:HB	1:A:180:VAL:HG13	0.43	1.91	2	1
1:A:23:THR:HA	1:A:26:ALA:HB3	0.43	1.91	4	1
1:A:156:LEU:CG	1:A:160:LEU:HD23	0.43	2.43	5	1
1:A:138:ILE:HG23	1:A:139:SER:N	0.43	2.29	11	3
1:A:99:LYS:O	1:A:99:LYS:HG3	0.43	2.13	12	1
1:A:41:GLU:HG3	1:A:128:ILE:CD1	0.43	2.43	13	1
1:A:129:GLN:HA	1:A:134:LEU:CD1	0.42	2.39	14	3
1:A:94:VAL:HA	1:A:97:ALA:HB2	0.42	1.91	1	2
1:A:54:LEU:C	1:A:56:LYS:H	0.42	2.18	14	2
1:A:149:VAL:HG12	1:A:153:GLN:OE1	0.42	2.14	13	1
1:A:23:THR:HG21	1:A:151:LYS:CD	0.42	2.44	7	1
1:A:104:VAL:HG21	1:A:183:LYS:CG	0.42	2.44	15	1
1:A:174:LEU:HD12	1:A:178:LEU:HD21	0.42	1.91	12	2
1:A:93:PHE:HE1	1:A:152:TYR:CD2	0.42	2.33	7	1
1:A:54:LEU:HD13	1:A:55:ASN:ND2	0.42	2.30	4	1
1:A:170:LEU:HD12	1:A:170:LEU:H	0.42	1.75	12	1
1:A:16:ILE:HD12	1:A:158:GLU:OE2	0.42	2.15	2	1
1:A:143:ILE:O	1:A:147:GLN:HG2	0.42	2.14	3	1
1:A:144:LYS:HB3	1:A:145:PRO:HD3	0.42	1.90	6	1
1:A:140:SER:O	1:A:144:LYS:HG2	0.42	2.15	13	1
1:A:156:LEU:O	1:A:160:LEU:HG	0.42	2.14	5	1
1:A:38:TYR:O	1:A:42:MET:HG3	0.41	2.15	4	1
1:A:96:TRP:CE3	1:A:99:LYS:HE3	0.41	2.49	6	1
1:A:152:TYR:HA	1:A:155:LEU:HD11	0.41	1.91	13	1
1:A:104:VAL:HG21	1:A:183:LYS:HG3	0.41	1.91	15	1
1:A:47:GLU:CB	1:A:124:PHE:HE1	0.41	2.29	4	1
1:A:76:LEU:O	1:A:80:GLU:HG2	0.41	2.16	7	1
1:A:97:ALA:HB1	1:A:176:VAL:HG21	0.41	1.92	12	1
1:A:37:THR:HG21	1:A:134:LEU:CD2	0.41	2.46	4	1
1:A:38:TYR:CZ	1:A:134:LEU:HD13	0.40	2.52	3	1
1:A:49:ILE:HG21	1:A:54:LEU:HA	0.40	1.92	11	1
1:A:59:ILE:O	1:A:113:SER:HB2	0.40	2.16	1	1
1:A:83:GLU:OE2	1:A:84:GLN:HG3	0.40	2.16	14	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	161/190 (85%)	150±1 (93±1%)	10±1 (6±1%)	1±1 (1±1%)	21	71
All	All	2415/2850 (85%)	2244 (93%)	153 (6%)	18 (1%)	21	71

All 6 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	54	LEU	11
1	A	46	VAL	3
1	A	74	ILE	1
1	A	77	LYS	1
1	A	123	THR	1
1	A	154	LEU	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	148/171 (87%)	129±3 (87±2%)	19±3 (13±2%)	6	47
All	All	2220/2565 (87%)	1932 (87%)	288 (13%)	6	47

All 47 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	28	VAL	15
1	A	31	LEU	15
1	A	54	LEU	15
1	A	64	ILE	15
1	A	72	ASN	15
1	A	85	LEU	15
1	A	118	LEU	15
1	A	119	GLU	15
1	A	42	MET	14
1	A	57	GLU	14
1	A	174	LEU	11

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Mol	Chain	Res	Type	Models (Total)
1	A	183	LYS	10
1	A	110	LYS	9
1	A	41	GLU	9
1	A	30	ASP	8
1	A	177	MET	8
1	A	159	LEU	8
1	A	33	GLU	7
1	A	89	VAL	7
1	A	75	PHE	6
1	A	88	ASP	6
1	A	35	LEU	4
1	A	170	LEU	4
1	A	29	ARG	4
1	A	46	VAL	4
1	A	148	ARG	4
1	A	158	GLU	3
1	A	56	LYS	3
1	A	71	HIS	3
1	A	48	GLU	2
1	A	178	LEU	2
1	A	136	ASN	2
1	A	155	LEU	2
1	A	66	GLU	1
1	A	83	GLU	1
1	A	102	MET	1
1	A	124	PHE	1
1	A	185	ASN	1
1	A	127	GLU	1
1	A	134	LEU	1
1	A	99	LYS	1
1	A	142	LEU	1
1	A	171	LYS	1
1	A	63	ASN	1
1	A	98	ASP	1
1	A	129	GLN	1
1	A	153	GLN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 93% 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	2490
Number of shifts mapped to atoms	2490
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	189	-0.90 ± 0.20	Should be checked
$^{13}\text{C}_\beta$	178	0.29 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	187	-0.64 ± 0.14	Should be applied
^{15}N	180	0.89 ± 0.27	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 2159 atoms were assigned a chemical shift out of a possible 2305. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	798/800 (100%)	323/323 (100%)	320/322 (99%)	155/155 (100%)
Sidechain	1191/1291 (92%)	802/839 (96%)	372/413 (90%)	17/39 (44%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	170/214 (79%)	85/103 (83%)	83/97 (86%)	2/14 (14%)
Overall	2159/2305 (94%)	1210/1265 (96%)	775/832 (93%)	174/208 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 2486 atoms were assigned a chemical shift out of a possible 2661. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	936/944 (99%)	380/383 (99%)	376/380 (99%)	180/181 (99%)
Sidechain	1358/1475 (92%)	914/956 (96%)	427/474 (90%)	17/45 (38%)
Aromatic	192/242 (79%)	96/117 (82%)	94/109 (86%)	2/16 (12%)
Overall	2486/2661 (93%)	1390/1456 (95%)	897/963 (93%)	199/242 (82%)

7.1.4 Statistically unusual chemical shifts [i](#)

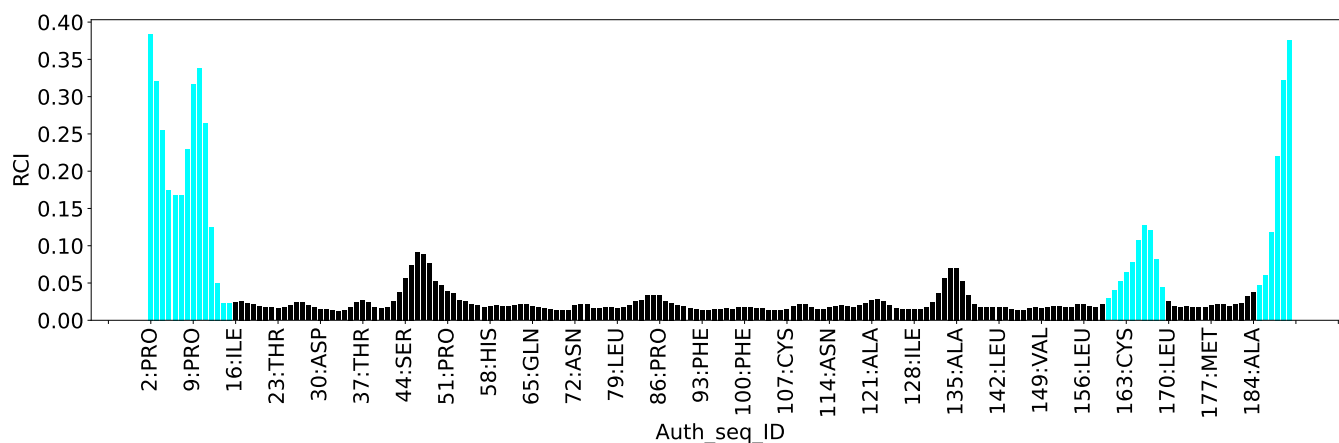
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	23	THR	HG1	5.70	0.08 – 2.19	21.6
1	A	27	TYR	HE1	5.00	5.59 – 7.82	-7.6
1	A	27	TYR	HE2	5.00	5.58 – 7.83	-7.6
1	A	99	LYS	HB2	0.20	0.58 – 2.97	-6.6
1	A	44	SER	HB3	2.22	2.49 – 5.20	-6.0
1	A	138	ILE	HB	0.31	0.35 – 3.22	-5.2

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping [i](#)

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

Total number of shifts	2488
Number of shifts mapped to atoms	2488
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	189	-0.87 ± 0.09	Should be checked
$^{13}\text{C}_\beta$	178	0.27 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	187	-0.62 ± 0.08	Should be applied
^{15}N	180	0.81 ± 0.19	Should be applied

7.2.3 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 94%, i.e. 2157 atoms were assigned a chemical shift out of a possible 2305. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	798/800 (100%)	323/323 (100%)	320/322 (99%)	155/155 (100%)
Sidechain	1191/1291 (92%)	802/839 (96%)	372/413 (90%)	17/39 (44%)
Aromatic	168/214 (79%)	85/103 (83%)	81/97 (84%)	2/14 (14%)
Overall	2157/2305 (94%)	1210/1265 (96%)	773/832 (93%)	174/208 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 2484 atoms were assigned a chemical shift out of a possible 2661. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	936/944 (99%)	380/383 (99%)	376/380 (99%)	180/181 (99%)
Sidechain	1358/1475 (92%)	914/956 (96%)	427/474 (90%)	17/45 (38%)
Aromatic	190/242 (79%)	96/117 (82%)	92/109 (84%)	2/16 (12%)
Overall	2484/2661 (93%)	1390/1456 (95%)	895/963 (93%)	199/242 (82%)

7.2.4 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.

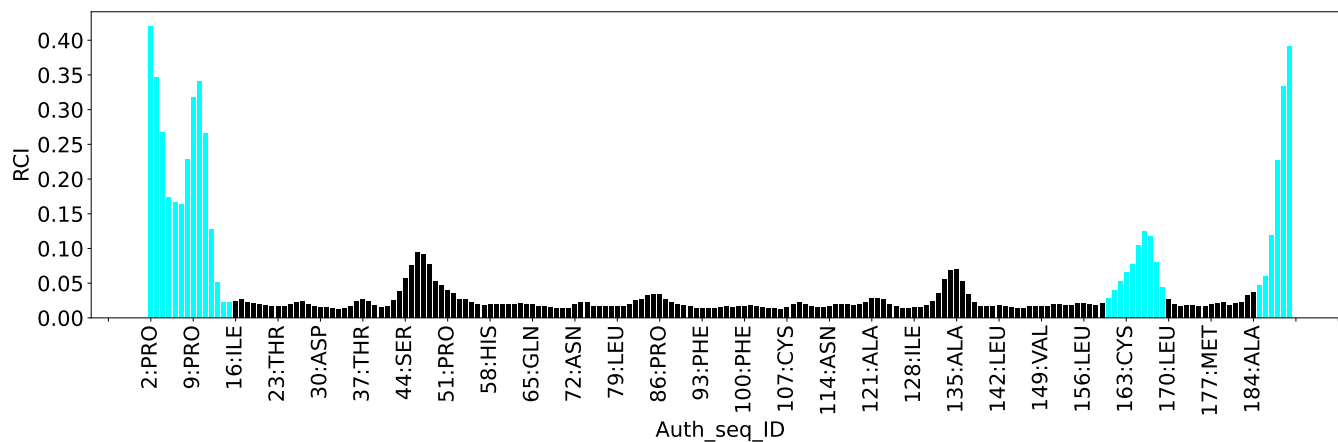
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	23	THR	HG1	5.68	0.08 – 2.19	21.5
2	A	27	TYR	HE1	5.00	5.59 – 7.82	-7.6
2	A	27	TYR	HE2	5.00	5.58 – 7.83	-7.6
2	A	99	LYS	HB2	0.18	0.58 – 2.97	-6.7
2	A	44	SER	HB3	2.22	2.49 – 5.20	-6.0
2	A	11	ARG	CZ	179.69	141.81 – 177.93	5.5
2	A	138	ILE	HB	0.30	0.35 – 3.22	-5.2

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-

defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	4993
Intra-residue ($ i-j =0$)	1236
Sequential ($ i-j =1$)	1275
Medium range ($ i-j >1$ and $ i-j <5$)	1387
Long range ($ i-j \geq 5$)	943
Inter-chain	0
Hydrogen bond restraints	152
Disulfide bond restraints	0
Total dihedral-angle restraints	306
Number of unmapped restraints	0
Number of restraints per residue	27.9
Number of long range restraints per residue ¹	5.0

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)	178.3	0.2
0.2-0.5 (Medium)	356.7	0.5
>0.5 (Large)	273.3	3.7

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	7.2	9.3
10.0-20.0 (Medium)	0.1	19.47
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

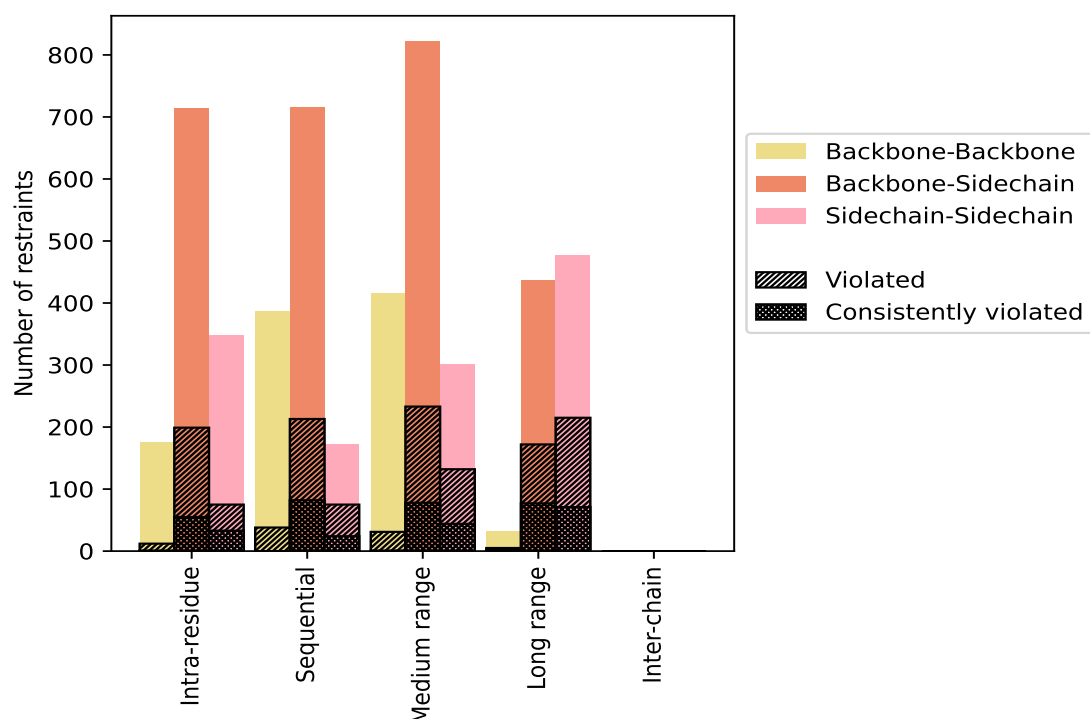
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1236	24.8	286	23.1	5.7	89	7.2	1.8
Backbone-Backbone	175	3.5	12	6.9	0.2	1	0.6	0.0
Backbone-Sidechain	714	14.3	199	27.9	4.0	55	7.7	1.1
Sidechain-Sidechain	347	6.9	75	21.6	1.5	33	9.5	0.7
Sequential ($i-j =1$)	1275	25.5	326	25.6	6.5	106	8.3	2.1
Backbone-Backbone	387	7.8	38	9.8	0.8	0	0.0	0.0
Backbone-Sidechain	716	14.3	213	29.7	4.3	82	11.5	1.6
Sidechain-Sidechain	172	3.4	75	43.6	1.5	24	14.0	0.5
Medium range ($i-j >1$ & $i-j <5$)	1387	27.8	384	27.7	7.7	123	8.9	2.5
Backbone-Backbone	416	8.3	31	7.5	0.6	1	0.2	0.0
Backbone-Sidechain	670	13.4	221	33.0	4.4	78	11.6	1.6
Sidechain-Sidechain	301	6.0	132	43.9	2.6	44	14.6	0.9
Long range ($i-j \geq 5$)	943	18.9	392	41.6	7.9	150	15.9	3.0
Backbone-Backbone	31	0.6	5	16.1	0.1	2	6.5	0.0
Backbone-Sidechain	436	8.7	172	39.4	3.4	77	17.7	1.5
Sidechain-Sidechain	476	9.5	215	45.2	4.3	71	14.9	1.4
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	152	3.0	12	7.9	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4993	100.0	1400	28.0	28.0	468	9.4	9.4
Backbone-Backbone	1009	20.2	86	8.5	1.7	4	0.4	0.1
Backbone-Sidechain	2688	53.8	817	30.4	16.4	292	10.9	5.8
Sidechain-Sidechain	1296	26.0	497	38.3	10.0	172	13.3	3.4

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	157	189	234	255	0	835	0.44	2.02	0.32	0.36
2	155	202	234	246	0	837	0.45	2.15	0.32	0.37
3	160	181	227	259	0	827	0.46	2.06	0.33	0.38
4	145	174	240	261	0	820	0.44	2.0	0.31	0.36
5	156	185	241	262	0	844	0.45	2.88	0.33	0.37
6	154	190	212	256	0	812	0.47	2.16	0.33	0.38
7	150	173	230	253	0	806	0.45	2.05	0.31	0.37
8	145	182	227	257	0	811	0.44	1.83	0.3	0.38
9	153	186	226	264	0	829	0.46	3.48	0.34	0.36
10	160	184	223	251	0	818	0.46	2.14	0.34	0.38

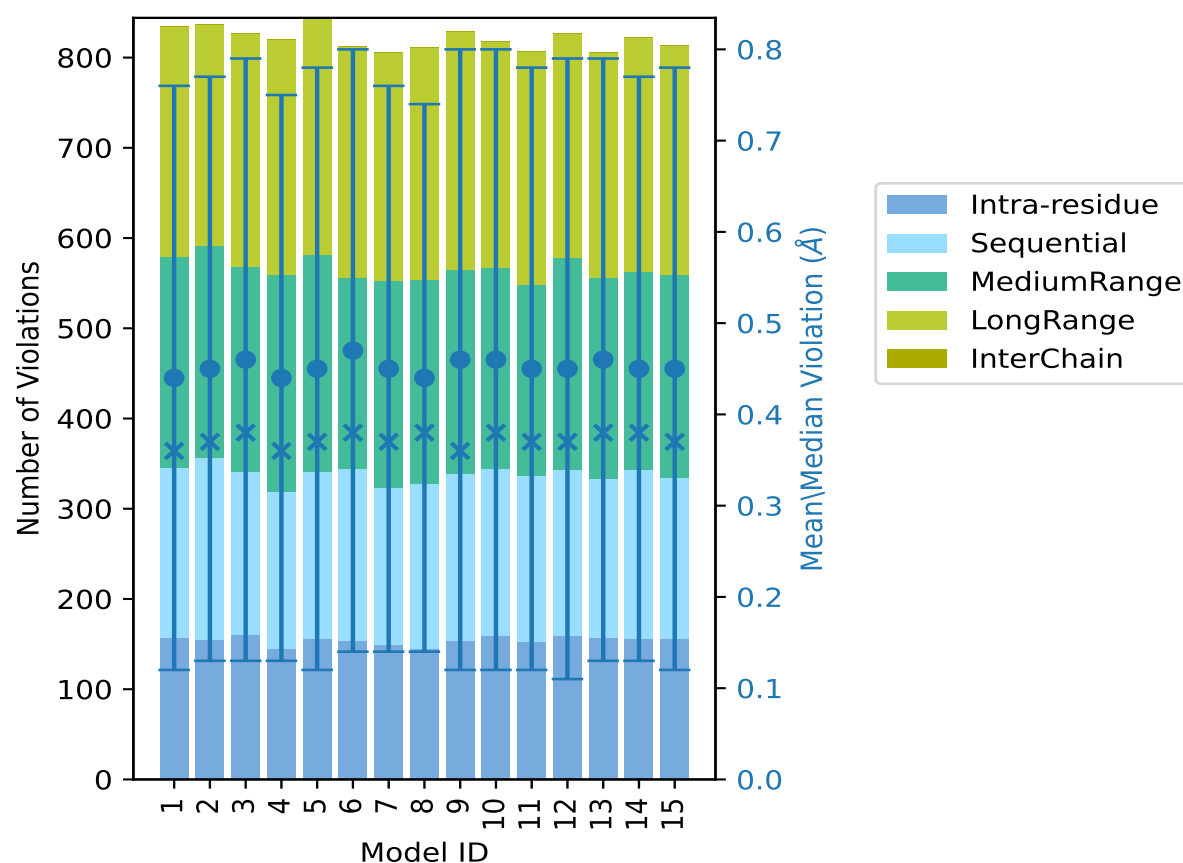
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	152	185	211	259	0	807	0.45	2.01	0.33	0.37
12	159	184	235	249	0	827	0.45	3.7	0.34	0.37
13	157	176	223	250	0	806	0.46	1.96	0.33	0.38
14	156	187	220	259	0	822	0.45	2.21	0.32	0.38
15	156	178	226	253	0	813	0.45	2.15	0.33	0.37

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

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



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

9.3 Distance violation statistics for the ensemble

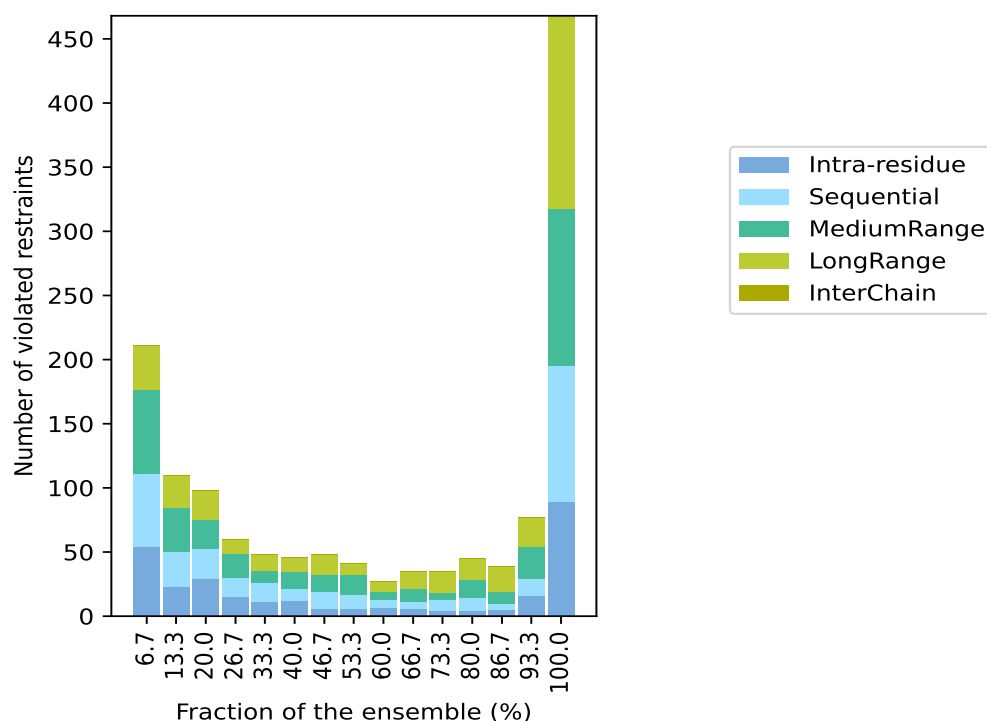
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3453(IR:950, SQ:949, MR:1003, LR:551, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
54	57	65	35	0	211	1	6.7
23	27	35	25	0	110	2	13.3
29	24	22	23	0	98	3	20.0
15	15	19	11	0	60	4	26.7
11	15	9	13	0	48	5	33.3
12	9	14	11	0	46	6	40.0
6	13	13	16	0	48	7	46.7
6	11	15	9	0	41	8	53.3
6	7	6	8	0	27	9	60.0
6	5	10	14	0	35	10	66.7
4	9	5	17	0	35	11	73.3
4	10	14	17	0	45	12	80.0
5	5	9	20	0	39	13	86.7
16	13	25	23	0	77	14	93.3
89	106	123	150	0	468	15	100.0

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

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

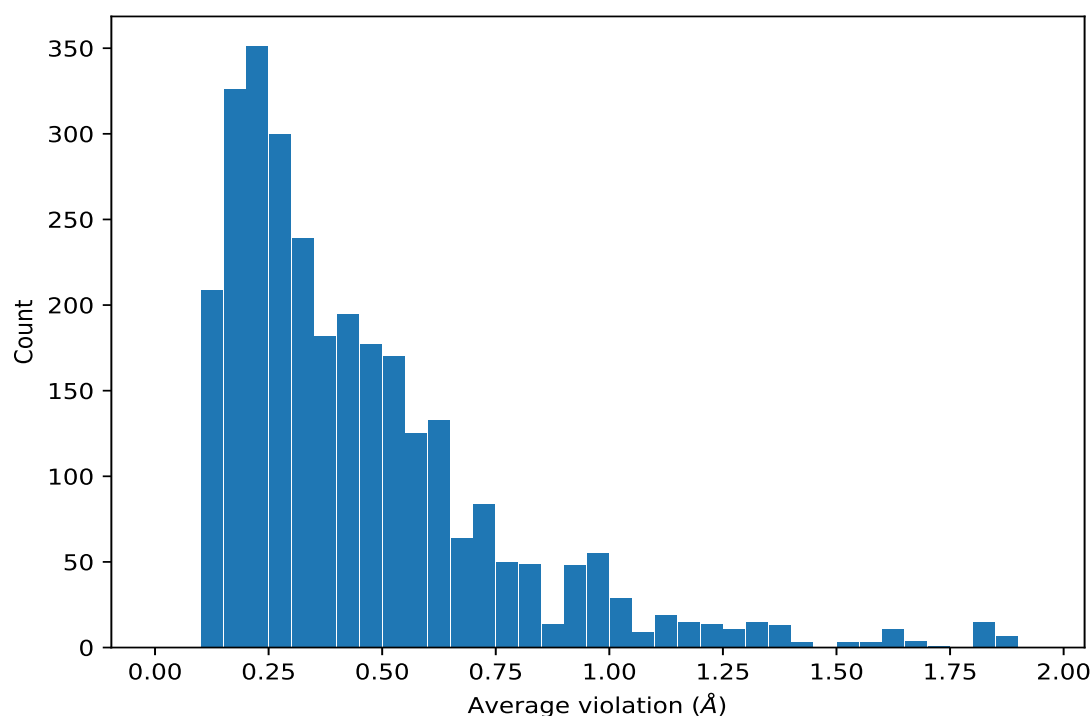
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,707)	1:18:A:ALA:HB2	1:21:A:LEU:HD23	15	1.86	0.07	1.85
(2,707)	1:18:A:ALA:HB2	1:21:A:LEU:HD22	15	1.86	0.07	1.85
(2,707)	1:18:A:ALA:HB3	1:21:A:LEU:HD21	15	1.86	0.07	1.85
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD23	15	1.86	0.07	1.85
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD21	15	1.86	0.07	1.85
(2,707)	1:18:A:ALA:HB3	1:21:A:LEU:HD23	15	1.86	0.07	1.85
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD22	15	1.86	0.07	1.85
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	15	1.82	0.08	1.82
(2,4259)	1:31:A:LEU:HD22	1:106:A:TYR:HD2	15	1.82	0.08	1.82
(2,4259)	1:31:A:LEU:HD21	1:106:A:TYR:HD2	15	1.82	0.08	1.82
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD12	15	1.81	0.45	2.01
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD13	15	1.81	0.45	2.01
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD11	15	1.81	0.45	2.01
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG21	15	1.81	0.19	1.86
(2,1569)	1:16:A:ILE:HD13	1:161:A:THR:HG21	15	1.81	0.19	1.86
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG22	15	1.81	0.19	1.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG22	15	1.81	0.19	1.86
(2,1569)	1:16:A:ILE:HD13	1:161:A:THR:HG23	15	1.81	0.19	1.86
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG23	15	1.81	0.19	1.86
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG21	15	1.81	0.19	1.86
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG23	15	1.81	0.19	1.86
(2,1569)	1:16:A:ILE:HD13	1:161:A:THR:HG22	15	1.81	0.19	1.86
(2,96)	1:180:A:VAL:HG21	1:181:A:PRO:HB2	15	1.65	0.04	1.66
(2,96)	1:180:A:VAL:HG23	1:181:A:PRO:HB2	15	1.65	0.04	1.66
(2,96)	1:180:A:VAL:HG22	1:181:A:PRO:HB2	15	1.65	0.04	1.66
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD11	15	1.62	0.06	1.63
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD13	15	1.62	0.06	1.63
(2,421)	1:53:A:ILE:HD13	1:138:A:ILE:HD11	15	1.62	0.06	1.63
(2,421)	1:53:A:ILE:HD13	1:138:A:ILE:HD12	15	1.62	0.06	1.63
(2,421)	1:53:A:ILE:HD11	1:138:A:ILE:HD11	15	1.62	0.06	1.63
(2,421)	1:53:A:ILE:HD11	1:138:A:ILE:HD12	15	1.62	0.06	1.63
(2,421)	1:53:A:ILE:HD11	1:138:A:ILE:HD13	15	1.62	0.06	1.63
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD12	15	1.62	0.06	1.63
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	15	1.6	0.14	1.61
(2,4359)	1:104:A:VAL:HG11	1:103:A:TYR:HD2	15	1.6	0.14	1.61
(2,4359)	1:104:A:VAL:HG12	1:103:A:TYR:HD2	15	1.6	0.14	1.61
(2,4549)	1:178:A:LEU:HD21	1:152:A:TYR:H	15	1.58	0.2	1.63
(2,4549)	1:178:A:LEU:HD22	1:152:A:TYR:H	15	1.58	0.2	1.63
(2,4549)	1:178:A:LEU:HD23	1:152:A:TYR:H	15	1.58	0.2	1.63
(2,52)	1:159:A:LEU:HD23	1:158:A:GLU:HB2	15	1.51	0.09	1.53
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	15	1.51	0.09	1.53
(2,52)	1:159:A:LEU:HD21	1:158:A:GLU:HB2	15	1.51	0.09	1.53
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	15	1.41	0.11	1.42
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	15	1.4	0.04	1.41
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD23	15	1.39	0.07	1.37
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD22	15	1.39	0.07	1.37
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD21	15	1.39	0.07	1.37
(2,4689)	1:18:A:ALA:H	1:16:A:ILE:HD12	15	1.39	0.07	1.37
(2,4689)	1:18:A:ALA:H	1:16:A:ILE:HD11	15	1.39	0.07	1.37
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	15	1.37	0.12	1.38
(2,4260)	1:156:A:LEU:HD11	1:172:A:ASP:HB2	15	1.34	0.15	1.33
(2,4260)	1:156:A:LEU:HD12	1:172:A:ASP:HB2	15	1.34	0.15	1.33
(2,4260)	1:156:A:LEU:HD12	1:172:A:ASP:HB3	15	1.34	0.15	1.33
(2,4260)	1:156:A:LEU:HD13	1:172:A:ASP:HB2	15	1.34	0.15	1.33
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	15	1.32	0.14	1.31
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	15	1.32	0.1	1.38
(2,4695)	1:23:A:THR:H	1:21:A:LEU:HD13	15	1.32	0.1	1.38
(2,4695)	1:23:A:THR:H	1:21:A:LEU:HD11	15	1.32	0.1	1.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4308)	1:106:A:TYR:HB3	1:184:A:ALA:HB1	15	1.32	0.15	1.32
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	15	1.32	0.15	1.32
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG2	15	1.32	0.15	1.32
(2,4308)	1:106:A:TYR:HB3	1:184:A:ALA:HB2	15	1.32	0.15	1.32
(2,4308)	1:106:A:TYR:HB3	1:184:A:ALA:HB3	15	1.32	0.15	1.32
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	15	1.3	0.03	1.31
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	15	1.29	0.03	1.29
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG22	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG21	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG22	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG23	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG23	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG21	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG23	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG21	15	1.28	0.12	1.29
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG22	15	1.28	0.12	1.29
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	15	1.23	0.03	1.24
(2,4494)	1:35:A:LEU:HD12	1:67:A:ILE:H	15	1.23	0.07	1.23
(2,4494)	1:35:A:LEU:HD13	1:66:A:GLU:H	15	1.23	0.07	1.23
(2,4494)	1:35:A:LEU:HD11	1:66:A:GLU:H	15	1.23	0.07	1.23
(2,4494)	1:35:A:LEU:HD11	1:67:A:ILE:H	15	1.23	0.07	1.23
(2,4494)	1:35:A:LEU:HD13	1:67:A:ILE:H	15	1.23	0.07	1.23
(2,4494)	1:35:A:LEU:HD12	1:66:A:GLU:H	15	1.23	0.07	1.23
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD22	15	1.22	0.08	1.23
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD11	15	1.22	0.08	1.23
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD23	15	1.22	0.08	1.23
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD13	15	1.22	0.08	1.23
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD21	15	1.22	0.08	1.23
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD12	15	1.22	0.08	1.23
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB2	15	1.15	0.13	1.18
(2,1438)	1:95:A:THR:HG21	1:97:A:ALA:HB2	15	1.15	0.13	1.18
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB1	15	1.15	0.13	1.18
(2,1438)	1:95:A:THR:HG21	1:97:A:ALA:HB3	15	1.15	0.13	1.18
(2,1438)	1:95:A:THR:HG22	1:97:A:ALA:HB2	15	1.15	0.13	1.18
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB3	15	1.15	0.13	1.18
(2,1438)	1:95:A:THR:HG22	1:97:A:ALA:HB1	15	1.15	0.13	1.18
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	15	1.15	0.07	1.14
(2,4336)	1:35:A:LEU:HD11	1:39:A:LEU:HB2	15	1.15	0.07	1.14
(2,4336)	1:35:A:LEU:HD12	1:39:A:LEU:HB2	15	1.15	0.07	1.14
(2,4507)	1:85:A:LEU:HD22	1:88:A:ASP:H	15	1.14	0.11	1.17
(2,4507)	1:85:A:LEU:HD21	1:88:A:ASP:H	15	1.14	0.11	1.17
(2,4507)	1:85:A:LEU:HD22	1:82:A:TYR:H	15	1.14	0.11	1.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4507)	1:85:A:LEU:HD23	1:82:A:TYR:H	15	1.14	0.11	1.17
(2,4507)	1:85:A:LEU:HD21	1:82:A:TYR:H	15	1.14	0.11	1.17
(2,4507)	1:85:A:LEU:HD23	1:88:A:ASP:H	15	1.14	0.11	1.17
(2,4535)	1:174:A:LEU:HD23	1:173:A:GLY:HA3	15	1.14	0.04	1.14
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	15	1.14	0.04	1.14
(2,4535)	1:174:A:LEU:HD22	1:173:A:GLY:HA3	15	1.14	0.04	1.14
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	15	1.13	0.11	1.15
(2,4719)	1:78:A:GLU:H	1:21:A:LEU:HD21	15	1.13	0.11	1.15
(2,4552)	1:21:A:LEU:HD23	1:82:A:TYR:HE2	15	1.13	0.09	1.14
(2,4552)	1:21:A:LEU:HD22	1:82:A:TYR:HE2	15	1.13	0.09	1.14
(2,4552)	1:21:A:LEU:HD21	1:82:A:TYR:HE2	15	1.13	0.09	1.14
(2,575)	1:89:A:VAL:HG13	1:93:A:PHE:HD2	15	1.12	0.06	1.11
(2,575)	1:89:A:VAL:HG12	1:93:A:PHE:HD2	15	1.12	0.06	1.11
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	15	1.12	0.06	1.11
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	15	1.12	0.04	1.12
(2,4515)	1:142:A:LEU:HD22	1:60:A:ILE:H	15	1.08	0.07	1.09
(2,4515)	1:142:A:LEU:HD23	1:60:A:ILE:H	15	1.08	0.07	1.09
(2,4515)	1:142:A:LEU:HD21	1:60:A:ILE:H	15	1.08	0.07	1.09
(2,4281)	1:177:A:MET:HE1	1:175:A:GLU:HA	15	1.06	0.13	1.05
(2,4281)	1:177:A:MET:HE3	1:175:A:GLU:HA	15	1.06	0.13	1.05
(2,4281)	1:177:A:MET:HE2	1:175:A:GLU:HA	15	1.06	0.13	1.05
(2,4281)	1:177:A:MET:HE2	1:181:A:PRO:HD3	15	1.06	0.13	1.05
(2,4281)	1:177:A:MET:HE1	1:181:A:PRO:HD3	15	1.06	0.13	1.05
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG22	15	1.04	0.07	1.03
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG23	15	1.04	0.07	1.03
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	15	1.04	0.07	1.03
(2,4295)	1:87:A:GLU:HB2	1:85:A:LEU:HD13	15	1.04	0.18	0.98
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG12	15	1.04	0.18	0.98
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG11	15	1.04	0.18	0.98
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG13	15	1.04	0.18	0.98
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	15	1.02	0.11	1.05
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD23	15	1.02	0.11	1.05
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD21	15	1.02	0.11	1.05
(2,586)	1:180:A:VAL:HG22	1:183:A:LYS:HG2	15	1.02	0.55	0.83
(2,586)	1:180:A:VAL:HG21	1:183:A:LYS:HG2	15	1.02	0.55	0.83
(2,586)	1:180:A:VAL:HG23	1:183:A:LYS:HG2	15	1.02	0.55	0.83
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	15	1.01	0.15	1.07
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG12	15	1.01	0.15	1.07
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG13	15	1.01	0.15	1.07
(2,4280)	1:177:A:MET:HE3	1:174:A:LEU:H	15	1.0	0.1	0.96
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	15	1.0	0.1	0.96
(2,4280)	1:177:A:MET:HE2	1:174:A:LEU:H	15	1.0	0.1	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4291)	1:121:A:ALA:HB3	1:120:A:HIS:HD2	15	1.0	0.06	1.02
(2,4291)	1:121:A:ALA:HB2	1:120:A:HIS:HD2	15	1.0	0.06	1.02
(2,4291)	1:121:A:ALA:HB1	1:120:A:HIS:HD2	15	1.0	0.06	1.02
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG22	15	0.99	0.72	0.5
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG21	15	0.99	0.72	0.5
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG23	15	0.99	0.72	0.5
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG22	15	0.99	0.72	0.5
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG21	15	0.99	0.72	0.5
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG23	15	0.99	0.72	0.5
(2,4692)	1:18:A:ALA:HB1	1:20:A:LEU:H	15	0.99	0.04	0.99
(2,4692)	1:18:A:ALA:HB2	1:20:A:LEU:H	15	0.99	0.04	0.99
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	15	0.99	0.04	0.99
(2,505)	1:174:A:LEU:HD21	1:157:A:LYS:HE3	15	0.99	0.78	0.56
(2,505)	1:174:A:LEU:HD23	1:157:A:LYS:HE3	15	0.99	0.78	0.56
(2,505)	1:174:A:LEU:HD22	1:157:A:LYS:HE3	15	0.99	0.78	0.56
(2,4534)	1:76:A:LEU:HD11	1:24:A:GLU:H	15	0.98	0.15	0.98
(2,4534)	1:76:A:LEU:HD13	1:73:A:ASN:H	15	0.98	0.15	0.98
(2,4534)	1:76:A:LEU:HD12	1:73:A:ASN:H	15	0.98	0.15	0.98
(2,4534)	1:76:A:LEU:HD12	1:24:A:GLU:H	15	0.98	0.15	0.98
(2,4534)	1:76:A:LEU:HD13	1:24:A:GLU:H	15	0.98	0.15	0.98
(2,4534)	1:76:A:LEU:HD11	1:73:A:ASN:H	15	0.98	0.15	0.98
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD12	15	0.97	0.16	1.0
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	15	0.97	0.16	1.0
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	15	0.97	0.16	1.0
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	15	0.97	0.1	0.97
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD11	15	0.97	0.11	1.0
(2,41)	1:31:A:LEU:HD13	1:67:A:ILE:HD12	15	0.97	0.11	1.0
(2,41)	1:31:A:LEU:HD12	1:67:A:ILE:HD11	15	0.97	0.11	1.0
(2,41)	1:31:A:LEU:HD12	1:67:A:ILE:HD12	15	0.97	0.11	1.0
(2,41)	1:31:A:LEU:HD13	1:67:A:ILE:HD11	15	0.97	0.11	1.0
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD12	15	0.97	0.11	1.0
(2,41)	1:31:A:LEU:HD13	1:67:A:ILE:HD13	15	0.97	0.11	1.0
(2,1370)	1:176:A:VAL:HG23	1:100:A:PHE:HE2	15	0.97	0.15	1.02
(2,1370)	1:176:A:VAL:HG21	1:100:A:PHE:HE2	15	0.97	0.15	1.02
(2,1370)	1:176:A:VAL:HG22	1:100:A:PHE:HE1	15	0.97	0.15	1.02
(2,1370)	1:176:A:VAL:HG21	1:100:A:PHE:HE1	15	0.97	0.15	1.02
(2,1370)	1:176:A:VAL:HG23	1:100:A:PHE:HE1	15	0.97	0.15	1.02
(2,1370)	1:176:A:VAL:HG22	1:100:A:PHE:HE2	15	0.97	0.15	1.02
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD11	15	0.97	0.16	0.96
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD12	15	0.97	0.16	0.96
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD11	15	0.97	0.16	0.96
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD12	15	0.97	0.16	0.96

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD13	15	0.97	0.16	0.96
(2,593)	1:64:A:ILE:HD12	1:67:A:ILE:HD12	15	0.97	0.16	0.96
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	15	0.96	0.08	0.98
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	15	0.96	0.13	0.92
(2,4285)	1:97:A:ALA:HB2	1:172:A:ASP:HB3	15	0.96	0.13	0.92
(2,4285)	1:97:A:ALA:HB1	1:172:A:ASP:HB3	15	0.96	0.13	0.92
(2,4522)	1:149:A:VAL:HG22	1:147:A:GLN:HA	15	0.95	0.09	0.92
(2,4522)	1:149:A:VAL:HG21	1:147:A:GLN:HA	15	0.95	0.09	0.92
(2,4522)	1:149:A:VAL:HG23	1:147:A:GLN:HA	15	0.95	0.09	0.92
(2,4490)	1:79:A:LEU:HD22	1:93:A:PHE:HZ	15	0.94	0.13	0.95
(2,4490)	1:79:A:LEU:HD23	1:93:A:PHE:HZ	15	0.94	0.13	0.95
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	15	0.94	0.13	0.95
(2,4490)	1:152:A:TYR:HE1	1:79:A:LEU:HD23	15	0.94	0.13	0.95
(2,4490)	1:152:A:TYR:HE1	1:79:A:LEU:HD22	15	0.94	0.13	0.95
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD11	15	0.94	0.1	0.96
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD12	15	0.94	0.1	0.96
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD13	15	0.94	0.1	0.96
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD11	15	0.94	0.1	0.96
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD13	15	0.94	0.1	0.96
(2,776)	1:121:A:ALA:HB2	1:138:A:ILE:HD13	15	0.94	0.1	0.96
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD12	15	0.94	0.1	0.96
(2,776)	1:121:A:ALA:HB2	1:138:A:ILE:HD12	15	0.94	0.1	0.96
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD11	15	0.94	0.07	0.95
(2,3618)	1:93:A:PHE:HE2	1:79:A:LEU:HD11	15	0.94	0.07	0.95
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD13	15	0.94	0.07	0.95
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD12	15	0.94	0.07	0.95
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	15	0.94	0.15	0.96
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	15	0.91	0.14	0.92
(2,436)	1:39:A:LEU:HD11	1:61:A:PHE:HD2	15	0.91	0.14	0.92
(2,436)	1:39:A:LEU:HD12	1:61:A:PHE:HD2	15	0.91	0.14	0.92
(2,393)	1:39:A:LEU:HD22	1:57:A:GLU:HB3	15	0.91	0.34	0.82
(2,393)	1:39:A:LEU:HD21	1:57:A:GLU:HB3	15	0.91	0.34	0.82
(2,393)	1:39:A:LEU:HD23	1:57:A:GLU:HB3	15	0.91	0.34	0.82
(2,3962)	1:135:A:ALA:HB3	1:137:A:SER:H	15	0.9	0.03	0.9
(2,3962)	1:135:A:ALA:HB1	1:137:A:SER:H	15	0.9	0.03	0.9
(2,3962)	1:135:A:ALA:HB2	1:137:A:SER:H	15	0.9	0.03	0.9
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	15	0.9	0.35	0.78
(2,4548)	1:49:A:ILE:HG22	1:38:A:TYR:HB3	15	0.9	0.18	0.92
(2,4548)	1:49:A:ILE:HG23	1:55:A:ASN:HB3	15	0.9	0.18	0.92
(2,4548)	1:49:A:ILE:HG22	1:55:A:ASN:HB3	15	0.9	0.18	0.92
(2,4548)	1:49:A:ILE:HG21	1:55:A:ASN:HB3	15	0.9	0.18	0.92
(2,4548)	1:49:A:ILE:HG21	1:38:A:TYR:HB3	15	0.9	0.18	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD11	15	0.9	0.08	0.91
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	15	0.9	0.08	0.91
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD13	15	0.9	0.08	0.91
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	15	0.9	0.15	0.88
(2,1866)	1:146:A:VAL:HG12	1:143:A:ILE:H	15	0.9	0.15	0.88
(2,1866)	1:146:A:VAL:HG13	1:143:A:ILE:H	15	0.9	0.15	0.88
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	15	0.89	0.04	0.89
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD12	15	0.86	0.04	0.86
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD13	15	0.86	0.04	0.86
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD11	15	0.86	0.04	0.86
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	15	0.86	0.03	0.86
(2,4171)	1:134:A:LEU:HD23	1:129:A:GLN:H	15	0.86	0.08	0.84
(2,4171)	1:134:A:LEU:HD21	1:129:A:GLN:H	15	0.86	0.08	0.84
(2,4171)	1:134:A:LEU:HD22	1:129:A:GLN:H	15	0.86	0.08	0.84
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	15	0.85	0.03	0.85
(2,2939)	1:178:A:LEU:HD12	1:177:A:MET:H	15	0.85	0.03	0.85
(2,2939)	1:178:A:LEU:HD13	1:177:A:MET:H	15	0.85	0.03	0.85
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG12	15	0.84	0.19	0.88
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG13	15	0.84	0.19	0.88
(2,1454)	1:103:A:TYR:HD1	1:149:A:VAL:HG12	15	0.84	0.19	0.88
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG11	15	0.84	0.19	0.88
(2,1454)	1:103:A:TYR:HD1	1:149:A:VAL:HG13	15	0.84	0.19	0.88
(2,1454)	1:103:A:TYR:HD1	1:149:A:VAL:HG11	15	0.84	0.19	0.88
(2,509)	1:174:A:LEU:HD21	1:156:A:LEU:HD22	15	0.84	0.14	0.83
(2,509)	1:174:A:LEU:HD21	1:156:A:LEU:HD21	15	0.84	0.14	0.83
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD22	15	0.84	0.14	0.83
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD21	15	0.84	0.14	0.83
(2,509)	1:174:A:LEU:HD21	1:156:A:LEU:HD23	15	0.84	0.14	0.83
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD23	15	0.84	0.14	0.83
(2,509)	1:174:A:LEU:HD23	1:156:A:LEU:HD23	15	0.84	0.14	0.83
(2,509)	1:174:A:LEU:HD23	1:156:A:LEU:HD21	15	0.84	0.14	0.83
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD11	15	0.83	0.16	0.85
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	15	0.83	0.16	0.85
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD13	15	0.83	0.16	0.85
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG23	15	0.82	0.05	0.84
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG22	15	0.82	0.05	0.84
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG21	15	0.82	0.05	0.84
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD22	15	0.82	0.09	0.81
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD21	15	0.82	0.09	0.81
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD23	15	0.82	0.09	0.81
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD21	15	0.82	0.09	0.81
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD23	15	0.82	0.09	0.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1263)	1:42:A:MET:HE1	1:39:A:LEU:HD23	15	0.82	0.09	0.81
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD22	15	0.82	0.09	0.81
(2,1263)	1:42:A:MET:HE1	1:39:A:LEU:HD22	15	0.82	0.09	0.81
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	15	0.82	0.51	0.96
(2,4447)	1:179:A:SER:HB3	1:182:A:LYS:HD3	15	0.82	0.51	0.96
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD12	15	0.81	0.06	0.82
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD11	15	0.81	0.06	0.82
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD13	15	0.81	0.06	0.82
(2,340)	1:102:A:MET:HE2	1:99:A:LYS:HE3	15	0.8	0.32	0.66
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	15	0.8	0.32	0.66
(2,340)	1:102:A:MET:HE1	1:99:A:LYS:HE3	15	0.8	0.32	0.66
(2,4475)	1:17:A:MET:HE3	1:17:A:MET:HB2	15	0.79	0.02	0.79
(2,4475)	1:17:A:MET:HE1	1:17:A:MET:HB2	15	0.79	0.02	0.79
(2,4475)	1:17:A:MET:HE2	1:17:A:MET:HB2	15	0.79	0.02	0.79
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG22	15	0.79	0.07	0.77
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG23	15	0.79	0.07	0.77
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG21	15	0.79	0.07	0.77
(2,4263)	1:178:A:LEU:HD23	1:175:A:GLU:HG2	15	0.79	0.25	0.8
(2,4263)	1:178:A:LEU:HD21	1:175:A:GLU:HG2	15	0.79	0.25	0.8
(2,4263)	1:178:A:LEU:HD22	1:175:A:GLU:HG2	15	0.79	0.25	0.8
(2,4195)	1:18:A:ALA:HB3	1:21:A:LEU:H	15	0.77	0.07	0.79
(2,4195)	1:18:A:ALA:HB1	1:21:A:LEU:H	15	0.77	0.07	0.79
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	15	0.77	0.07	0.79
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	15	0.76	0.16	0.81
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG21	15	0.76	0.21	0.77
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG23	15	0.76	0.21	0.77
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG22	15	0.76	0.21	0.77
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	15	0.75	0.12	0.71
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD2	15	0.75	0.12	0.71
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	15	0.75	0.05	0.74
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG13	15	0.75	0.05	0.74
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG11	15	0.75	0.05	0.74
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	15	0.75	0.04	0.74
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG12	15	0.75	0.04	0.74
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG11	15	0.75	0.04	0.74
(2,1368)	1:79:A:LEU:HD23	1:17:A:MET:HE2	15	0.75	0.08	0.75
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE1	15	0.75	0.08	0.75
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE2	15	0.75	0.08	0.75
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE3	15	0.75	0.08	0.75
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE2	15	0.75	0.08	0.75
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE1	15	0.75	0.08	0.75
(2,1558)	1:20:A:LEU:HD22	1:89:A:VAL:HA	15	0.74	0.19	0.81

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1558)	1:20:A:LEU:HD21	1:89:A:VAL:HA	15	0.74	0.19	0.81
(2,1558)	1:20:A:LEU:HD23	1:89:A:VAL:HA	15	0.74	0.19	0.81
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG23	15	0.74	0.08	0.73
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG22	15	0.74	0.08	0.73
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	15	0.74	0.08	0.73
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	15	0.74	0.07	0.75
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD12	15	0.74	0.07	0.75
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD11	15	0.74	0.07	0.75
(2,378)	1:142:A:LEU:HD22	1:60:A:ILE:HG23	15	0.74	0.04	0.74
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG21	15	0.74	0.04	0.74
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG22	15	0.74	0.04	0.74
(2,378)	1:142:A:LEU:HD22	1:60:A:ILE:HG22	15	0.74	0.04	0.74
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG23	15	0.74	0.04	0.74
(2,378)	1:142:A:LEU:HD21	1:60:A:ILE:HG21	15	0.74	0.04	0.74
(2,378)	1:142:A:LEU:HD21	1:60:A:ILE:HG22	15	0.74	0.04	0.74
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG22	15	0.73	0.05	0.75
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG21	15	0.73	0.05	0.75
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG23	15	0.73	0.05	0.75
(2,4328)	1:156:A:LEU:HD23	1:155:A:LEU:H	15	0.73	0.26	0.67
(2,4328)	1:156:A:LEU:HD22	1:155:A:LEU:H	15	0.73	0.26	0.67
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	15	0.73	0.26	0.67
(2,4328)	1:156:A:LEU:HD22	1:152:A:TYR:H	15	0.73	0.26	0.67
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	15	0.72	0.03	0.73
(2,31)	1:35:A:LEU:HD13	1:69:A:ASP:HB2	15	0.72	0.03	0.73
(2,31)	1:35:A:LEU:HD11	1:69:A:ASP:HB2	15	0.72	0.03	0.73
(2,4530)	1:60:A:ILE:HG21	1:57:A:GLU:HG2	15	0.72	0.11	0.71
(2,4530)	1:60:A:ILE:HG22	1:57:A:GLU:HG2	15	0.72	0.11	0.71
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG3	15	0.72	0.11	0.71
(2,4530)	1:60:A:ILE:HG21	1:57:A:GLU:HG3	15	0.72	0.11	0.71
(2,4530)	1:60:A:ILE:HG22	1:57:A:GLU:HG3	15	0.72	0.11	0.71
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG2	15	0.72	0.11	0.71
(2,1988)	1:49:A:ILE:HG23	1:55:A:ASN:H	15	0.72	0.05	0.73
(2,1988)	1:49:A:ILE:HG22	1:55:A:ASN:H	15	0.72	0.05	0.73
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	15	0.72	0.05	0.73
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	15	0.72	0.09	0.71
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD22	15	0.72	0.09	0.71
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD23	15	0.72	0.09	0.71
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG12	15	0.71	0.26	0.56
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG11	15	0.71	0.26	0.56
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG11	15	0.71	0.26	0.56
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG12	15	0.71	0.26	0.56
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG13	15	0.71	0.26	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3770)	1:117:A:ILE:HD12	1:118:A:LEU:H	15	0.71	0.05	0.7
(2,3770)	1:117:A:ILE:HD11	1:118:A:LEU:H	15	0.71	0.05	0.7
(2,3770)	1:117:A:ILE:HD13	1:118:A:LEU:H	15	0.71	0.05	0.7
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	15	0.7	0.08	0.69
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD22	15	0.7	0.08	0.69
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD23	15	0.7	0.08	0.69
(2,4322)	1:20:A:LEU:HD11	1:152:A:TYR:H	15	0.7	0.15	0.7
(2,4322)	1:20:A:LEU:HD13	1:152:A:TYR:H	15	0.7	0.15	0.7
(2,4322)	1:20:A:LEU:HD12	1:152:A:TYR:H	15	0.7	0.15	0.7
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	15	0.7	0.03	0.7
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD11	15	0.7	0.08	0.7
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD13	15	0.7	0.08	0.7
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD12	15	0.7	0.08	0.7
(2,581)	1:180:A:VAL:HG22	1:183:A:LYS:H	15	0.7	0.1	0.71
(2,581)	1:180:A:VAL:HG21	1:183:A:LYS:H	15	0.7	0.1	0.71
(2,581)	1:180:A:VAL:HG23	1:183:A:LYS:H	15	0.7	0.1	0.71
(2,5)	1:95:A:THR:HG22	1:94:A:VAL:HB	15	0.7	0.05	0.7
(2,5)	1:95:A:THR:HG23	1:94:A:VAL:HB	15	0.7	0.05	0.7
(2,5)	1:95:A:THR:HG21	1:94:A:VAL:HB	15	0.7	0.05	0.7
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	15	0.7	0.13	0.7
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	15	0.69	0.08	0.7
(2,454)	1:53:A:ILE:HG22	1:60:A:ILE:HG22	15	0.69	0.09	0.68
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG23	15	0.69	0.09	0.68
(2,454)	1:53:A:ILE:HG22	1:60:A:ILE:HG23	15	0.69	0.09	0.68
(2,454)	1:53:A:ILE:HG23	1:60:A:ILE:HG21	15	0.69	0.09	0.68
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG21	15	0.69	0.09	0.68
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG22	15	0.69	0.09	0.68
(2,454)	1:53:A:ILE:HG22	1:60:A:ILE:HG21	15	0.69	0.09	0.68
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD22	15	0.69	0.14	0.68
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD23	15	0.69	0.14	0.68
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	15	0.69	0.14	0.68
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	15	0.68	0.42	0.53
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD21	15	0.68	0.42	0.53
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD22	15	0.68	0.42	0.53
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	15	0.68	0.09	0.7
(2,687)	1:184:A:ALA:HB2	1:181:A:PRO:HD3	15	0.68	0.09	0.7
(2,687)	1:184:A:ALA:HB3	1:181:A:PRO:HD3	15	0.68	0.09	0.7
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	15	0.67	0.13	0.68
(2,1517)	1:39:A:LEU:HD13	1:61:A:PHE:HB2	15	0.67	0.13	0.68
(2,1517)	1:39:A:LEU:HD11	1:61:A:PHE:HB2	15	0.67	0.13	0.68
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD11	15	0.67	0.09	0.68
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD12	15	0.67	0.09	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	15	0.67	0.09	0.68
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	15	0.67	0.22	0.78
(2,29)	1:35:A:LEU:HD12	1:33:A:GLU:H	15	0.67	0.22	0.78
(2,29)	1:35:A:LEU:HD13	1:33:A:GLU:H	15	0.67	0.22	0.78
(2,3705)	1:74:A:ILE:HG21	1:74:A:ILE:H	15	0.67	0.01	0.67
(2,3705)	1:74:A:ILE:HG23	1:74:A:ILE:H	15	0.67	0.01	0.67
(2,3705)	1:74:A:ILE:HG22	1:74:A:ILE:H	15	0.67	0.01	0.67
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	15	0.67	0.05	0.67
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD11	15	0.67	0.08	0.69
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD13	15	0.67	0.08	0.69
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD12	15	0.67	0.08	0.69
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD12	15	0.66	0.09	0.66
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	15	0.66	0.09	0.66
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD11	15	0.66	0.09	0.66
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	15	0.66	0.19	0.67
(2,4576)	1:62:A:GLY:H	1:106:A:TYR:HD2	15	0.66	0.19	0.67
(2,705)	1:18:A:ALA:HB2	1:21:A:LEU:HG	15	0.66	0.05	0.65
(2,705)	1:18:A:ALA:HB3	1:21:A:LEU:HG	15	0.66	0.05	0.65
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	15	0.66	0.05	0.65
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	15	0.66	0.09	0.69
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD13	15	0.66	0.09	0.69
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD11	15	0.66	0.09	0.69
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	15	0.66	0.13	0.66
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	15	0.65	0.09	0.63
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE1	15	0.65	0.09	0.63
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE3	15	0.65	0.09	0.63
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD12	15	0.65	0.15	0.69
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	15	0.65	0.15	0.69
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	15	0.65	0.15	0.69
(2,4516)	1:138:A:ILE:HD13	1:39:A:LEU:H	15	0.65	0.15	0.69
(2,1267)	1:94:A:VAL:HG22	1:97:A:ALA:H	15	0.65	0.05	0.66
(2,1267)	1:94:A:VAL:HG23	1:97:A:ALA:H	15	0.65	0.05	0.66
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	15	0.65	0.05	0.66
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	15	0.64	0.02	0.65
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG23	15	0.64	0.06	0.64
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG21	15	0.64	0.06	0.64
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG22	15	0.64	0.06	0.64
(2,3907)	1:138:A:ILE:HD13	1:142:A:LEU:H	15	0.64	0.03	0.64
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	15	0.64	0.03	0.64
(2,3907)	1:138:A:ILE:HD12	1:142:A:LEU:H	15	0.64	0.03	0.64
(2,3931)	1:156:A:LEU:HD22	1:177:A:MET:H	15	0.63	0.11	0.67
(2,3931)	1:156:A:LEU:HD21	1:177:A:MET:H	15	0.63	0.11	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	15	0.63	0.11	0.67
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD11	15	0.63	0.04	0.63
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	15	0.63	0.04	0.63
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD12	15	0.63	0.04	0.63
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	15	0.63	0.05	0.65
(2,4123)	1:28:A:VAL:HG21	1:72:A:ASN:H	15	0.63	0.05	0.65
(2,4123)	1:28:A:VAL:HG23	1:72:A:ASN:H	15	0.63	0.05	0.65
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	15	0.63	0.03	0.62
(2,76)	1:116:A:LEU:HD21	1:56:A:LYS:H	15	0.63	0.03	0.62
(2,76)	1:116:A:LEU:HD23	1:56:A:LYS:H	15	0.63	0.03	0.62
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	15	0.63	0.26	0.77
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	15	0.62	0.28	0.41
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG12	15	0.62	0.06	0.63
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG11	15	0.62	0.06	0.63
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	15	0.62	0.06	0.63
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD1	15	0.62	0.08	0.64
(2,4551)	1:21:A:LEU:HD23	1:75:A:PHE:HD1	15	0.62	0.08	0.64
(2,4551)	1:21:A:LEU:HD22	1:75:A:PHE:HD1	15	0.62	0.08	0.64
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD2	15	0.62	0.08	0.64
(2,4551)	1:21:A:LEU:HD23	1:75:A:PHE:HD2	15	0.62	0.08	0.64
(2,497)	1:142:A:LEU:HD11	1:138:A:ILE:HA	15	0.62	0.06	0.64
(2,497)	1:142:A:LEU:HD13	1:138:A:ILE:HA	15	0.62	0.06	0.64
(2,497)	1:142:A:LEU:HD12	1:138:A:ILE:HA	15	0.62	0.06	0.64
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	15	0.62	0.03	0.62
(2,3810)	1:150:A:THR:HG23	1:150:A:THR:H	15	0.62	0.03	0.62
(2,3810)	1:150:A:THR:HG22	1:150:A:THR:H	15	0.62	0.03	0.62
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG22	15	0.62	0.06	0.62
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG23	15	0.62	0.06	0.62
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG23	15	0.62	0.06	0.62
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG21	15	0.62	0.06	0.62
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG22	15	0.62	0.06	0.62
(2,775)	1:121:A:ALA:HB1	1:60:A:ILE:HG23	15	0.62	0.06	0.62
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG21	15	0.62	0.06	0.62
(2,775)	1:121:A:ALA:HB1	1:60:A:ILE:HG21	15	0.62	0.06	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	15	0.62	0.02	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD12	15	0.62	0.02	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD11	15	0.62	0.02	0.62
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD11	15	0.62	0.03	0.62
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD13	15	0.62	0.03	0.62
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD12	15	0.62	0.03	0.62
(2,4570)	1:128:A:ILE:HG21	1:38:A:TYR:H	15	0.62	0.08	0.61
(2,4570)	1:128:A:ILE:HG22	1:38:A:TYR:H	15	0.62	0.08	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4570)	1:128:A:ILE:HG23	1:38:A:TYR:H	15	0.62	0.08	0.61
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG21	15	0.62	0.09	0.63
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG23	15	0.62	0.09	0.63
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	15	0.62	0.09	0.63
(2,356)	1:138:A:ILE:HD13	1:60:A:ILE:HD13	15	0.62	0.09	0.65
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD12	15	0.62	0.09	0.65
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD11	15	0.62	0.09	0.65
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD12	15	0.62	0.09	0.65
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD13	15	0.62	0.09	0.65
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD11	15	0.62	0.09	0.65
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD13	15	0.62	0.09	0.65
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	15	0.62	0.02	0.62
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD13	15	0.62	0.02	0.62
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD11	15	0.62	0.02	0.62
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD13	15	0.61	0.03	0.61
(2,88)	1:60:A:ILE:HD12	1:117:A:ILE:HD12	15	0.61	0.03	0.61
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD13	15	0.61	0.03	0.61
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD11	15	0.61	0.03	0.61
(2,88)	1:60:A:ILE:HD12	1:117:A:ILE:HD11	15	0.61	0.03	0.61
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD12	15	0.61	0.03	0.61
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD11	15	0.61	0.03	0.61
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD12	15	0.61	0.03	0.61
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG23	15	0.61	0.03	0.6
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG21	15	0.61	0.03	0.6
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG22	15	0.61	0.03	0.6
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG22	15	0.61	0.09	0.59
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG21	15	0.61	0.09	0.59
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG23	15	0.61	0.09	0.59
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	15	0.61	0.08	0.6
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	15	0.61	0.11	0.63
(2,4352)	1:28:A:VAL:HG23	1:25:A:LYS:HG2	15	0.61	0.11	0.63
(2,4352)	1:28:A:VAL:HG22	1:25:A:LYS:HG2	15	0.61	0.11	0.63
(2,4511)	1:46:A:VAL:HG23	1:46:A:VAL:HB	15	0.61	0.02	0.62
(2,4511)	1:46:A:VAL:HG22	1:46:A:VAL:HB	15	0.61	0.02	0.62
(2,4511)	1:46:A:VAL:HG21	1:46:A:VAL:HB	15	0.61	0.02	0.62
(2,4511)	1:46:A:VAL:HG12	1:46:A:VAL:HB	15	0.61	0.02	0.62
(2,4511)	1:46:A:VAL:HG11	1:46:A:VAL:HB	15	0.61	0.02	0.62
(2,612)	1:28:A:VAL:HG13	1:68:A:TYR:HE1	15	0.61	0.07	0.62
(2,612)	1:28:A:VAL:HG12	1:68:A:TYR:HE1	15	0.61	0.07	0.62
(2,612)	1:28:A:VAL:HG11	1:68:A:TYR:HE1	15	0.61	0.07	0.62
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	15	0.6	0.01	0.6
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	15	0.6	0.02	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG21	15	0.6	0.05	0.61
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG22	15	0.6	0.05	0.61
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG23	15	0.6	0.05	0.61
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG22	15	0.59	0.11	0.59
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG23	15	0.59	0.11	0.59
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG21	15	0.59	0.11	0.59
(2,585)	1:180:A:VAL:HG21	1:181:A:PRO:HG3	15	0.59	0.05	0.6
(2,585)	1:180:A:VAL:HG23	1:181:A:PRO:HG3	15	0.59	0.05	0.6
(2,585)	1:180:A:VAL:HG22	1:181:A:PRO:HG3	15	0.59	0.05	0.6
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG21	15	0.59	0.05	0.58
(2,411)	1:138:A:ILE:HG23	1:117:A:ILE:HG22	15	0.59	0.05	0.58
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG22	15	0.59	0.05	0.58
(2,411)	1:138:A:ILE:HG21	1:117:A:ILE:HG23	15	0.59	0.05	0.58
(2,411)	1:138:A:ILE:HG21	1:117:A:ILE:HG22	15	0.59	0.05	0.58
(2,411)	1:138:A:ILE:HG23	1:117:A:ILE:HG21	15	0.59	0.05	0.58
(2,411)	1:138:A:ILE:HG23	1:117:A:ILE:HG23	15	0.59	0.05	0.58
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	15	0.59	0.03	0.59
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD22	15	0.59	0.03	0.59
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD21	15	0.59	0.03	0.59
(2,4218)	1:85:A:LEU:HD12	1:84:A:GLN:H	15	0.59	0.08	0.61
(2,4218)	1:85:A:LEU:HD11	1:84:A:GLN:H	15	0.59	0.08	0.61
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	15	0.59	0.08	0.61
(2,528)	1:46:A:VAL:HG21	1:41:A:GLU:HB3	15	0.59	0.11	0.61
(2,528)	1:46:A:VAL:HG22	1:41:A:GLU:HB3	15	0.59	0.11	0.61
(2,528)	1:46:A:VAL:HG23	1:41:A:GLU:HB3	15	0.59	0.11	0.61
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD23	15	0.59	0.08	0.61
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	15	0.59	0.08	0.61
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD21	15	0.59	0.08	0.61
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	15	0.58	0.05	0.59
(2,1498)	1:49:A:ILE:HG23	1:43:A:THR:H	15	0.58	0.05	0.59
(2,1498)	1:49:A:ILE:HG22	1:43:A:THR:H	15	0.58	0.05	0.59
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	15	0.58	0.16	0.6
(2,1516)	1:39:A:LEU:HD13	1:61:A:PHE:HB3	15	0.58	0.16	0.6
(2,1516)	1:39:A:LEU:HD11	1:61:A:PHE:HB3	15	0.58	0.16	0.6
(2,608)	1:28:A:VAL:HG13	1:75:A:PHE:H	15	0.58	0.08	0.57
(2,608)	1:28:A:VAL:HG12	1:75:A:PHE:H	15	0.58	0.08	0.57
(2,608)	1:28:A:VAL:HG11	1:75:A:PHE:H	15	0.58	0.08	0.57
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD22	15	0.58	0.05	0.59
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD21	15	0.58	0.05	0.59
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD23	15	0.58	0.05	0.59
(2,3896)	1:134:A:LEU:HD23	1:132:A:HIS:H	15	0.58	0.06	0.58
(2,3896)	1:134:A:LEU:HD21	1:132:A:HIS:H	15	0.58	0.06	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3896)	1:134:A:LEU:HD22	1:132:A:HIS:H	15	0.58	0.06	0.58
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	15	0.58	0.08	0.57
(2,3930)	1:184:A:ALA:HB2	1:107:A:CYS:H	15	0.58	0.08	0.57
(2,3930)	1:184:A:ALA:HB3	1:107:A:CYS:H	15	0.58	0.08	0.57
(2,610)	1:28:A:VAL:HG13	1:74:A:ILE:H	15	0.58	0.04	0.59
(2,610)	1:28:A:VAL:HG12	1:74:A:ILE:H	15	0.58	0.04	0.59
(2,610)	1:28:A:VAL:HG11	1:74:A:ILE:H	15	0.58	0.04	0.59
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	15	0.58	0.06	0.61
(2,77)	1:76:A:LEU:HD11	1:80:A:GLU:HG3	15	0.58	0.06	0.61
(2,77)	1:76:A:LEU:HD13	1:80:A:GLU:HG3	15	0.58	0.06	0.61
(2,4635)	1:23:A:THR:HG21	1:22:A:GLN:H	15	0.57	0.05	0.58
(2,4635)	1:23:A:THR:HG22	1:22:A:GLN:H	15	0.57	0.05	0.58
(2,4635)	1:23:A:THR:HG23	1:22:A:GLN:H	15	0.57	0.05	0.58
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	15	0.57	0.03	0.57
(2,34)	1:39:A:LEU:HD12	1:35:A:LEU:H	15	0.57	0.03	0.57
(2,34)	1:39:A:LEU:HD13	1:35:A:LEU:H	15	0.57	0.03	0.57
(2,372)	1:95:A:THR:HG21	1:92:A:CYS:H	15	0.57	0.04	0.57
(2,372)	1:95:A:THR:HG22	1:92:A:CYS:H	15	0.57	0.04	0.57
(2,372)	1:95:A:THR:HG23	1:92:A:CYS:H	15	0.57	0.04	0.57
(2,3689)	1:60:A:ILE:HD12	1:61:A:PHE:H	15	0.57	0.02	0.58
(2,3689)	1:60:A:ILE:HD11	1:61:A:PHE:H	15	0.57	0.02	0.58
(2,3689)	1:60:A:ILE:HD13	1:61:A:PHE:H	15	0.57	0.02	0.58
(2,55)	1:142:A:LEU:HD13	1:106:A:TYR:HH	15	0.57	0.13	0.62
(2,55)	1:142:A:LEU:HD11	1:106:A:TYR:HH	15	0.57	0.13	0.62
(2,55)	1:142:A:LEU:HD12	1:106:A:TYR:HH	15	0.57	0.13	0.62
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	15	0.57	0.05	0.57
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD11	15	0.57	0.12	0.54
(2,405)	1:117:A:ILE:HD12	1:138:A:ILE:HD12	15	0.57	0.12	0.54
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD13	15	0.57	0.12	0.54
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD11	15	0.57	0.12	0.54
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD13	15	0.57	0.12	0.54
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD12	15	0.57	0.12	0.54
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD12	15	0.57	0.12	0.54
(2,1243)	1:21:A:LEU:HD21	1:21:A:LEU:HB2	15	0.56	0.01	0.56
(2,1243)	1:21:A:LEU:HD23	1:21:A:LEU:HB2	15	0.56	0.01	0.56
(2,1243)	1:21:A:LEU:HD22	1:21:A:LEU:HB2	15	0.56	0.01	0.56
(2,1470)	1:53:A:ILE:HG23	1:54:A:LEU:HA	15	0.56	0.02	0.56
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	15	0.56	0.02	0.56
(2,1470)	1:53:A:ILE:HG21	1:54:A:LEU:HA	15	0.56	0.02	0.56
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	15	0.55	0.05	0.56
(2,4814)	1:31:A:LEU:HD23	1:69:A:ASP:H	15	0.55	0.05	0.56
(2,4814)	1:31:A:LEU:HD22	1:69:A:ASP:H	15	0.55	0.05	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,60)	1:174:A:LEU:HD22	1:178:A:LEU:H	15	0.55	0.12	0.51
(2,60)	1:174:A:LEU:HD21	1:178:A:LEU:H	15	0.55	0.12	0.51
(2,60)	1:174:A:LEU:HD23	1:178:A:LEU:H	15	0.55	0.12	0.51
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD11	15	0.55	0.02	0.55
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	15	0.55	0.02	0.55
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD13	15	0.55	0.02	0.55
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	15	0.55	0.03	0.55
(2,508)	1:155:A:LEU:HD21	1:155:A:LEU:HB2	15	0.55	0.03	0.55
(2,508)	1:155:A:LEU:HD22	1:155:A:LEU:HB2	15	0.55	0.03	0.55
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	15	0.55	0.02	0.55
(2,4794)	1:115:A:GLN:HG2	1:115:A:GLN:H	15	0.55	0.02	0.55
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB2	15	0.55	0.13	0.57
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	15	0.55	0.13	0.57
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB3	15	0.55	0.13	0.57
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG23	15	0.54	0.03	0.53
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	15	0.54	0.03	0.53
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG22	15	0.54	0.03	0.53
(2,3789)	1:128:A:ILE:HG22	1:128:A:ILE:H	15	0.54	0.03	0.55
(2,3789)	1:128:A:ILE:HG21	1:128:A:ILE:H	15	0.54	0.03	0.55
(2,3789)	1:128:A:ILE:HG23	1:128:A:ILE:H	15	0.54	0.03	0.55
(2,4539)	1:95:A:THR:HG21	1:91:A:HIS:HB2	15	0.54	0.15	0.51
(2,4539)	1:95:A:THR:HG22	1:91:A:HIS:HB2	15	0.54	0.15	0.51
(2,4539)	1:95:A:THR:HG23	1:91:A:HIS:HB2	15	0.54	0.15	0.51
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	15	0.54	0.04	0.53
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD22	15	0.54	0.04	0.53
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD21	15	0.54	0.04	0.53
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	15	0.53	0.08	0.54
(2,2116)	1:97:A:ALA:HB3	1:100:A:PHE:H	15	0.53	0.08	0.54
(2,2116)	1:97:A:ALA:HB2	1:100:A:PHE:H	15	0.53	0.08	0.54
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	15	0.53	0.06	0.52
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE1	15	0.53	0.06	0.52
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE3	15	0.53	0.06	0.52
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	15	0.53	0.03	0.53
(2,1392)	1:31:A:LEU:HD21	1:27:A:TYR:H	15	0.53	0.03	0.53
(2,1392)	1:31:A:LEU:HD23	1:27:A:TYR:H	15	0.53	0.03	0.53
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	15	0.53	0.03	0.52
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD13	15	0.53	0.03	0.52
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD12	15	0.53	0.03	0.52
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	15	0.53	0.11	0.58
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD23	15	0.53	0.11	0.58
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD21	15	0.53	0.11	0.58
(2,309)	1:79:A:LEU:HD21	1:79:A:LEU:H	15	0.53	0.03	0.53

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,309)	1:79:A:LEU:HD22	1:79:A:LEU:H	15	0.53	0.03	0.53
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	15	0.53	0.03	0.53
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	15	0.53	0.04	0.52
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG23	15	0.53	0.04	0.52
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG22	15	0.53	0.04	0.52
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	15	0.53	0.06	0.53
(2,4069)	1:23:A:THR:HG21	1:24:A:GLU:H	15	0.53	0.06	0.54
(2,4069)	1:23:A:THR:HG22	1:24:A:GLU:H	15	0.53	0.06	0.54
(2,4069)	1:23:A:THR:HG23	1:24:A:GLU:H	15	0.53	0.06	0.54
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	15	0.53	0.05	0.53
(2,4185)	1:178:A:LEU:HD11	1:179:A:SER:H	15	0.53	0.05	0.53
(2,4185)	1:178:A:LEU:HD12	1:179:A:SER:H	15	0.53	0.05	0.53
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	15	0.53	0.04	0.53
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	15	0.53	0.02	0.53
(2,3131)	1:49:A:ILE:HG22	1:49:A:ILE:H	15	0.53	0.02	0.53
(2,3131)	1:49:A:ILE:HG21	1:49:A:ILE:H	15	0.53	0.02	0.53
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	15	0.53	0.04	0.53
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD21	15	0.53	0.04	0.53
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD22	15	0.53	0.04	0.53
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD12	15	0.52	0.04	0.51
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	15	0.52	0.04	0.51
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD11	15	0.52	0.04	0.51
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB2	15	0.52	0.11	0.53
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	15	0.52	0.11	0.53
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB3	15	0.52	0.11	0.53
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	15	0.52	0.04	0.52
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	15	0.52	0.03	0.53
(2,1965)	1:39:A:LEU:HD11	1:39:A:LEU:H	15	0.52	0.03	0.53
(2,1965)	1:39:A:LEU:HD12	1:39:A:LEU:H	15	0.52	0.03	0.53
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	15	0.52	0.05	0.52
(2,3309)	1:28:A:VAL:HG22	1:31:A:LEU:H	15	0.52	0.05	0.52
(2,3309)	1:28:A:VAL:HG21	1:31:A:LEU:H	15	0.52	0.05	0.52
(2,4358)	1:177:A:MET:HE3	1:173:A:GLY:HA3	15	0.52	0.18	0.55
(2,4358)	1:177:A:MET:HE1	1:176:A:VAL:HA	15	0.52	0.18	0.55
(2,4358)	1:177:A:MET:HE2	1:173:A:GLY:HA3	15	0.52	0.18	0.55
(2,4358)	1:177:A:MET:HE1	1:173:A:GLY:HA3	15	0.52	0.18	0.55
(2,1555)	1:18:A:ALA:HB3	1:22:A:GLN:HB3	15	0.52	0.15	0.53
(2,1555)	1:18:A:ALA:HB1	1:22:A:GLN:HB3	15	0.52	0.15	0.53
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	15	0.52	0.15	0.53
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD11	15	0.52	0.11	0.49
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD13	15	0.52	0.11	0.49
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD12	15	0.52	0.11	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,11)	1:79:A:LEU:HD12	1:79:A:LEU:H	15	0.52	0.04	0.53
(2,11)	1:79:A:LEU:HD13	1:79:A:LEU:H	15	0.52	0.04	0.53
(2,11)	1:79:A:LEU:HD11	1:79:A:LEU:H	15	0.52	0.04	0.53
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD11	15	0.52	0.09	0.53
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD12	15	0.52	0.09	0.53
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD13	15	0.52	0.09	0.53
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	15	0.52	0.09	0.51
(2,3737)	1:95:A:THR:HG23	1:95:A:THR:H	15	0.51	0.03	0.52
(2,3737)	1:95:A:THR:HG21	1:95:A:THR:H	15	0.51	0.03	0.52
(2,3737)	1:95:A:THR:HG22	1:95:A:THR:H	15	0.51	0.03	0.52
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	15	0.51	0.05	0.52
(2,4208)	1:64:A:ILE:HG21	1:66:A:GLU:H	15	0.51	0.05	0.52
(2,4208)	1:64:A:ILE:HG23	1:66:A:GLU:H	15	0.51	0.05	0.52
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	15	0.51	0.04	0.51
(2,1854)	1:143:A:ILE:HD11	1:147:A:GLN:H	15	0.51	0.04	0.51
(2,1854)	1:143:A:ILE:HD13	1:147:A:GLN:H	15	0.51	0.04	0.51
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD12	15	0.51	0.17	0.56
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD13	15	0.51	0.17	0.56
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG23	15	0.51	0.17	0.56
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG22	15	0.51	0.17	0.56
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG21	15	0.51	0.17	0.56
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD11	15	0.51	0.17	0.56
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	15	0.51	0.08	0.51
(2,3372)	1:141:A:TYR:HE1	1:141:A:TYR:H	15	0.51	0.08	0.51
(2,467)	1:178:A:LEU:HD23	1:175:A:GLU:H	15	0.51	0.1	0.55
(2,467)	1:178:A:LEU:HD21	1:175:A:GLU:H	15	0.51	0.1	0.55
(2,467)	1:178:A:LEU:HD22	1:175:A:GLU:H	15	0.51	0.1	0.55
(2,441)	1:31:A:LEU:HD13	1:61:A:PHE:HE1	15	0.51	0.09	0.53
(2,441)	1:31:A:LEU:HD12	1:61:A:PHE:HE1	15	0.51	0.09	0.53
(2,441)	1:31:A:LEU:HD11	1:61:A:PHE:HE1	15	0.51	0.09	0.53
(2,1244)	1:20:A:LEU:HD12	1:21:A:LEU:H	15	0.5	0.05	0.5
(2,1244)	1:20:A:LEU:HD11	1:21:A:LEU:H	15	0.5	0.05	0.5
(2,1244)	1:20:A:LEU:HD13	1:21:A:LEU:H	15	0.5	0.05	0.5
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	15	0.5	0.08	0.49
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE1	15	0.5	0.08	0.49
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE3	15	0.5	0.08	0.49
(2,700)	1:23:A:THR:HG21	1:21:A:LEU:H	15	0.5	0.09	0.52
(2,700)	1:23:A:THR:HG22	1:21:A:LEU:H	15	0.5	0.09	0.52
(2,700)	1:23:A:THR:HG23	1:21:A:LEU:H	15	0.5	0.09	0.52
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	15	0.5	0.07	0.51
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	15	0.5	0.03	0.5
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD13	15	0.5	0.02	0.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD11	15	0.5	0.02	0.5
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD12	15	0.5	0.02	0.5
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	15	0.5	0.16	0.51
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	15	0.49	0.02	0.49
(2,3772)	1:118:A:LEU:HD22	1:119:A:GLU:H	15	0.49	0.02	0.49
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG23	15	0.49	0.18	0.53
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG21	15	0.49	0.18	0.53
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	15	0.49	0.18	0.53
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD21	15	0.49	0.05	0.48
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	15	0.49	0.05	0.48
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD22	15	0.49	0.05	0.48
(2,94)	1:180:A:VAL:HG23	1:103:A:TYR:HA	15	0.49	0.1	0.48
(2,94)	1:180:A:VAL:HG22	1:103:A:TYR:HA	15	0.49	0.1	0.48
(2,94)	1:180:A:VAL:HG21	1:103:A:TYR:HA	15	0.49	0.1	0.48
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD13	15	0.49	0.11	0.52
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD11	15	0.49	0.11	0.52
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD12	15	0.49	0.11	0.52
(2,3683)	1:59:A:ILE:HG23	1:59:A:ILE:H	15	0.49	0.02	0.49
(2,3683)	1:59:A:ILE:HG21	1:59:A:ILE:H	15	0.49	0.02	0.49
(2,3683)	1:59:A:ILE:HG22	1:59:A:ILE:H	15	0.49	0.02	0.49
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	15	0.49	0.07	0.52
(2,836)	1:64:A:ILE:HG21	1:65:A:GLN:HG3	15	0.49	0.07	0.52
(2,836)	1:64:A:ILE:HG23	1:65:A:GLN:HG3	15	0.49	0.07	0.52
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	15	0.49	0.11	0.51
(2,658)	1:104:A:VAL:HG13	1:184:A:ALA:HA	15	0.49	0.11	0.51
(2,658)	1:104:A:VAL:HG11	1:184:A:ALA:HA	15	0.49	0.11	0.51
(2,3771)	1:118:A:LEU:HD11	1:119:A:GLU:H	15	0.49	0.01	0.48
(2,3771)	1:118:A:LEU:HD13	1:119:A:GLU:H	15	0.49	0.01	0.48
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	15	0.49	0.01	0.48
(2,3913)	1:176:A:VAL:HG21	1:100:A:PHE:H	15	0.48	0.1	0.5
(2,3913)	1:176:A:VAL:HG22	1:100:A:PHE:H	15	0.48	0.1	0.5
(2,3913)	1:176:A:VAL:HG23	1:100:A:PHE:H	15	0.48	0.1	0.5
(2,3943)	1:18:A:ALA:HB1	1:17:A:MET:H	15	0.48	0.09	0.5
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	15	0.48	0.09	0.5
(2,3943)	1:18:A:ALA:HB2	1:17:A:MET:H	15	0.48	0.09	0.5
(2,4150)	1:118:A:LEU:HD11	1:115:A:GLN:H	15	0.48	0.02	0.48
(2,4150)	1:118:A:LEU:HD13	1:115:A:GLN:H	15	0.48	0.02	0.48
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	15	0.48	0.02	0.48
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD13	15	0.47	0.07	0.46
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD11	15	0.47	0.07	0.46
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD12	15	0.47	0.07	0.46
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	15	0.47	0.04	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,419)	1:53:A:ILE:HD11	1:49:A:ILE:HB	15	0.47	0.04	0.47
(2,419)	1:53:A:ILE:HD12	1:49:A:ILE:HB	15	0.47	0.04	0.47
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	15	0.47	0.05	0.46
(2,35)	1:39:A:LEU:HD12	1:65:A:GLN:HG3	15	0.47	0.05	0.46
(2,35)	1:39:A:LEU:HD13	1:65:A:GLN:HG3	15	0.47	0.05	0.46
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD13	15	0.47	0.14	0.48
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	15	0.47	0.14	0.48
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD12	15	0.47	0.14	0.48
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	15	0.46	0.04	0.47
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB2	15	0.46	0.04	0.47
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB3	15	0.46	0.04	0.47
(2,3169)	1:53:A:ILE:HG23	1:54:A:LEU:H	15	0.46	0.02	0.47
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	15	0.46	0.02	0.47
(2,3169)	1:53:A:ILE:HG21	1:54:A:LEU:H	15	0.46	0.02	0.47
(2,4160)	1:53:A:ILE:HG22	1:122:A:GLY:H	15	0.46	0.05	0.47
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	15	0.46	0.05	0.47
(2,4160)	1:53:A:ILE:HG23	1:122:A:GLY:H	15	0.46	0.05	0.47
(2,4223)	1:159:A:LEU:HD11	1:156:A:LEU:H	15	0.46	0.04	0.47
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	15	0.46	0.04	0.47
(2,4223)	1:159:A:LEU:HD13	1:156:A:LEU:H	15	0.46	0.04	0.47
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG21	15	0.46	0.08	0.46
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG23	15	0.46	0.08	0.46
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	15	0.46	0.08	0.46
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG23	15	0.46	0.03	0.46
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG22	15	0.46	0.03	0.46
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG21	15	0.46	0.03	0.46
(2,4037)	1:21:A:LEU:HD21	1:22:A:GLN:H	15	0.46	0.02	0.46
(2,4037)	1:21:A:LEU:HD23	1:22:A:GLN:H	15	0.46	0.02	0.46
(2,4037)	1:21:A:LEU:HD22	1:22:A:GLN:H	15	0.46	0.02	0.46
(2,1838)	1:16:A:ILE:HD11	1:158:A:GLU:H	15	0.46	0.17	0.49
(2,1838)	1:16:A:ILE:HD12	1:158:A:GLU:H	15	0.46	0.17	0.49
(2,1838)	1:16:A:ILE:HD13	1:158:A:GLU:H	15	0.46	0.17	0.49
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD11	15	0.46	0.06	0.46
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD13	15	0.46	0.06	0.46
(2,87)	1:67:A:ILE:HG22	1:31:A:LEU:HD12	15	0.46	0.06	0.46
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD12	15	0.46	0.06	0.46
(2,87)	1:67:A:ILE:HG22	1:31:A:LEU:HD11	15	0.46	0.06	0.46
(2,87)	1:67:A:ILE:HG21	1:31:A:LEU:HD13	15	0.46	0.06	0.46
(2,87)	1:67:A:ILE:HG21	1:31:A:LEU:HD11	15	0.46	0.06	0.46
(2,498)	1:142:A:LEU:HD12	1:60:A:ILE:HA	15	0.46	0.02	0.46
(2,498)	1:142:A:LEU:HD11	1:60:A:ILE:HA	15	0.46	0.02	0.46
(2,498)	1:142:A:LEU:HD13	1:60:A:ILE:HA	15	0.46	0.02	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	15	0.46	0.05	0.47
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG22	15	0.46	0.05	0.47
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG23	15	0.46	0.05	0.47
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD21	15	0.46	0.05	0.44
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD22	15	0.46	0.05	0.44
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD23	15	0.46	0.05	0.44
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	15	0.46	0.1	0.48
(2,3904)	1:31:A:LEU:HD23	1:72:A:ASN:H	15	0.46	0.1	0.48
(2,3904)	1:31:A:LEU:HD22	1:72:A:ASN:H	15	0.46	0.1	0.48
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD23	15	0.46	0.1	0.46
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD21	15	0.46	0.1	0.46
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD22	15	0.46	0.1	0.46
(2,415)	1:37:A:THR:HG23	1:36:A:GLU:HG3	15	0.46	0.05	0.45
(2,415)	1:37:A:THR:HG21	1:36:A:GLU:HG3	15	0.46	0.05	0.45
(2,415)	1:37:A:THR:HG22	1:36:A:GLU:HG3	15	0.46	0.05	0.45
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD21	15	0.46	0.07	0.48
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD22	15	0.46	0.07	0.48
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD23	15	0.46	0.07	0.48
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD13	15	0.46	0.04	0.45
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD12	15	0.46	0.04	0.45
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD11	15	0.46	0.04	0.45
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD13	15	0.46	0.04	0.45
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD12	15	0.46	0.04	0.45
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD11	15	0.46	0.04	0.45
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG22	15	0.45	0.12	0.46
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG23	15	0.45	0.12	0.46
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG21	15	0.45	0.12	0.46
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	15	0.45	0.05	0.46
(2,3032)	1:20:A:LEU:HD23	1:20:A:LEU:H	15	0.45	0.03	0.45
(2,3032)	1:20:A:LEU:HD22	1:20:A:LEU:H	15	0.45	0.03	0.45
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	15	0.45	0.03	0.45
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	15	0.45	0.02	0.45
(2,1421)	1:116:A:LEU:HD22	1:116:A:LEU:H	15	0.45	0.02	0.45
(2,1421)	1:116:A:LEU:HD21	1:116:A:LEU:H	15	0.45	0.02	0.45
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	15	0.45	0.1	0.44
(2,1519)	1:39:A:LEU:HD13	1:65:A:GLN:H	15	0.45	0.1	0.44
(2,1519)	1:39:A:LEU:HD11	1:65:A:GLN:H	15	0.45	0.1	0.44
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD21	15	0.45	0.04	0.43
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD23	15	0.45	0.04	0.43
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	15	0.45	0.04	0.43
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG23	15	0.45	0.07	0.45
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG22	15	0.45	0.07	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG21	15	0.45	0.07	0.45
(2,4348)	1:60:A:ILE:HD12	1:113:A:SER:H	15	0.44	0.11	0.44
(2,4348)	1:60:A:ILE:HD11	1:113:A:SER:H	15	0.44	0.11	0.44
(2,4348)	1:60:A:ILE:HD13	1:113:A:SER:H	15	0.44	0.11	0.44
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	15	0.44	0.07	0.47
(2,3163)	1:42:A:MET:HE1	1:54:A:LEU:H	15	0.44	0.07	0.47
(2,3163)	1:42:A:MET:HE3	1:54:A:LEU:H	15	0.44	0.07	0.47
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	15	0.44	0.02	0.44
(2,380)	1:31:A:LEU:HD23	1:70:A:PHE:H	15	0.44	0.02	0.44
(2,380)	1:31:A:LEU:HD22	1:70:A:PHE:H	15	0.44	0.02	0.44
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD12	15	0.44	0.05	0.45
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD13	15	0.44	0.05	0.45
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD11	15	0.44	0.05	0.45
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	15	0.44	0.09	0.43
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	15	0.44	0.05	0.43
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG13	15	0.44	0.05	0.43
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG11	15	0.44	0.05	0.43
(2,16)	1:79:A:LEU:HD11	1:75:A:PHE:HA	15	0.44	0.04	0.44
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	15	0.44	0.04	0.44
(2,16)	1:79:A:LEU:HD13	1:75:A:PHE:HA	15	0.44	0.04	0.44
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	15	0.43	0.06	0.45
(2,3670)	1:43:A:THR:HG22	1:44:A:SER:H	15	0.43	0.06	0.45
(2,3670)	1:43:A:THR:HG21	1:44:A:SER:H	15	0.43	0.06	0.45
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE2	15	0.43	0.04	0.44
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE3	15	0.43	0.04	0.44
(2,4373)	1:182:A:LYS:HD3	1:182:A:LYS:HE2	15	0.43	0.04	0.44
(2,4373)	1:167:A:LYS:HD3	1:167:A:LYS:HE2	15	0.43	0.04	0.44
(2,4172)	1:18:A:ALA:HB3	1:22:A:GLN:HE22	15	0.43	0.22	0.38
(2,4172)	1:18:A:ALA:HB1	1:22:A:GLN:HE22	15	0.43	0.22	0.38
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	15	0.43	0.22	0.38
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	15	0.43	0.03	0.44
(2,1280)	1:35:A:LEU:HD23	1:31:A:LEU:HA	15	0.43	0.03	0.44
(2,1280)	1:35:A:LEU:HD21	1:31:A:LEU:HA	15	0.43	0.03	0.44
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	15	0.43	0.03	0.42
(2,3833)	1:178:A:LEU:HD11	1:178:A:LEU:H	15	0.43	0.03	0.42
(2,3833)	1:178:A:LEU:HD12	1:178:A:LEU:H	15	0.43	0.03	0.42
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	15	0.43	0.03	0.43
(2,427)	1:35:A:LEU:HD11	1:35:A:LEU:HA	15	0.43	0.03	0.43
(2,427)	1:35:A:LEU:HD12	1:35:A:LEU:HA	15	0.43	0.03	0.43
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG21	15	0.43	0.11	0.44
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG22	15	0.43	0.11	0.44
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG23	15	0.43	0.11	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	15	0.43	0.2	0.38
(2,729)	1:97:A:ALA:HB2	1:100:A:PHE:HE1	15	0.43	0.2	0.38
(2,729)	1:97:A:ALA:HB1	1:100:A:PHE:HE1	15	0.43	0.2	0.38
(2,3264)	1:94:A:VAL:HG23	1:172:A:ASP:H	15	0.43	0.09	0.43
(2,3264)	1:94:A:VAL:HG21	1:172:A:ASP:H	15	0.43	0.09	0.43
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	15	0.43	0.09	0.43
(2,3816)	1:156:A:LEU:HD23	1:156:A:LEU:H	15	0.42	0.05	0.42
(2,3816)	1:156:A:LEU:HD22	1:156:A:LEU:H	15	0.42	0.05	0.42
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	15	0.42	0.05	0.42
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD12	15	0.42	0.08	0.46
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	15	0.42	0.08	0.46
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD13	15	0.42	0.08	0.46
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG23	15	0.42	0.07	0.42
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG21	15	0.42	0.07	0.42
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG22	15	0.42	0.07	0.42
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	15	0.42	0.09	0.42
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG11	15	0.42	0.09	0.42
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG13	15	0.42	0.09	0.42
(2,43)	1:128:A:ILE:HG21	1:38:A:TYR:H	15	0.42	0.08	0.41
(2,43)	1:128:A:ILE:HG22	1:38:A:TYR:H	15	0.42	0.08	0.41
(2,43)	1:128:A:ILE:HG23	1:38:A:TYR:H	15	0.42	0.08	0.41
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD23	15	0.42	0.05	0.43
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	15	0.42	0.05	0.43
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD22	15	0.42	0.05	0.43
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	15	0.42	0.09	0.42
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD12	15	0.42	0.09	0.44
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD11	15	0.42	0.09	0.44
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD13	15	0.42	0.09	0.44
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	15	0.42	0.02	0.41
(2,1351)	1:94:A:VAL:HG13	1:96:A:TRP:H	15	0.42	0.02	0.41
(2,1351)	1:94:A:VAL:HG11	1:96:A:TRP:H	15	0.42	0.02	0.41
(2,2151)	1:105:A:THR:HG23	1:105:A:THR:H	15	0.42	0.03	0.41
(2,2151)	1:105:A:THR:HG22	1:105:A:THR:H	15	0.42	0.03	0.41
(2,2151)	1:105:A:THR:HG21	1:105:A:THR:H	15	0.42	0.03	0.41
(2,4495)	1:154:A:LEU:HD11	1:154:A:LEU:HG	15	0.41	0.01	0.42
(2,4495)	1:154:A:LEU:HD12	1:154:A:LEU:HG	15	0.41	0.01	0.42
(2,4495)	1:154:A:LEU:HD13	1:154:A:LEU:HG	15	0.41	0.01	0.42
(2,4495)	1:154:A:LEU:HG	1:154:A:LEU:HD23	15	0.41	0.01	0.42
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	15	0.41	0.09	0.42
(2,4021)	1:18:A:ALA:HB1	1:20:A:LEU:H	15	0.41	0.04	0.41
(2,4021)	1:18:A:ALA:HB2	1:20:A:LEU:H	15	0.41	0.04	0.41
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	15	0.41	0.04	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4186)	1:178:A:LEU:HD21	1:179:A:SER:H	15	0.41	0.02	0.41
(2,4186)	1:178:A:LEU:HD22	1:179:A:SER:H	15	0.41	0.02	0.41
(2,4186)	1:178:A:LEU:HD23	1:179:A:SER:H	15	0.41	0.02	0.41
(2,4518)	1:128:A:ILE:HG21	1:124:A:PHE:HZ	15	0.41	0.08	0.45
(2,4518)	1:128:A:ILE:HG22	1:124:A:PHE:HZ	15	0.41	0.08	0.45
(2,4518)	1:128:A:ILE:HG23	1:124:A:PHE:HZ	15	0.41	0.08	0.45
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	15	0.4	0.05	0.39
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD13	15	0.4	0.05	0.39
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD12	15	0.4	0.05	0.39
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	15	0.4	0.09	0.41
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG22	15	0.4	0.09	0.41
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG23	15	0.4	0.09	0.41
(2,3768)	1:117:A:ILE:HD13	1:117:A:ILE:H	15	0.4	0.05	0.39
(2,3768)	1:117:A:ILE:HD12	1:117:A:ILE:H	15	0.4	0.05	0.39
(2,3768)	1:117:A:ILE:HD11	1:117:A:ILE:H	15	0.4	0.05	0.39
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD23	15	0.4	0.11	0.38
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD22	15	0.4	0.11	0.38
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	15	0.4	0.11	0.38
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	15	0.4	0.09	0.44
(2,425)	1:35:A:LEU:HD12	1:35:A:LEU:H	15	0.4	0.09	0.44
(2,425)	1:35:A:LEU:HD13	1:35:A:LEU:H	15	0.4	0.09	0.44
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	15	0.4	0.01	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB1	15	0.4	0.01	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB3	15	0.4	0.01	0.4
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	15	0.4	0.01	0.4
(2,3289)	1:21:A:LEU:HD12	1:21:A:LEU:H	15	0.4	0.05	0.4
(2,3289)	1:21:A:LEU:HD13	1:21:A:LEU:H	15	0.4	0.05	0.4
(2,3289)	1:21:A:LEU:HD11	1:21:A:LEU:H	15	0.4	0.05	0.4
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	15	0.39	0.06	0.4
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG23	15	0.39	0.06	0.4
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG22	15	0.39	0.06	0.4
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG23	15	0.39	0.07	0.38
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG21	15	0.39	0.07	0.38
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG22	15	0.39	0.07	0.38
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	15	0.39	0.06	0.39
(2,1752)	1:76:A:LEU:HD21	1:78:A:GLU:H	15	0.39	0.03	0.38
(2,1752)	1:76:A:LEU:HD22	1:78:A:GLU:H	15	0.39	0.03	0.38
(2,1752)	1:76:A:LEU:HD23	1:78:A:GLU:H	15	0.39	0.03	0.38
(2,623)	1:146:A:VAL:HG22	1:146:A:VAL:HB	15	0.39	0.01	0.39
(2,623)	1:146:A:VAL:HG23	1:146:A:VAL:HB	15	0.39	0.01	0.39
(2,623)	1:146:A:VAL:HG21	1:146:A:VAL:HB	15	0.39	0.01	0.39
(2,500)	1:142:A:LEU:HD23	1:142:A:LEU:HD11	15	0.39	0.02	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,500)	1:142:A:LEU:HD21	1:142:A:LEU:HD13	15	0.39	0.02	0.39
(2,500)	1:142:A:LEU:HD23	1:142:A:LEU:HD13	15	0.39	0.02	0.39
(2,500)	1:142:A:LEU:HD21	1:142:A:LEU:HD12	15	0.39	0.02	0.39
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD12	15	0.39	0.02	0.39
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD13	15	0.39	0.02	0.39
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD11	15	0.39	0.02	0.39
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG23	15	0.39	0.13	0.38
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG21	15	0.39	0.13	0.38
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG22	15	0.39	0.13	0.38
(2,313)	1:20:A:LEU:HD12	1:22:A:GLN:H	15	0.39	0.09	0.36
(2,313)	1:20:A:LEU:HD11	1:22:A:GLN:H	15	0.39	0.09	0.36
(2,313)	1:20:A:LEU:HD13	1:22:A:GLN:H	15	0.39	0.09	0.36
(2,3933)	1:94:A:VAL:HG21	1:95:A:THR:H	15	0.39	0.05	0.39
(2,3933)	1:94:A:VAL:HG22	1:95:A:THR:H	15	0.39	0.05	0.39
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	15	0.39	0.05	0.39
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	15	0.39	0.03	0.39
(2,438)	1:39:A:LEU:HD11	1:42:A:MET:HB2	15	0.39	0.03	0.39
(2,438)	1:39:A:LEU:HD12	1:42:A:MET:HB2	15	0.39	0.03	0.39
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	15	0.38	0.07	0.4
(2,4338)	1:39:A:LEU:HD13	1:39:A:LEU:HG	15	0.38	0.07	0.4
(2,4338)	1:39:A:LEU:HD13	1:43:A:THR:HG22	15	0.38	0.07	0.4
(2,4338)	1:39:A:LEU:HD11	1:39:A:LEU:HG	15	0.38	0.07	0.4
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	15	0.38	0.02	0.38
(2,4264)	1:16:A:ILE:HD11	1:19:A:GLU:HB3	15	0.38	0.18	0.39
(2,4264)	1:16:A:ILE:HD12	1:19:A:GLU:HB3	15	0.38	0.18	0.39
(2,4264)	1:16:A:ILE:HD13	1:19:A:GLU:HB3	15	0.38	0.18	0.39
(2,3872)	1:60:A:ILE:HD12	1:62:A:GLY:H	15	0.38	0.04	0.39
(2,3872)	1:60:A:ILE:HD11	1:62:A:GLY:H	15	0.38	0.04	0.39
(2,3872)	1:60:A:ILE:HD13	1:62:A:GLY:H	15	0.38	0.04	0.39
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD22	15	0.38	0.08	0.39
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD21	15	0.38	0.08	0.39
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD22	15	0.38	0.08	0.39
(2,103)	1:28:A:VAL:HG13	1:31:A:LEU:HD21	15	0.38	0.08	0.39
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD23	15	0.38	0.08	0.39
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD21	15	0.38	0.08	0.39
(2,103)	1:28:A:VAL:HG13	1:31:A:LEU:HD22	15	0.38	0.08	0.39
(2,3889)	1:85:A:LEU:HD21	1:84:A:GLN:H	15	0.38	0.09	0.4
(2,3889)	1:85:A:LEU:HD23	1:84:A:GLN:H	15	0.38	0.09	0.4
(2,3889)	1:85:A:LEU:HD22	1:84:A:GLN:H	15	0.38	0.09	0.4
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	15	0.38	0.08	0.36
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD22	15	0.38	0.08	0.36
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD23	15	0.38	0.08	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2171)	1:174:A:LEU:HD23	1:174:A:LEU:H	15	0.38	0.05	0.37
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	15	0.38	0.05	0.37
(2,2171)	1:174:A:LEU:HD22	1:174:A:LEU:H	15	0.38	0.05	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG23	15	0.38	0.02	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG21	15	0.38	0.02	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG22	15	0.38	0.02	0.37
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	15	0.37	0.1	0.4
(2,328)	1:42:A:MET:HE2	1:60:A:ILE:HB	15	0.37	0.1	0.4
(2,328)	1:42:A:MET:HE1	1:60:A:ILE:HB	15	0.37	0.1	0.4
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	15	0.37	0.06	0.38
(2,3937)	1:184:A:ALA:HB1	1:182:A:LYS:H	15	0.37	0.06	0.38
(2,3937)	1:184:A:ALA:HB2	1:182:A:LYS:H	15	0.37	0.06	0.38
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	15	0.37	0.02	0.37
(2,89)	1:116:A:LEU:HD11	1:117:A:ILE:H	15	0.37	0.02	0.37
(2,89)	1:116:A:LEU:HD12	1:117:A:ILE:H	15	0.37	0.02	0.37
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD12	15	0.37	0.04	0.37
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD13	15	0.37	0.04	0.37
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD11	15	0.37	0.04	0.37
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	15	0.37	0.07	0.37
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	15	0.37	0.07	0.37
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD12	15	0.37	0.07	0.37
(2,1210)	1:134:A:LEU:HD12	1:134:A:LEU:HA	15	0.37	0.08	0.36
(2,1210)	1:134:A:LEU:HD13	1:134:A:LEU:HA	15	0.37	0.08	0.36
(2,1210)	1:134:A:LEU:HD11	1:134:A:LEU:HA	15	0.37	0.08	0.36
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	15	0.37	0.06	0.35
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG23	15	0.36	0.08	0.36
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG22	15	0.36	0.08	0.36
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG21	15	0.36	0.08	0.36
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	15	0.36	0.04	0.37
(2,437)	1:39:A:LEU:HD11	1:42:A:MET:HG3	15	0.36	0.04	0.37
(2,437)	1:39:A:LEU:HD12	1:42:A:MET:HG3	15	0.36	0.04	0.37
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD21	15	0.36	0.13	0.35
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD23	15	0.36	0.13	0.35
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	15	0.36	0.13	0.35
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	15	0.36	0.07	0.35
(2,2835)	1:146:A:VAL:HG11	1:148:A:ARG:H	15	0.36	0.07	0.35
(2,2835)	1:146:A:VAL:HG12	1:148:A:ARG:H	15	0.36	0.07	0.35
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG22	15	0.36	0.05	0.36
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG21	15	0.36	0.05	0.36
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG23	15	0.36	0.05	0.36
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	15	0.36	0.05	0.36
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	15	0.36	0.02	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD22	15	0.36	0.02	0.36
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	15	0.36	0.09	0.38
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB2	15	0.36	0.09	0.38
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB3	15	0.36	0.09	0.38
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	15	0.36	0.04	0.35
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD21	15	0.36	0.04	0.35
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD22	15	0.36	0.04	0.35
(2,3257)	1:170:A:LEU:HD23	1:160:A:LEU:H	15	0.35	0.1	0.35
(2,3257)	1:170:A:LEU:HD22	1:160:A:LEU:H	15	0.35	0.1	0.35
(2,3257)	1:170:A:LEU:HD21	1:160:A:LEU:H	15	0.35	0.1	0.35
(2,2763)	1:146:A:VAL:HG22	1:147:A:GLN:H	15	0.35	0.04	0.36
(2,2763)	1:146:A:VAL:HG23	1:147:A:GLN:H	15	0.35	0.04	0.36
(2,2763)	1:146:A:VAL:HG21	1:147:A:GLN:H	15	0.35	0.04	0.36
(2,3686)	1:60:A:ILE:HG23	1:60:A:ILE:H	15	0.35	0.01	0.35
(2,3686)	1:60:A:ILE:HG21	1:60:A:ILE:H	15	0.35	0.01	0.35
(2,3686)	1:60:A:ILE:HG22	1:60:A:ILE:H	15	0.35	0.01	0.35
(2,567)	1:116:A:LEU:HD13	1:116:A:LEU:HG	15	0.35	0.01	0.35
(2,567)	1:116:A:LEU:HD12	1:116:A:LEU:HG	15	0.35	0.01	0.35
(2,567)	1:116:A:LEU:HD11	1:116:A:LEU:HG	15	0.35	0.01	0.35
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD11	15	0.35	0.07	0.34
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD13	15	0.35	0.07	0.34
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	15	0.35	0.07	0.34
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	15	0.35	0.13	0.37
(2,652)	1:177:A:MET:HE3	1:179:A:SER:H	15	0.35	0.13	0.37
(2,652)	1:177:A:MET:HE2	1:179:A:SER:H	15	0.35	0.13	0.37
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD11	15	0.34	0.08	0.32
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD12	15	0.34	0.08	0.32
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD13	15	0.34	0.08	0.32
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	15	0.34	0.11	0.38
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG23	15	0.34	0.11	0.38
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG21	15	0.34	0.11	0.38
(2,2288)	1:21:A:LEU:HD12	1:22:A:GLN:H	15	0.34	0.11	0.38
(2,2288)	1:21:A:LEU:HD13	1:22:A:GLN:H	15	0.34	0.11	0.38
(2,2288)	1:21:A:LEU:HD11	1:22:A:GLN:H	15	0.34	0.11	0.38
(2,40)	1:31:A:LEU:HD11	1:67:A:ILE:HB	15	0.34	0.04	0.34
(2,40)	1:31:A:LEU:HD13	1:67:A:ILE:HB	15	0.34	0.04	0.34
(2,40)	1:31:A:LEU:HD12	1:67:A:ILE:HB	15	0.34	0.04	0.34
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	15	0.34	0.07	0.36
(2,4068)	1:26:A:ALA:HB3	1:24:A:GLU:H	15	0.34	0.07	0.36
(2,4068)	1:26:A:ALA:HB2	1:24:A:GLU:H	15	0.34	0.07	0.36
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD13	15	0.33	0.03	0.33
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD12	15	0.33	0.03	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	15	0.33	0.03	0.33
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD22	15	0.33	0.08	0.34
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD21	15	0.33	0.08	0.34
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD23	15	0.33	0.08	0.34
(2,2675)	1:117:A:ILE:HD12	1:113:A:SER:H	15	0.33	0.12	0.33
(2,2675)	1:117:A:ILE:HD11	1:113:A:SER:H	15	0.33	0.12	0.33
(2,2675)	1:117:A:ILE:HD13	1:113:A:SER:H	15	0.33	0.12	0.33
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	15	0.33	0.05	0.31
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD12	15	0.33	0.05	0.31
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD13	15	0.33	0.05	0.31
(2,1170)	1:18:A:ALA:HB2	1:18:A:ALA:HA	15	0.33	0.02	0.33
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	15	0.33	0.02	0.33
(2,1170)	1:18:A:ALA:HB3	1:18:A:ALA:HA	15	0.33	0.02	0.33
(2,1590)	1:18:A:ALA:HB3	1:20:A:LEU:HA	15	0.33	0.07	0.34
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	15	0.33	0.07	0.34
(2,1590)	1:18:A:ALA:HB1	1:20:A:LEU:HA	15	0.33	0.07	0.34
(2,394)	1:39:A:LEU:HD22	1:39:A:LEU:HB3	15	0.32	0.01	0.33
(2,394)	1:39:A:LEU:HD21	1:39:A:LEU:HB3	15	0.32	0.01	0.33
(2,394)	1:39:A:LEU:HD23	1:39:A:LEU:HB3	15	0.32	0.01	0.33
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD11	15	0.32	0.03	0.33
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD13	15	0.32	0.03	0.33
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD12	15	0.32	0.03	0.33
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	15	0.32	0.04	0.33
(2,630)	1:64:A:ILE:HG21	1:35:A:LEU:HG	15	0.32	0.04	0.33
(2,630)	1:64:A:ILE:HG23	1:35:A:LEU:HG	15	0.32	0.04	0.33
(2,589)	1:64:A:ILE:HD11	1:35:A:LEU:HB3	15	0.32	0.06	0.32
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	15	0.32	0.06	0.32
(2,589)	1:64:A:ILE:HD13	1:35:A:LEU:HB3	15	0.32	0.06	0.32
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG21	15	0.32	0.05	0.33
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG22	15	0.32	0.05	0.33
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG23	15	0.32	0.05	0.33
(2,4064)	1:17:A:MET:HE2	1:20:A:LEU:H	15	0.32	0.08	0.32
(2,4064)	1:17:A:MET:HE3	1:20:A:LEU:H	15	0.32	0.08	0.32
(2,4064)	1:17:A:MET:HE1	1:20:A:LEU:H	15	0.32	0.08	0.32
(2,4193)	1:20:A:LEU:HD23	1:21:A:LEU:H	15	0.32	0.04	0.32
(2,4193)	1:20:A:LEU:HD22	1:21:A:LEU:H	15	0.32	0.04	0.32
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	15	0.32	0.04	0.32
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	15	0.32	0.09	0.3
(2,577)	1:89:A:VAL:HG11	1:93:A:PHE:HE2	15	0.31	0.07	0.32
(2,577)	1:89:A:VAL:HG13	1:93:A:PHE:HE2	15	0.31	0.07	0.32
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	15	0.31	0.07	0.32
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	15	0.31	0.09	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2638)	1:180:A:VAL:HG23	1:104:A:VAL:H	15	0.31	0.09	0.29
(2,2638)	1:180:A:VAL:HG21	1:104:A:VAL:H	15	0.31	0.09	0.29
(2,4078)	1:28:A:VAL:HG21	1:30:A:ASP:H	15	0.31	0.07	0.31
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	15	0.31	0.07	0.31
(2,4078)	1:28:A:VAL:HG22	1:30:A:ASP:H	15	0.31	0.07	0.31
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	15	0.31	0.07	0.32
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG22	15	0.31	0.07	0.32
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG21	15	0.31	0.07	0.32
(2,851)	1:134:A:LEU:HD23	1:129:A:GLN:HB3	15	0.31	0.1	0.29
(2,851)	1:134:A:LEU:HD21	1:129:A:GLN:HB3	15	0.31	0.1	0.29
(2,851)	1:134:A:LEU:HD22	1:129:A:GLN:HB3	15	0.31	0.1	0.29
(2,3740)	1:95:A:THR:HG23	1:96:A:TRP:H	15	0.31	0.02	0.31
(2,3740)	1:95:A:THR:HG21	1:96:A:TRP:H	15	0.31	0.02	0.31
(2,3740)	1:95:A:THR:HG22	1:96:A:TRP:H	15	0.31	0.02	0.31
(2,3031)	1:20:A:LEU:HD12	1:20:A:LEU:H	15	0.31	0.07	0.3
(2,3031)	1:20:A:LEU:HD11	1:20:A:LEU:H	15	0.31	0.07	0.3
(2,3031)	1:20:A:LEU:HD13	1:20:A:LEU:H	15	0.31	0.07	0.3
(2,3130)	1:49:A:ILE:HD12	1:49:A:ILE:H	15	0.31	0.02	0.31
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	15	0.31	0.02	0.31
(2,3130)	1:49:A:ILE:HD11	1:49:A:ILE:H	15	0.31	0.02	0.31
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	15	0.31	0.04	0.31
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD12	15	0.31	0.04	0.31
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD13	15	0.31	0.04	0.31
(2,761)	1:37:A:THR:HG23	1:36:A:GLU:HG2	15	0.31	0.06	0.31
(2,761)	1:37:A:THR:HG21	1:36:A:GLU:HG2	15	0.31	0.06	0.31
(2,761)	1:37:A:THR:HG22	1:36:A:GLU:HG2	15	0.31	0.06	0.31
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	15	0.31	0.06	0.32
(2,2399)	1:117:A:ILE:HD12	1:116:A:LEU:H	15	0.3	0.05	0.31
(2,2399)	1:117:A:ILE:HD11	1:116:A:LEU:H	15	0.3	0.05	0.31
(2,2399)	1:117:A:ILE:HD13	1:116:A:LEU:H	15	0.3	0.05	0.31
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD12	15	0.3	0.09	0.29
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	15	0.3	0.09	0.29
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD11	15	0.3	0.09	0.29
(2,17)	1:39:A:LEU:HD22	1:42:A:MET:HG2	15	0.3	0.05	0.3
(2,17)	1:39:A:LEU:HD21	1:42:A:MET:HG2	15	0.3	0.05	0.3
(2,17)	1:39:A:LEU:HD23	1:42:A:MET:HG2	15	0.3	0.05	0.3
(2,1512)	1:142:A:LEU:HD12	1:117:A:ILE:H	15	0.3	0.1	0.29
(2,1512)	1:142:A:LEU:HD13	1:117:A:ILE:H	15	0.3	0.1	0.29
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	15	0.3	0.1	0.29
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD12	15	0.3	0.05	0.29
(2,93)	1:89:A:VAL:HG12	1:79:A:LEU:HD13	15	0.3	0.05	0.29
(2,93)	1:89:A:VAL:HG12	1:79:A:LEU:HD12	15	0.3	0.05	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD13	15	0.3	0.05	0.29
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD13	15	0.3	0.05	0.29
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD12	15	0.3	0.05	0.29
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD11	15	0.3	0.05	0.29
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD11	15	0.3	0.05	0.29
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD13	15	0.3	0.06	0.31
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	15	0.3	0.06	0.31
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD12	15	0.3	0.06	0.31
(2,3988)	1:21:A:LEU:HD13	1:83:A:GLU:H	15	0.3	0.04	0.29
(2,3988)	1:21:A:LEU:HD11	1:83:A:GLU:H	15	0.3	0.04	0.29
(2,3988)	1:21:A:LEU:HD12	1:83:A:GLU:H	15	0.3	0.04	0.29
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	15	0.3	0.06	0.31
(2,36)	1:39:A:LEU:HD12	1:65:A:GLN:HG2	15	0.3	0.06	0.31
(2,36)	1:39:A:LEU:HD13	1:65:A:GLN:HG2	15	0.3	0.06	0.31
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD13	15	0.3	0.07	0.29
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	15	0.3	0.07	0.29
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD12	15	0.3	0.07	0.29
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD21	15	0.29	0.06	0.31
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD22	15	0.29	0.06	0.31
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD23	15	0.29	0.06	0.31
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	15	0.29	0.01	0.29
(2,448)	1:31:A:LEU:HD13	1:31:A:LEU:HG	15	0.29	0.01	0.29
(2,448)	1:31:A:LEU:HD12	1:31:A:LEU:HG	15	0.29	0.01	0.29
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	15	0.29	0.06	0.3
(2,116)	1:177:A:MET:HE1	1:100:A:PHE:HB2	15	0.29	0.06	0.3
(2,116)	1:177:A:MET:HE3	1:100:A:PHE:HB2	15	0.29	0.06	0.3
(2,472)	1:178:A:LEU:HD23	1:178:A:LEU:HG	15	0.29	0.02	0.3
(2,472)	1:178:A:LEU:HD21	1:178:A:LEU:HG	15	0.29	0.02	0.3
(2,472)	1:178:A:LEU:HD22	1:178:A:LEU:HG	15	0.29	0.02	0.3
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG23	15	0.29	0.06	0.29
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG21	15	0.29	0.06	0.29
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG22	15	0.29	0.06	0.29
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	15	0.29	0.03	0.3
(2,1371)	1:31:A:LEU:HD12	1:29:A:ARG:H	15	0.29	0.06	0.3
(2,1371)	1:31:A:LEU:HD11	1:29:A:ARG:H	15	0.29	0.06	0.3
(2,1371)	1:31:A:LEU:HD13	1:29:A:ARG:H	15	0.29	0.06	0.3
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	15	0.29	0.01	0.28
(2,433)	1:35:A:LEU:HD13	1:35:A:LEU:HG	15	0.29	0.01	0.28
(2,433)	1:35:A:LEU:HD11	1:35:A:LEU:HG	15	0.29	0.01	0.28
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG12	15	0.28	0.04	0.27
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG13	15	0.28	0.04	0.27
(2,733)	1:97:A:ALA:HB2	1:176:A:VAL:HG12	15	0.28	0.04	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,733)	1:97:A:ALA:HB1	1:176:A:VAL:HG12	15	0.28	0.04	0.27
(2,733)	1:97:A:ALA:HB1	1:176:A:VAL:HG13	15	0.28	0.04	0.27
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG11	15	0.28	0.04	0.27
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	15	0.28	0.06	0.27
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG2	15	0.28	0.06	0.27
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	15	0.28	0.03	0.27
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG11	15	0.28	0.03	0.29
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG13	15	0.28	0.03	0.29
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG12	15	0.28	0.03	0.29
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	15	0.27	0.03	0.28
(2,3976)	1:37:A:THR:HG21	1:38:A:TYR:H	15	0.27	0.03	0.28
(2,3976)	1:37:A:THR:HG22	1:38:A:TYR:H	15	0.27	0.03	0.28
(2,4430)	1:11:A:ARG:HG2	1:11:A:ARG:HD2	15	0.27	0.08	0.25
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	15	0.27	0.08	0.25
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD3	15	0.27	0.08	0.25
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	15	0.27	0.13	0.22
(2,4268)	1:99:A:LYS:HG2	1:101:A:GLN:H	15	0.27	0.13	0.22
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	15	0.27	0.04	0.26
(2,4234)	1:54:A:LEU:HD21	1:53:A:ILE:H	15	0.27	0.03	0.28
(2,4234)	1:54:A:LEU:HD22	1:53:A:ILE:H	15	0.27	0.03	0.28
(2,4234)	1:54:A:LEU:HD23	1:53:A:ILE:H	15	0.27	0.03	0.28
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	15	0.27	0.04	0.27
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD22	15	0.27	0.03	0.26
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD21	15	0.27	0.03	0.26
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD23	15	0.27	0.03	0.26
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	15	0.27	0.04	0.25
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	15	0.27	0.05	0.26
(2,3934)	1:42:A:MET:HE3	1:60:A:ILE:H	15	0.27	0.05	0.26
(2,3934)	1:42:A:MET:HE2	1:60:A:ILE:H	15	0.27	0.05	0.26
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	15	0.26	0.01	0.27
(2,402)	1:35:A:LEU:HD23	1:35:A:LEU:HG	15	0.26	0.01	0.27
(2,402)	1:35:A:LEU:HD21	1:35:A:LEU:HG	15	0.26	0.01	0.27
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	15	0.26	0.07	0.28
(2,422)	1:49:A:ILE:HG21	1:124:A:PHE:HB3	15	0.26	0.07	0.28
(2,422)	1:49:A:ILE:HG23	1:124:A:PHE:HB3	15	0.26	0.07	0.28
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	15	0.26	0.09	0.27
(2,618)	1:43:A:THR:HG22	1:45:A:GLY:H	15	0.26	0.09	0.27
(2,618)	1:43:A:THR:HG21	1:45:A:GLY:H	15	0.26	0.09	0.27
(2,2446)	1:74:A:ILE:HG21	1:73:A:ASN:H	15	0.26	0.03	0.26
(2,2446)	1:74:A:ILE:HG23	1:73:A:ASN:H	15	0.26	0.03	0.26
(2,2446)	1:74:A:ILE:HG22	1:73:A:ASN:H	15	0.26	0.03	0.26
(2,3915)	1:121:A:ALA:HB2	1:119:A:GLU:H	15	0.26	0.06	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3915)	1:121:A:ALA:HB1	1:119:A:GLU:H	15	0.26	0.06	0.25
(2,3915)	1:121:A:ALA:HB3	1:119:A:GLU:H	15	0.26	0.06	0.25
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	15	0.26	0.07	0.26
(2,4016)	1:64:A:ILE:HG22	1:61:A:PHE:H	15	0.26	0.07	0.26
(2,4016)	1:64:A:ILE:HG21	1:61:A:PHE:H	15	0.26	0.07	0.26
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE1	15	0.26	0.1	0.22
(2,557)	1:60:A:ILE:HD13	1:42:A:MET:HE3	15	0.26	0.1	0.22
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE3	15	0.26	0.1	0.22
(2,557)	1:60:A:ILE:HD13	1:42:A:MET:HE1	15	0.26	0.1	0.22
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE3	15	0.26	0.1	0.22
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE1	15	0.26	0.1	0.22
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE2	15	0.26	0.1	0.22
(2,1533)	1:53:A:ILE:HG22	1:117:A:ILE:H	15	0.26	0.06	0.27
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	15	0.26	0.06	0.27
(2,1533)	1:53:A:ILE:HG23	1:117:A:ILE:H	15	0.26	0.06	0.27
(2,409)	1:156:A:LEU:HD13	1:156:A:LEU:HG	15	0.26	0.01	0.26
(2,409)	1:156:A:LEU:HD11	1:156:A:LEU:HG	15	0.26	0.01	0.26
(2,409)	1:156:A:LEU:HD12	1:156:A:LEU:HG	15	0.26	0.01	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG23	15	0.26	0.02	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG21	15	0.26	0.02	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	15	0.26	0.02	0.26
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG23	15	0.26	0.05	0.25
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG21	15	0.26	0.05	0.25
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	15	0.26	0.05	0.25
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	15	0.26	0.02	0.26
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	15	0.26	0.08	0.27
(2,4553)	1:64:A:ILE:HG21	1:65:A:GLN:HE21	15	0.26	0.08	0.27
(2,4553)	1:64:A:ILE:HG23	1:65:A:GLN:HE21	15	0.26	0.08	0.27
(2,4553)	1:64:A:ILE:HG22	1:36:A:GLU:H	15	0.26	0.08	0.27
(2,408)	1:156:A:LEU:HD12	1:156:A:LEU:HB3	15	0.25	0.02	0.25
(2,408)	1:156:A:LEU:HD13	1:156:A:LEU:HB3	15	0.25	0.02	0.25
(2,408)	1:156:A:LEU:HD11	1:156:A:LEU:HB3	15	0.25	0.02	0.25
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	15	0.25	0.03	0.26
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG3	15	0.25	0.03	0.26
(2,615)	1:28:A:VAL:HG13	1:28:A:VAL:HB	15	0.25	0.02	0.25
(2,615)	1:28:A:VAL:HG12	1:28:A:VAL:HB	15	0.25	0.02	0.25
(2,615)	1:28:A:VAL:HG11	1:28:A:VAL:HB	15	0.25	0.02	0.25
(2,1302)	1:156:A:LEU:HD11	1:174:A:LEU:HB3	15	0.25	0.02	0.25
(2,1302)	1:156:A:LEU:HD12	1:174:A:LEU:HB3	15	0.25	0.02	0.25
(2,1302)	1:156:A:LEU:HD13	1:174:A:LEU:HB3	15	0.25	0.02	0.25
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	15	0.25	0.04	0.25
(2,3866)	1:35:A:LEU:HD22	1:65:A:GLN:HE21	15	0.25	0.04	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3866)	1:35:A:LEU:HD23	1:65:A:GLN:HE21	15	0.25	0.04	0.25
(2,609)	1:28:A:VAL:HG11	1:29:A:ARG:H	15	0.25	0.05	0.26
(2,609)	1:28:A:VAL:HG13	1:29:A:ARG:H	15	0.25	0.05	0.26
(2,609)	1:28:A:VAL:HG12	1:29:A:ARG:H	15	0.25	0.05	0.26
(2,3639)	1:18:A:ALA:HB1	1:18:A:ALA:H	15	0.25	0.08	0.26
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	15	0.25	0.08	0.26
(2,3639)	1:18:A:ALA:HB2	1:18:A:ALA:H	15	0.25	0.08	0.26
(2,4229)	1:28:A:VAL:HG13	1:73:A:ASN:H	15	0.25	0.06	0.25
(2,4229)	1:28:A:VAL:HG12	1:73:A:ASN:H	15	0.25	0.06	0.25
(2,4229)	1:28:A:VAL:HG11	1:73:A:ASN:H	15	0.25	0.06	0.25
(2,74)	1:54:A:LEU:HD12	1:51:A:PRO:HB2	15	0.24	0.03	0.24
(2,74)	1:54:A:LEU:HD13	1:51:A:PRO:HB2	15	0.24	0.03	0.24
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	15	0.24	0.03	0.24
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	15	0.24	0.03	0.25
(2,3995)	1:17:A:MET:HE3	1:85:A:LEU:H	15	0.24	0.04	0.26
(2,3995)	1:17:A:MET:HE1	1:85:A:LEU:H	15	0.24	0.04	0.26
(2,3995)	1:17:A:MET:HE2	1:85:A:LEU:H	15	0.24	0.04	0.26
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	15	0.24	0.05	0.23
(2,2630)	1:150:A:THR:HG23	1:154:A:LEU:H	15	0.24	0.05	0.23
(2,2630)	1:150:A:THR:HG22	1:154:A:LEU:H	15	0.24	0.05	0.23
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG21	15	0.23	0.08	0.23
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG23	15	0.23	0.08	0.23
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG22	15	0.23	0.08	0.23
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG23	15	0.23	0.08	0.23
(2,423)	1:42:A:MET:HE3	1:49:A:ILE:HG23	15	0.23	0.08	0.23
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG22	15	0.23	0.08	0.23
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG21	15	0.23	0.08	0.23
(2,423)	1:42:A:MET:HE3	1:49:A:ILE:HG21	15	0.23	0.08	0.23
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	15	0.23	0.03	0.23
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD22	15	0.23	0.03	0.23
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	15	0.23	0.01	0.23
(2,3982)	1:53:A:ILE:HD12	1:121:A:ALA:H	15	0.23	0.01	0.23
(2,3982)	1:53:A:ILE:HD13	1:121:A:ALA:H	15	0.23	0.01	0.23
(2,696)	1:49:A:ILE:HD13	1:49:A:ILE:HG12	15	0.22	0.01	0.23
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	15	0.22	0.01	0.23
(2,696)	1:49:A:ILE:HD12	1:49:A:ILE:HG12	15	0.22	0.01	0.23
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	15	0.22	0.01	0.22
(2,727)	1:143:A:ILE:HD12	1:143:A:ILE:HG12	15	0.22	0.01	0.22
(2,727)	1:143:A:ILE:HD11	1:143:A:ILE:HG12	15	0.22	0.01	0.22
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	15	0.22	0.02	0.22
(2,3647)	1:26:A:ALA:HB1	1:26:A:ALA:H	15	0.22	0.02	0.22
(2,3647)	1:26:A:ALA:HB3	1:26:A:ALA:H	15	0.22	0.02	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	15	0.22	0.05	0.23
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD12	15	0.22	0.05	0.23
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD13	15	0.22	0.05	0.23
(2,1500)	1:49:A:ILE:HG23	1:53:A:ILE:HB	15	0.22	0.05	0.23
(2,1500)	1:49:A:ILE:HG21	1:53:A:ILE:HB	15	0.22	0.05	0.23
(2,1500)	1:49:A:ILE:HG22	1:53:A:ILE:HB	15	0.22	0.05	0.23
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	15	0.22	0.05	0.23
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	15	0.22	0.02	0.21
(2,383)	1:31:A:LEU:HD21	1:31:A:LEU:HA	15	0.22	0.02	0.21
(2,383)	1:31:A:LEU:HD23	1:31:A:LEU:HA	15	0.22	0.02	0.21
(2,1336)	1:46:A:VAL:HG13	1:46:A:VAL:HA	15	0.21	0.02	0.21
(2,1336)	1:46:A:VAL:HG12	1:46:A:VAL:HA	15	0.21	0.02	0.21
(2,1336)	1:46:A:VAL:HG11	1:46:A:VAL:HA	15	0.21	0.02	0.21
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	15	0.21	0.04	0.21
(2,2585)	1:94:A:VAL:HG13	1:95:A:THR:H	15	0.21	0.04	0.21
(2,2585)	1:94:A:VAL:HG11	1:95:A:THR:H	15	0.21	0.04	0.21
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	15	0.21	0.02	0.21
(2,602)	1:28:A:VAL:HG21	1:28:A:VAL:HB	15	0.21	0.02	0.21
(2,602)	1:28:A:VAL:HG23	1:28:A:VAL:HB	15	0.21	0.02	0.21
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	15	0.21	0.06	0.17
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB2	15	0.21	0.06	0.17
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB3	15	0.21	0.06	0.17
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	15	0.2	0.04	0.19
(2,3844)	1:184:A:ALA:HB1	1:185:A:ASN:H	15	0.2	0.04	0.19
(2,3844)	1:184:A:ALA:HB2	1:185:A:ASN:H	15	0.2	0.04	0.19
(2,788)	1:143:A:ILE:HG23	1:143:A:ILE:HB	15	0.2	0.04	0.22
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	15	0.2	0.04	0.22
(2,788)	1:143:A:ILE:HG22	1:143:A:ILE:HB	15	0.2	0.04	0.22
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	15	0.2	0.02	0.2
(2,4030)	1:118:A:LEU:HD22	1:118:A:LEU:H	15	0.2	0.02	0.2
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	15	0.2	0.01	0.19
(2,492)	1:159:A:LEU:HD23	1:160:A:LEU:H	15	0.2	0.04	0.21
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	15	0.2	0.04	0.21
(2,492)	1:159:A:LEU:HD21	1:160:A:LEU:H	15	0.2	0.04	0.21
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	15	0.2	0.04	0.19
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	15	0.2	0.03	0.2
(2,332)	1:42:A:MET:HE3	1:60:A:ILE:HG13	15	0.2	0.03	0.2
(2,332)	1:42:A:MET:HE2	1:60:A:ILE:HG13	15	0.2	0.03	0.2
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	15	0.2	0.03	0.2
(2,600)	1:28:A:VAL:HG22	1:28:A:VAL:HA	15	0.2	0.03	0.2
(2,600)	1:28:A:VAL:HG21	1:28:A:VAL:HA	15	0.2	0.03	0.2
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	15	0.19	0.01	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,677)	1:146:A:VAL:HG12	1:146:A:VAL:HB	15	0.19	0.01	0.19
(2,677)	1:146:A:VAL:HG11	1:146:A:VAL:HB	15	0.19	0.01	0.19
(2,512)	1:170:A:LEU:HD22	1:170:A:LEU:HG	15	0.19	0.02	0.19
(2,512)	1:170:A:LEU:HD21	1:170:A:LEU:HG	15	0.19	0.02	0.19
(2,512)	1:170:A:LEU:HD23	1:170:A:LEU:HG	15	0.19	0.02	0.19
(2,3640)	1:18:A:ALA:HB1	1:19:A:GLU:H	15	0.18	0.03	0.18
(2,3640)	1:18:A:ALA:HB2	1:19:A:GLU:H	15	0.18	0.03	0.18
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	15	0.18	0.03	0.18
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD22	15	0.18	0.03	0.18
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD21	15	0.18	0.03	0.18
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD23	15	0.18	0.03	0.18
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	15	0.17	0.02	0.17
(2,364)	1:156:A:LEU:HD21	1:156:A:LEU:HG	15	0.17	0.02	0.17
(2,364)	1:156:A:LEU:HD22	1:156:A:LEU:HG	15	0.17	0.02	0.17
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	15	0.17	0.02	0.17
(2,977)	1:104:A:VAL:HG13	1:104:A:VAL:HA	15	0.17	0.02	0.17
(2,977)	1:104:A:VAL:HG11	1:104:A:VAL:HA	15	0.17	0.02	0.17
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	15	0.17	0.04	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG22	15	0.17	0.01	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG21	15	0.17	0.01	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG23	15	0.17	0.01	0.17
(2,392)	1:39:A:LEU:HD22	1:42:A:MET:HB2	15	0.17	0.02	0.17
(2,392)	1:39:A:LEU:HD21	1:42:A:MET:HB2	15	0.17	0.02	0.17
(2,392)	1:39:A:LEU:HD23	1:42:A:MET:HB2	15	0.17	0.02	0.17
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG11	15	0.16	0.02	0.16
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG13	15	0.16	0.02	0.16
(2,4504)	1:190:A:VAL:HG23	1:190:A:VAL:HB	15	0.16	0.02	0.16
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG12	15	0.16	0.02	0.16
(2,4504)	1:190:A:VAL:HG22	1:190:A:VAL:HB	15	0.16	0.02	0.16
(2,403)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	15	0.16	0.01	0.16
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	15	0.16	0.01	0.16
(2,403)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	15	0.16	0.01	0.16
(2,995)	1:117:A:ILE:HG23	1:117:A:ILE:HA	15	0.14	0.01	0.14
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	15	0.14	0.01	0.14
(2,995)	1:117:A:ILE:HG22	1:117:A:ILE:HA	15	0.14	0.01	0.14
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	15	0.13	0.01	0.13
(2,329)	1:89:A:VAL:HG11	1:17:A:MET:HE1	15	0.13	0.02	0.12
(2,329)	1:89:A:VAL:HG13	1:17:A:MET:HE2	15	0.13	0.02	0.12
(2,329)	1:89:A:VAL:HG13	1:17:A:MET:HE3	15	0.13	0.02	0.12
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE1	15	0.13	0.02	0.12
(2,329)	1:89:A:VAL:HG11	1:17:A:MET:HE2	15	0.13	0.02	0.12
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE2	15	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE3	15	0.13	0.02	0.12
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	15	0.12	0.01	0.12
(2,635)	1:176:A:VAL:HG13	1:176:A:VAL:HB	15	0.12	0.01	0.12
(2,635)	1:176:A:VAL:HG11	1:176:A:VAL:HB	15	0.12	0.01	0.12
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG21	14	1.19	0.38	1.24
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG23	14	1.19	0.38	1.24
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG22	14	1.19	0.38	1.24
(2,3861)	1:143:A:ILE:HG22	1:147:A:GLN:HE22	14	0.82	0.37	0.6
(2,3861)	1:143:A:ILE:HG21	1:147:A:GLN:HE22	14	0.82	0.37	0.6
(2,3861)	1:143:A:ILE:HG23	1:147:A:GLN:HE22	14	0.82	0.37	0.6
(2,4547)	1:102:A:MET:HE3	1:64:A:ILE:HA	14	0.8	0.31	0.74
(2,4547)	1:102:A:MET:HE2	1:64:A:ILE:HA	14	0.8	0.31	0.74
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	14	0.8	0.31	0.74
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	14	0.77	0.14	0.82
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	14	0.59	0.13	0.6
(2,824)	1:134:A:LEU:HD21	1:33:A:GLU:HG3	14	0.59	0.13	0.6
(2,824)	1:134:A:LEU:HD23	1:33:A:GLU:HG3	14	0.59	0.13	0.6
(2,4609)	1:141:A:TYR:HE1	1:33:A:GLU:H	14	0.54	0.08	0.54
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	14	0.54	0.08	0.54
(2,66)	1:118:A:LEU:HD23	1:114:A:ASN:HD21	14	0.53	0.08	0.55
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	14	0.53	0.08	0.55
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG11	14	0.52	0.17	0.56
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG13	14	0.52	0.17	0.56
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG12	14	0.52	0.17	0.56
(2,4492)	1:79:A:LEU:HD23	1:25:A:LYS:HG3	14	0.51	0.24	0.5
(2,4492)	1:79:A:LEU:HD21	1:25:A:LYS:HG3	14	0.51	0.24	0.5
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	14	0.51	0.24	0.5
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	14	0.51	0.14	0.54
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HB3	14	0.51	0.14	0.54
(2,4331)	1:95:A:THR:HG22	1:92:A:CYS:HG	14	0.5	0.19	0.55
(2,4331)	1:95:A:THR:HG21	1:92:A:CYS:HG	14	0.5	0.19	0.55
(2,4331)	1:95:A:THR:HG23	1:92:A:CYS:HG	14	0.5	0.19	0.55
(2,316)	1:20:A:LEU:HD11	1:152:A:TYR:HB3	14	0.48	0.21	0.5
(2,316)	1:20:A:LEU:HD13	1:152:A:TYR:HB3	14	0.48	0.21	0.5
(2,316)	1:20:A:LEU:HD12	1:152:A:TYR:HB3	14	0.48	0.21	0.5
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD12	14	0.45	0.08	0.46
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	14	0.45	0.08	0.46
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD11	14	0.45	0.08	0.46
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	14	0.44	0.12	0.38
(2,4272)	1:174:A:LEU:HD23	1:175:A:GLU:HB2	14	0.42	0.15	0.45
(2,4272)	1:174:A:LEU:HD21	1:175:A:GLU:HB2	14	0.42	0.15	0.45
(2,4272)	1:174:A:LEU:HD22	1:175:A:GLU:HB2	14	0.42	0.15	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1522)	1:76:A:LEU:HD13	1:68:A:TYR:HE1	14	0.41	0.14	0.4
(2,1522)	1:76:A:LEU:HD11	1:68:A:TYR:HE1	14	0.41	0.14	0.4
(2,1522)	1:76:A:LEU:HD12	1:68:A:TYR:HE1	14	0.41	0.14	0.4
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	14	0.41	0.1	0.45
(2,4776)	1:11:A:ARG:HG3	1:11:A:ARG:H	14	0.41	0.1	0.45
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG22	14	0.41	0.03	0.42
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG22	14	0.41	0.03	0.42
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG21	14	0.41	0.03	0.42
(2,624)	1:39:A:LEU:HD12	1:43:A:THR:HG22	14	0.41	0.03	0.42
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG21	14	0.41	0.03	0.42
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG23	14	0.41	0.03	0.42
(2,624)	1:39:A:LEU:HD12	1:43:A:THR:HG23	14	0.41	0.03	0.42
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD11	14	0.37	0.09	0.36
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD12	14	0.37	0.09	0.36
(2,387)	1:31:A:LEU:HD22	1:67:A:ILE:HD12	14	0.37	0.09	0.36
(2,387)	1:31:A:LEU:HD21	1:67:A:ILE:HD11	14	0.37	0.09	0.36
(2,387)	1:31:A:LEU:HD22	1:67:A:ILE:HD11	14	0.37	0.09	0.36
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD13	14	0.37	0.09	0.36
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	14	0.37	0.07	0.36
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG12	14	0.37	0.07	0.36
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG11	14	0.37	0.07	0.36
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	14	0.36	0.13	0.42
(2,1317)	1:43:A:THR:HG22	1:57:A:GLU:HB3	14	0.36	0.13	0.42
(2,1317)	1:43:A:THR:HG21	1:57:A:GLU:HB3	14	0.36	0.13	0.42
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD22	14	0.35	0.08	0.33
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD23	14	0.35	0.08	0.33
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	14	0.35	0.08	0.33
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG23	14	0.34	0.08	0.34
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG21	14	0.34	0.08	0.34
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG22	14	0.34	0.08	0.34
(2,4292)	1:48:A:GLU:HB3	1:49:A:ILE:HG21	14	0.34	0.08	0.34
(2,4292)	1:48:A:GLU:HB3	1:49:A:ILE:HG23	14	0.34	0.08	0.34
(2,4292)	1:48:A:GLU:HB3	1:49:A:ILE:HG22	14	0.34	0.08	0.34
(2,1254)	1:17:A:MET:HE3	1:82:A:TYR:H	14	0.32	0.11	0.3
(2,1254)	1:17:A:MET:HE1	1:82:A:TYR:H	14	0.32	0.11	0.3
(2,1254)	1:17:A:MET:HE2	1:82:A:TYR:H	14	0.32	0.11	0.3
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	14	0.32	0.37	0.14
(2,592)	1:64:A:ILE:HD13	1:31:A:LEU:HD23	14	0.32	0.11	0.29
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD23	14	0.32	0.11	0.29
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD22	14	0.32	0.11	0.29
(2,592)	1:64:A:ILE:HD12	1:31:A:LEU:HD21	14	0.32	0.11	0.29
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD21	14	0.32	0.11	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,592)	1:64:A:ILE:HD12	1:31:A:LEU:HD22	14	0.32	0.11	0.29
(2,1543)	1:128:A:ILE:HD11	1:132:A:HIS:HD2	14	0.31	0.12	0.32
(2,1543)	1:128:A:ILE:HD12	1:132:A:HIS:HD2	14	0.31	0.12	0.32
(2,1543)	1:128:A:ILE:HD13	1:132:A:HIS:HD2	14	0.31	0.12	0.32
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG22	14	0.31	0.07	0.32
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG23	14	0.31	0.07	0.32
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG21	14	0.31	0.07	0.32
(2,644)	1:105:A:THR:HG22	1:108:A:LYS:HD3	14	0.31	0.07	0.33
(2,644)	1:105:A:THR:HG21	1:108:A:LYS:HD3	14	0.31	0.07	0.33
(2,644)	1:105:A:THR:HG23	1:108:A:LYS:HD3	14	0.31	0.07	0.33
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	14	0.3	0.17	0.21
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD13	14	0.3	0.17	0.21
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD12	14	0.3	0.17	0.21
(2,362)	1:156:A:LEU:HD23	1:152:A:TYR:HB2	14	0.3	0.14	0.28
(2,362)	1:156:A:LEU:HD22	1:152:A:TYR:HB2	14	0.3	0.14	0.28
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	14	0.3	0.14	0.28
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG23	14	0.29	0.11	0.28
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG22	14	0.29	0.11	0.28
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG21	14	0.29	0.11	0.28
(2,3344)	1:170:A:LEU:HD13	1:171:A:LYS:H	14	0.29	0.09	0.29
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	14	0.29	0.09	0.29
(2,3344)	1:170:A:LEU:HD12	1:171:A:LYS:H	14	0.29	0.09	0.29
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	14	0.28	0.12	0.24
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	14	0.27	0.05	0.26
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD23	14	0.27	0.05	0.26
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD21	14	0.27	0.05	0.26
(2,1744)	1:76:A:LEU:HD21	1:77:A:LYS:H	14	0.27	0.06	0.3
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	14	0.27	0.06	0.3
(2,1744)	1:76:A:LEU:HD23	1:77:A:LYS:H	14	0.27	0.06	0.3
(2,4232)	1:117:A:ILE:HG22	1:116:A:LEU:H	14	0.27	0.07	0.28
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	14	0.27	0.07	0.28
(2,4232)	1:117:A:ILE:HG21	1:116:A:LEU:H	14	0.27	0.07	0.28
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	14	0.27	0.11	0.28
(2,3794)	1:135:A:ALA:HB1	1:135:A:ALA:H	14	0.27	0.02	0.27
(2,3794)	1:135:A:ALA:HB2	1:135:A:ALA:H	14	0.27	0.02	0.27
(2,3794)	1:135:A:ALA:HB3	1:135:A:ALA:H	14	0.27	0.02	0.27
(2,4521)	1:54:A:LEU:HD11	1:54:A:LEU:HA	14	0.26	0.06	0.28
(2,4521)	1:54:A:LEU:HD13	1:52:A:GLY:HA2	14	0.26	0.06	0.28
(2,4521)	1:54:A:LEU:HD12	1:52:A:GLY:HA2	14	0.26	0.06	0.28
(2,4521)	1:54:A:LEU:HD12	1:54:A:LEU:HA	14	0.26	0.06	0.28
(2,4521)	1:54:A:LEU:HD11	1:52:A:GLY:HA2	14	0.26	0.06	0.28
(2,4521)	1:54:A:LEU:HD13	1:54:A:LEU:HA	14	0.26	0.06	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	14	0.26	0.09	0.26
(2,1402)	1:35:A:LEU:HD11	1:65:A:GLN:HB2	14	0.26	0.09	0.26
(2,1402)	1:35:A:LEU:HD12	1:65:A:GLN:HB2	14	0.26	0.09	0.26
(2,171)	1:74:A:ILE:HG23	1:78:A:GLU:HG3	14	0.25	0.08	0.24
(2,171)	1:74:A:ILE:HG21	1:78:A:GLU:HG3	14	0.25	0.08	0.24
(2,171)	1:74:A:ILE:HG22	1:78:A:GLU:HG3	14	0.25	0.08	0.24
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	14	0.25	0.08	0.27
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG21	14	0.25	0.08	0.27
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG23	14	0.25	0.08	0.27
(2,1369)	1:156:A:LEU:HD13	1:170:A:LEU:HB3	14	0.25	0.1	0.22
(2,1369)	1:156:A:LEU:HD11	1:170:A:LEU:HB3	14	0.25	0.1	0.22
(2,1369)	1:156:A:LEU:HD12	1:170:A:LEU:HB3	14	0.25	0.1	0.22
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	14	0.25	0.05	0.24
(2,418)	1:53:A:ILE:HD11	1:124:A:PHE:HB3	14	0.25	0.05	0.24
(2,418)	1:53:A:ILE:HD12	1:124:A:PHE:HB3	14	0.25	0.05	0.24
(2,42)	1:53:A:ILE:HG23	1:120:A:HIS:HD2	14	0.25	0.1	0.25
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	14	0.25	0.1	0.25
(2,42)	1:53:A:ILE:HG21	1:120:A:HIS:HD2	14	0.25	0.1	0.25
(2,468)	1:178:A:LEU:HD23	1:175:A:GLU:HA	14	0.24	0.09	0.26
(2,468)	1:178:A:LEU:HD21	1:175:A:GLU:HA	14	0.24	0.09	0.26
(2,468)	1:178:A:LEU:HD22	1:175:A:GLU:HA	14	0.24	0.09	0.26
(2,4046)	1:159:A:LEU:HD23	1:159:A:LEU:H	14	0.24	0.05	0.22
(2,4046)	1:159:A:LEU:HD21	1:159:A:LEU:H	14	0.24	0.05	0.22
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	14	0.24	0.05	0.22
(2,3223)	1:117:A:ILE:HD11	1:139:A:SER:H	14	0.24	0.04	0.24
(2,3223)	1:117:A:ILE:HD13	1:139:A:SER:H	14	0.24	0.04	0.24
(2,3223)	1:117:A:ILE:HD12	1:139:A:SER:H	14	0.24	0.04	0.24
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG23	14	0.24	0.04	0.22
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG22	14	0.24	0.04	0.22
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	14	0.24	0.04	0.22
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	14	0.23	0.06	0.24
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG21	14	0.23	0.06	0.24
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG22	14	0.23	0.06	0.24
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD21	14	0.23	0.06	0.22
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD22	14	0.23	0.06	0.22
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD23	14	0.23	0.06	0.22
(2,3796)	1:135:A:ALA:HB3	1:136:A:ASN:HD22	14	0.22	0.07	0.24
(2,3796)	1:135:A:ALA:HB1	1:136:A:ASN:HD22	14	0.22	0.07	0.24
(2,3796)	1:135:A:ALA:HB2	1:136:A:ASN:HD22	14	0.22	0.07	0.24
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	14	0.22	0.08	0.2
(2,4110)	1:64:A:ILE:HG22	1:62:A:GLY:H	14	0.22	0.08	0.2
(2,4110)	1:64:A:ILE:HG21	1:62:A:GLY:H	14	0.22	0.08	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,475)	1:59:A:ILE:HG23	1:116:A:LEU:HB3	14	0.22	0.05	0.24
(2,475)	1:59:A:ILE:HG21	1:116:A:LEU:HB3	14	0.22	0.05	0.24
(2,475)	1:59:A:ILE:HG22	1:116:A:LEU:HB3	14	0.22	0.05	0.24
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG22	14	0.21	0.07	0.22
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG22	14	0.21	0.07	0.22
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG23	14	0.21	0.07	0.22
(2,1536)	1:60:A:ILE:HD13	1:53:A:ILE:HG21	14	0.21	0.07	0.22
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG21	14	0.21	0.07	0.22
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG21	14	0.21	0.07	0.22
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG23	14	0.21	0.07	0.22
(2,1536)	1:60:A:ILE:HD13	1:53:A:ILE:HG22	14	0.21	0.07	0.22
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG2	14	0.21	0.04	0.21
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	14	0.21	0.04	0.21
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	14	0.2	0.04	0.22
(2,622)	1:43:A:THR:HG22	1:42:A:MET:HG3	14	0.2	0.04	0.22
(2,622)	1:43:A:THR:HG21	1:42:A:MET:HG3	14	0.2	0.04	0.22
(2,4116)	1:79:A:LEU:HD11	1:78:A:GLU:H	14	0.2	0.07	0.18
(2,4116)	1:79:A:LEU:HD13	1:78:A:GLU:H	14	0.2	0.07	0.18
(2,4116)	1:79:A:LEU:HD12	1:78:A:GLU:H	14	0.2	0.07	0.18
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD13	14	0.2	0.04	0.22
(2,377)	1:142:A:LEU:HD21	1:117:A:ILE:HD12	14	0.2	0.04	0.22
(2,377)	1:142:A:LEU:HD21	1:117:A:ILE:HD11	14	0.2	0.04	0.22
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD11	14	0.2	0.04	0.22
(2,377)	1:142:A:LEU:HD21	1:117:A:ILE:HD13	14	0.2	0.04	0.22
(2,377)	1:142:A:LEU:HD22	1:117:A:ILE:HD11	14	0.2	0.04	0.22
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD12	14	0.2	0.04	0.22
(2,377)	1:142:A:LEU:HD22	1:117:A:ILE:HD12	14	0.2	0.04	0.22
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	14	0.2	0.05	0.21
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG22	14	0.2	0.05	0.21
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG23	14	0.2	0.05	0.21
(2,4435)	1:94:A:VAL:HG22	1:94:A:VAL:HA	14	0.2	0.03	0.2
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG23	14	0.2	0.03	0.2
(2,4435)	1:94:A:VAL:HG21	1:94:A:VAL:HA	14	0.2	0.03	0.2
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG22	14	0.2	0.03	0.2
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG21	14	0.2	0.03	0.2
(2,4435)	1:94:A:VAL:HG23	1:94:A:VAL:HA	14	0.2	0.03	0.2
(2,3978)	1:23:A:THR:HG21	1:22:A:GLN:H	14	0.19	0.04	0.19
(2,3978)	1:23:A:THR:HG22	1:22:A:GLN:H	14	0.19	0.04	0.19
(2,3978)	1:23:A:THR:HG23	1:22:A:GLN:H	14	0.19	0.04	0.19
(2,3682)	1:54:A:LEU:HD23	1:55:A:ASN:HD21	14	0.18	0.03	0.18
(2,3682)	1:54:A:LEU:HD21	1:55:A:ASN:HD21	14	0.18	0.03	0.18
(2,3682)	1:54:A:LEU:HD22	1:55:A:ASN:HD21	14	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	14	0.17	0.08	0.15
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	14	0.16	0.03	0.17
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD21	14	0.16	0.04	0.14
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD22	14	0.16	0.04	0.14
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD23	14	0.16	0.04	0.14
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	14	0.16	0.03	0.16
(2,553)	1:16:A:ILE:HG23	1:16:A:ILE:H	14	0.16	0.03	0.16
(2,553)	1:16:A:ILE:HG22	1:16:A:ILE:H	14	0.16	0.03	0.16
(2,1092)	1:59:A:ILE:HG22	1:59:A:ILE:HA	14	0.15	0.02	0.15
(2,1092)	1:59:A:ILE:HG23	1:59:A:ILE:HA	14	0.15	0.02	0.15
(2,1092)	1:59:A:ILE:HG21	1:59:A:ILE:HA	14	0.15	0.02	0.15
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	14	0.15	0.03	0.16
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	14	0.14	0.02	0.14
(2,386)	1:31:A:LEU:HD23	1:31:A:LEU:HG	14	0.14	0.02	0.14
(2,386)	1:31:A:LEU:HD22	1:31:A:LEU:HG	14	0.14	0.02	0.14
(2,3779)	1:121:A:ALA:HB2	1:121:A:ALA:H	14	0.13	0.01	0.14
(2,3779)	1:121:A:ALA:HB1	1:121:A:ALA:H	14	0.13	0.01	0.14
(2,3779)	1:121:A:ALA:HB3	1:121:A:ALA:H	14	0.13	0.01	0.14
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	14	0.13	0.01	0.13
(2,541)	1:116:A:LEU:HD21	1:116:A:LEU:HB3	14	0.13	0.01	0.13
(2,541)	1:116:A:LEU:HD23	1:116:A:LEU:HB3	14	0.13	0.01	0.13
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	14	0.13	0.02	0.12
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	14	0.13	0.01	0.12
(2,4546)	1:67:A:ILE:HG23	1:67:A:ILE:HB	14	0.11	0.01	0.11
(2,4546)	1:67:A:ILE:HG22	1:67:A:ILE:HB	14	0.11	0.01	0.11
(2,4546)	1:16:A:ILE:HG21	1:16:A:ILE:HB	14	0.11	0.01	0.11
(2,4546)	1:67:A:ILE:HG21	1:67:A:ILE:HB	14	0.11	0.01	0.11
(2,4546)	1:16:A:ILE:HG23	1:16:A:ILE:HB	14	0.11	0.01	0.11
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	14	0.11	0.01	0.11
(2,1141)	1:43:A:THR:HG23	1:43:A:THR:HB	14	0.11	0.01	0.11
(2,1141)	1:43:A:THR:HG22	1:43:A:THR:HB	14	0.11	0.01	0.11
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD23	13	0.98	0.08	1.0
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD21	13	0.98	0.08	1.0
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD22	13	0.98	0.08	1.0
(2,4554)	1:146:A:VAL:HG22	1:143:A:ILE:HG12	13	0.77	0.2	0.8
(2,4554)	1:146:A:VAL:HG21	1:110:A:LYS:HD2	13	0.77	0.2	0.8
(2,4554)	1:146:A:VAL:HG22	1:110:A:LYS:HD3	13	0.77	0.2	0.8
(2,4554)	1:146:A:VAL:HG23	1:110:A:LYS:HD2	13	0.77	0.2	0.8
(2,4554)	1:146:A:VAL:HG23	1:110:A:LYS:HD3	13	0.77	0.2	0.8
(2,4554)	1:146:A:VAL:HG22	1:110:A:LYS:HD2	13	0.77	0.2	0.8
(2,4554)	1:146:A:VAL:HG21	1:143:A:ILE:HG12	13	0.77	0.2	0.8
(2,4554)	1:146:A:VAL:HG21	1:110:A:LYS:HD3	13	0.77	0.2	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	13	0.75	0.15	0.76
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG22	13	0.75	0.15	0.79
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG23	13	0.75	0.15	0.79
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG21	13	0.75	0.15	0.79
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD11	13	0.73	0.28	0.7
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD13	13	0.73	0.28	0.7
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD12	13	0.73	0.28	0.7
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD12	13	0.62	0.44	0.51
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD11	13	0.62	0.44	0.51
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD13	13	0.62	0.44	0.51
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	13	0.62	0.21	0.7
(2,4766)	1:8:A:PHE:HD2	1:7:A:GLU:HB3	13	0.62	0.21	0.7
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB3	13	0.62	0.21	0.7
(2,461)	1:134:A:LEU:HD21	1:33:A:GLU:HG2	13	0.61	0.15	0.63
(2,461)	1:134:A:LEU:HD22	1:33:A:GLU:HG2	13	0.61	0.15	0.63
(2,461)	1:134:A:LEU:HD23	1:33:A:GLU:HG2	13	0.61	0.15	0.63
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD13	13	0.6	0.45	0.49
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD12	13	0.6	0.45	0.49
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD11	13	0.6	0.45	0.49
(2,4262)	1:31:A:LEU:HD13	1:103:A:TYR:HE1	13	0.6	0.45	0.49
(2,4262)	1:31:A:LEU:HD11	1:103:A:TYR:HE1	13	0.6	0.45	0.49
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	13	0.58	0.51	0.2
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	13	0.56	0.19	0.62
(2,4584)	1:170:A:LEU:HD23	1:90:A:GLY:H	13	0.56	0.19	0.62
(2,4584)	1:170:A:LEU:HD22	1:90:A:GLY:H	13	0.56	0.19	0.62
(2,318)	1:20:A:LEU:HD21	1:152:A:TYR:HD1	13	0.54	0.22	0.5
(2,318)	1:20:A:LEU:HD23	1:152:A:TYR:HD1	13	0.54	0.22	0.5
(2,318)	1:20:A:LEU:HD23	1:152:A:TYR:HD2	13	0.54	0.22	0.5
(2,318)	1:20:A:LEU:HD22	1:152:A:TYR:HD1	13	0.54	0.22	0.5
(2,4265)	1:142:A:LEU:HD12	1:110:A:LYS:HB2	13	0.43	0.2	0.42
(2,4265)	1:142:A:LEU:HD11	1:110:A:LYS:HB2	13	0.43	0.2	0.42
(2,4265)	1:142:A:LEU:HD13	1:110:A:LYS:HB2	13	0.43	0.2	0.42
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	13	0.42	0.08	0.4
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD2	13	0.42	0.08	0.4
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	13	0.38	0.15	0.34
(2,4772)	1:32:A:HIS:HE1	1:69:A:ASP:HA	13	0.38	0.15	0.34
(2,4258)	1:95:A:THR:HG23	1:75:A:PHE:HD2	13	0.35	0.19	0.33
(2,4258)	1:95:A:THR:HG21	1:75:A:PHE:HD2	13	0.35	0.19	0.33
(2,4258)	1:95:A:THR:HG22	1:75:A:PHE:HD1	13	0.35	0.19	0.33
(2,4258)	1:95:A:THR:HG23	1:75:A:PHE:HD1	13	0.35	0.19	0.33
(2,4258)	1:95:A:THR:HG21	1:75:A:PHE:HD1	13	0.35	0.19	0.33
(2,4258)	1:95:A:THR:HG22	1:75:A:PHE:HD2	13	0.35	0.19	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	13	0.3	0.09	0.32
(2,1350)	1:35:A:LEU:HD12	1:36:A:GLU:H	13	0.3	0.09	0.32
(2,1350)	1:35:A:LEU:HD13	1:36:A:GLU:H	13	0.3	0.09	0.32
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	13	0.3	0.1	0.29
(2,1282)	1:64:A:ILE:HG21	1:35:A:LEU:H	13	0.3	0.1	0.29
(2,1282)	1:64:A:ILE:HG23	1:35:A:LEU:H	13	0.3	0.1	0.29
(2,1264)	1:60:A:ILE:HG21	1:42:A:MET:HE3	13	0.3	0.06	0.29
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE3	13	0.3	0.06	0.29
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE1	13	0.3	0.06	0.29
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE1	13	0.3	0.06	0.29
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE2	13	0.3	0.06	0.29
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE3	13	0.3	0.06	0.29
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE2	13	0.3	0.06	0.29
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	13	0.3	0.07	0.31
(2,3969)	1:184:A:ALA:HB3	1:108:A:LYS:H	13	0.3	0.07	0.31
(2,3969)	1:184:A:ALA:HB1	1:108:A:LYS:H	13	0.3	0.07	0.31
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	13	0.28	0.1	0.26
(2,449)	1:53:A:ILE:HG22	1:125:A:PHE:HZ	13	0.27	0.07	0.29
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	13	0.27	0.07	0.29
(2,449)	1:53:A:ILE:HG23	1:125:A:PHE:HZ	13	0.27	0.07	0.29
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD12	13	0.27	0.1	0.23
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD11	13	0.27	0.1	0.23
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD13	13	0.27	0.1	0.23
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD12	13	0.27	0.11	0.25
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD13	13	0.27	0.11	0.25
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD11	13	0.27	0.11	0.25
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	13	0.26	0.08	0.3
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	13	0.26	0.08	0.23
(2,3979)	1:18:A:ALA:HB3	1:22:A:GLN:H	13	0.25	0.07	0.27
(2,3979)	1:18:A:ALA:HB1	1:22:A:GLN:H	13	0.25	0.07	0.27
(2,3979)	1:18:A:ALA:HB2	1:22:A:GLN:H	13	0.25	0.07	0.27
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	13	0.24	0.12	0.2
(2,61)	1:155:A:LEU:HD21	1:21:A:LEU:H	13	0.24	0.12	0.2
(2,61)	1:155:A:LEU:HD22	1:21:A:LEU:H	13	0.24	0.12	0.2
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	13	0.23	0.04	0.24
(2,1165)	1:161:A:THR:HG22	1:161:A:THR:HA	13	0.23	0.04	0.24
(2,1165)	1:161:A:THR:HG21	1:161:A:THR:HA	13	0.23	0.04	0.24
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG22	13	0.22	0.06	0.2
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	13	0.22	0.06	0.2
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG23	13	0.22	0.06	0.2
(2,3956)	1:74:A:ILE:HG21	1:78:A:GLU:H	13	0.2	0.08	0.15
(2,3956)	1:74:A:ILE:HG22	1:78:A:GLU:H	13	0.2	0.08	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3956)	1:74:A:ILE:HG23	1:78:A:GLU:H	13	0.2	0.08	0.15
(2,1444)	1:43:A:THR:HG23	1:39:A:LEU:HB2	13	0.19	0.05	0.19
(2,1444)	1:43:A:THR:HG22	1:39:A:LEU:HB2	13	0.19	0.05	0.19
(2,1444)	1:43:A:THR:HG21	1:39:A:LEU:HB2	13	0.19	0.05	0.19
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	13	0.18	0.04	0.18
(2,379)	1:142:A:LEU:HD21	1:138:A:ILE:HD13	13	0.18	0.06	0.16
(2,379)	1:142:A:LEU:HD22	1:138:A:ILE:HD11	13	0.18	0.06	0.16
(2,379)	1:142:A:LEU:HD22	1:138:A:ILE:HD13	13	0.18	0.06	0.16
(2,379)	1:142:A:LEU:HD21	1:138:A:ILE:HD12	13	0.18	0.06	0.16
(2,379)	1:142:A:LEU:HD22	1:138:A:ILE:HD12	13	0.18	0.06	0.16
(2,379)	1:142:A:LEU:HD23	1:138:A:ILE:HD11	13	0.18	0.06	0.16
(2,379)	1:142:A:LEU:HD21	1:138:A:ILE:HD11	13	0.18	0.06	0.16
(2,379)	1:142:A:LEU:HD23	1:138:A:ILE:HD12	13	0.18	0.06	0.16
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG22	13	0.16	0.04	0.15
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG23	13	0.16	0.04	0.15
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG21	13	0.16	0.04	0.15
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	13	0.16	0.03	0.14
(2,3981)	1:53:A:ILE:HG22	1:121:A:ALA:H	13	0.15	0.05	0.14
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	13	0.15	0.05	0.14
(2,3981)	1:53:A:ILE:HG23	1:121:A:ALA:H	13	0.15	0.05	0.14
(2,642)	1:150:A:THR:HG21	1:154:A:LEU:HG	13	0.14	0.03	0.14
(2,642)	1:150:A:THR:HG23	1:154:A:LEU:HG	13	0.14	0.03	0.14
(2,642)	1:150:A:THR:HG22	1:154:A:LEU:HG	13	0.14	0.03	0.14
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	13	0.13	0.02	0.13
(2,1331)	1:89:A:VAL:HG23	1:89:A:VAL:HA	13	0.13	0.02	0.12
(2,1331)	1:89:A:VAL:HG22	1:89:A:VAL:HA	13	0.13	0.02	0.12
(2,1331)	1:89:A:VAL:HG21	1:89:A:VAL:HA	13	0.13	0.02	0.12
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG11	12	1.38	1.19	0.94
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG13	12	1.38	1.19	0.94
(2,1397)	1:188:A:MET:HE3	1:190:A:VAL:HG13	12	1.38	1.19	0.94
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG12	12	1.38	1.19	0.94
(2,1397)	1:188:A:MET:HE1	1:190:A:VAL:HG12	12	1.38	1.19	0.94
(2,1397)	1:188:A:MET:HE3	1:190:A:VAL:HG12	12	1.38	1.19	0.94
(2,1397)	1:188:A:MET:HE1	1:190:A:VAL:HG13	12	1.38	1.19	0.94
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	12	1.02	0.06	1.03
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD11	12	0.72	0.05	0.73
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD12	12	0.72	0.05	0.73
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD13	12	0.72	0.05	0.73
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD13	12	0.62	0.47	0.38
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	12	0.62	0.47	0.38
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD12	12	0.62	0.47	0.38
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	12	0.62	0.3	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	12	0.55	0.35	0.48
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	12	0.54	0.2	0.55
(2,1592)	1:135:A:ALA:HB2	1:129:A:GLN:HE22	12	0.47	0.29	0.41
(2,1592)	1:135:A:ALA:HB3	1:129:A:GLN:HE22	12	0.47	0.29	0.41
(2,1592)	1:135:A:ALA:HB1	1:129:A:GLN:HE22	12	0.47	0.29	0.41
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD11	12	0.43	0.06	0.42
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD12	12	0.43	0.06	0.42
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD13	12	0.43	0.06	0.42
(2,4022)	1:143:A:ILE:HD13	1:147:A:GLN:HE22	12	0.43	0.29	0.4
(2,4022)	1:143:A:ILE:HD12	1:147:A:GLN:HE22	12	0.43	0.29	0.4
(2,4022)	1:143:A:ILE:HD11	1:147:A:GLN:HE22	12	0.43	0.29	0.4
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	12	0.41	0.02	0.42
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	12	0.39	0.11	0.41
(2,1547)	1:95:A:THR:HG21	1:78:A:GLU:HB2	12	0.36	0.12	0.34
(2,1547)	1:95:A:THR:HG22	1:78:A:GLU:HB2	12	0.36	0.12	0.34
(2,1547)	1:95:A:THR:HG23	1:78:A:GLU:HB2	12	0.36	0.12	0.34
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB2	12	0.34	0.11	0.34
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	12	0.34	0.11	0.34
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	12	0.34	0.13	0.42
(2,4785)	1:56:A:LYS:HE2	1:56:A:LYS:H	12	0.34	0.13	0.42
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	12	0.33	0.1	0.32
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	12	0.33	0.06	0.34
(2,19)	1:79:A:LEU:HD12	1:92:A:CYS:HG	12	0.31	0.11	0.32
(2,19)	1:79:A:LEU:HD13	1:92:A:CYS:HG	12	0.31	0.11	0.32
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	12	0.31	0.12	0.3
(2,4197)	1:16:A:ILE:HG23	1:158:A:GLU:H	12	0.31	0.12	0.3
(2,4197)	1:16:A:ILE:HG21	1:158:A:GLU:H	12	0.31	0.12	0.3
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD21	12	0.27	0.08	0.26
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD22	12	0.27	0.08	0.26
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD23	12	0.27	0.08	0.26
(2,473)	1:59:A:ILE:HG21	1:112:A:ASP:HB2	12	0.26	0.1	0.26
(2,473)	1:59:A:ILE:HG22	1:112:A:ASP:HB2	12	0.26	0.1	0.26
(2,473)	1:59:A:ILE:HG23	1:112:A:ASP:HB2	12	0.26	0.1	0.26
(2,1526)	1:178:A:LEU:HD21	1:176:A:VAL:H	12	0.26	0.04	0.27
(2,1526)	1:178:A:LEU:HD22	1:176:A:VAL:H	12	0.26	0.04	0.27
(2,1526)	1:178:A:LEU:HD23	1:176:A:VAL:H	12	0.26	0.04	0.27
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD11	12	0.25	0.08	0.23
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD13	12	0.25	0.08	0.23
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD12	12	0.25	0.08	0.23
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	12	0.23	0.07	0.21
(2,4750)	1:120:A:HIS:HD2	1:121:A:ALA:HA	12	0.23	0.07	0.21
(2,704)	1:18:A:ALA:HB3	1:21:A:LEU:HB3	12	0.22	0.1	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,704)	1:18:A:ALA:HB1	1:21:A:LEU:HB3	12	0.22	0.1	0.18
(2,704)	1:18:A:ALA:HB2	1:21:A:LEU:HB3	12	0.22	0.1	0.18
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD11	12	0.22	0.08	0.2
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD13	12	0.22	0.08	0.2
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD12	12	0.22	0.08	0.2
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD12	12	0.22	0.08	0.19
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD11	12	0.22	0.08	0.19
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD13	12	0.22	0.08	0.19
(2,3713)	1:76:A:LEU:HD13	1:77:A:LYS:H	12	0.22	0.05	0.22
(2,3713)	1:76:A:LEU:HD11	1:77:A:LYS:H	12	0.22	0.05	0.22
(2,3713)	1:76:A:LEU:HD12	1:77:A:LYS:H	12	0.22	0.05	0.22
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	12	0.22	0.04	0.22
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	12	0.21	0.08	0.22
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD11	12	0.21	0.08	0.22
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD13	12	0.21	0.08	0.22
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG23	12	0.2	0.08	0.22
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG22	12	0.2	0.08	0.22
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG21	12	0.2	0.08	0.22
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD21	12	0.2	0.06	0.18
(2,4586)	1:93:A:PHE:H	1:176:A:VAL:HG13	12	0.2	0.06	0.18
(2,4586)	1:93:A:PHE:H	1:176:A:VAL:HG12	12	0.2	0.06	0.18
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD23	12	0.2	0.06	0.18
(2,478)	1:59:A:ILE:HG23	1:60:A:ILE:HG22	12	0.2	0.05	0.22
(2,478)	1:59:A:ILE:HG23	1:60:A:ILE:HG23	12	0.2	0.05	0.22
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG23	12	0.2	0.05	0.22
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG21	12	0.2	0.05	0.22
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG22	12	0.2	0.05	0.22
(2,478)	1:59:A:ILE:HG22	1:60:A:ILE:HG23	12	0.2	0.05	0.22
(2,478)	1:59:A:ILE:HG23	1:60:A:ILE:HG21	12	0.2	0.05	0.22
(2,478)	1:59:A:ILE:HG22	1:60:A:ILE:HG21	12	0.2	0.05	0.22
(2,369)	1:138:A:ILE:HD13	1:60:A:ILE:HG23	12	0.2	0.06	0.19
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG21	12	0.2	0.06	0.19
(2,369)	1:138:A:ILE:HD12	1:60:A:ILE:HG21	12	0.2	0.06	0.19
(2,369)	1:138:A:ILE:HD13	1:60:A:ILE:HG22	12	0.2	0.06	0.19
(2,369)	1:138:A:ILE:HD12	1:60:A:ILE:HG22	12	0.2	0.06	0.19
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG23	12	0.2	0.06	0.19
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG22	12	0.2	0.06	0.19
(2,369)	1:138:A:ILE:HD12	1:60:A:ILE:HG23	12	0.2	0.06	0.19
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD13	12	0.19	0.04	0.19
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD11	12	0.19	0.04	0.19
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD12	12	0.19	0.04	0.19
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD11	12	0.19	0.04	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD12	12	0.19	0.04	0.2
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD13	12	0.19	0.04	0.2
(2,39)	1:31:A:LEU:HD13	1:34:A:CYS:H	12	0.19	0.05	0.19
(2,39)	1:31:A:LEU:HD11	1:34:A:CYS:H	12	0.19	0.05	0.19
(2,39)	1:31:A:LEU:HD12	1:34:A:CYS:H	12	0.19	0.05	0.19
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD21	12	0.18	0.07	0.18
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD23	12	0.18	0.07	0.18
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD22	12	0.18	0.07	0.18
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	12	0.17	0.04	0.17
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB2	12	0.17	0.04	0.17
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	12	0.16	0.03	0.16
(2,3691)	1:64:A:ILE:HG22	1:65:A:GLN:H	12	0.16	0.03	0.16
(2,3691)	1:64:A:ILE:HG21	1:65:A:GLN:H	12	0.16	0.03	0.16
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD13	12	0.16	0.04	0.15
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD11	12	0.16	0.04	0.15
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD12	12	0.16	0.04	0.15
(2,334)	1:42:A:MET:HE3	1:53:A:ILE:HD12	12	0.15	0.09	0.12
(2,334)	1:42:A:MET:HE3	1:53:A:ILE:HD13	12	0.15	0.09	0.12
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD13	12	0.15	0.09	0.12
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD11	12	0.15	0.09	0.12
(2,334)	1:42:A:MET:HE3	1:53:A:ILE:HD11	12	0.15	0.09	0.12
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD12	12	0.15	0.09	0.12
(2,334)	1:42:A:MET:HE2	1:53:A:ILE:HD12	12	0.15	0.09	0.12
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	12	0.14	0.03	0.14
(2,420)	1:53:A:ILE:HD12	1:60:A:ILE:HG13	12	0.12	0.01	0.12
(2,420)	1:53:A:ILE:HD13	1:60:A:ILE:HG13	12	0.12	0.01	0.12
(2,420)	1:53:A:ILE:HD11	1:60:A:ILE:HG13	12	0.12	0.01	0.12
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	12	0.12	0.01	0.12
(2,4749)	1:15:A:PHE:HD2	1:14:A:GLU:HG2	11	0.71	0.3	0.61
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG3	11	0.71	0.3	0.61
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG2	11	0.71	0.3	0.61
(2,4749)	1:15:A:PHE:HD2	1:14:A:GLU:HG3	11	0.71	0.3	0.61
(2,120)	1:161:A:THR:HG21	1:158:A:GLU:HG2	11	0.57	0.13	0.62
(2,120)	1:161:A:THR:HG22	1:158:A:GLU:HG2	11	0.57	0.13	0.62
(2,120)	1:161:A:THR:HG23	1:158:A:GLU:HG2	11	0.57	0.13	0.62
(2,4423)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	11	0.47	0.26	0.37
(2,4423)	1:116:A:LEU:HD23	1:56:A:LYS:HE2	11	0.47	0.26	0.37
(2,4423)	1:174:A:LEU:HD13	1:157:A:LYS:HE2	11	0.47	0.26	0.37
(2,4423)	1:174:A:LEU:HD12	1:157:A:LYS:HE2	11	0.47	0.26	0.37
(2,4423)	1:174:A:LEU:HD11	1:157:A:LYS:HE2	11	0.47	0.26	0.37
(2,4423)	1:54:A:LEU:HD13	1:56:A:LYS:HE3	11	0.47	0.26	0.37
(2,1439)	1:102:A:MET:HE3	1:106:A:TYR:HD2	11	0.46	0.33	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1439)	1:102:A:MET:HE1	1:106:A:TYR:HD2	11	0.46	0.33	0.39
(2,1439)	1:102:A:MET:HE2	1:106:A:TYR:HD2	11	0.46	0.33	0.39
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	11	0.43	0.35	0.18
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD3	11	0.41	0.18	0.34
(2,4486)	1:104:A:VAL:HG12	1:183:A:LYS:HD3	11	0.41	0.18	0.34
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD2	11	0.41	0.18	0.34
(2,4486)	1:104:A:VAL:HG11	1:183:A:LYS:HD3	11	0.41	0.18	0.34
(2,4486)	1:104:A:VAL:HG13	1:108:A:LYS:HD3	11	0.41	0.18	0.34
(2,4486)	1:104:A:VAL:HG13	1:183:A:LYS:HD3	11	0.41	0.18	0.34
(2,4486)	1:104:A:VAL:HG12	1:183:A:LYS:HG2	11	0.41	0.18	0.34
(2,1630)	1:178:A:LEU:HD21	1:153:A:GLN:H	11	0.36	0.12	0.37
(2,1630)	1:178:A:LEU:HD22	1:153:A:GLN:H	11	0.36	0.12	0.37
(2,1630)	1:178:A:LEU:HD23	1:153:A:GLN:H	11	0.36	0.12	0.37
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	11	0.36	0.18	0.33
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	11	0.35	0.13	0.32
(2,3652)	1:161:A:THR:HG21	1:162:A:CYS:H	11	0.34	0.1	0.37
(2,3652)	1:161:A:THR:HG23	1:162:A:CYS:H	11	0.34	0.1	0.37
(2,3652)	1:161:A:THR:HG22	1:162:A:CYS:H	11	0.34	0.1	0.37
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG23	11	0.32	0.19	0.29
(2,3477)	1:103:A:TYR:HE2	1:149:A:VAL:HG22	11	0.32	0.19	0.29
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG22	11	0.32	0.19	0.29
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG21	11	0.32	0.19	0.29
(2,4561)	1:23:A:THR:HG22	1:16:A:ILE:HA	11	0.29	0.16	0.22
(2,4561)	1:23:A:THR:HG21	1:16:A:ILE:HA	11	0.29	0.16	0.22
(2,4561)	1:23:A:THR:HG23	1:16:A:ILE:HA	11	0.29	0.16	0.22
(2,406)	1:156:A:LEU:HD13	1:93:A:PHE:HZ	11	0.29	0.11	0.26
(2,406)	1:156:A:LEU:HD11	1:93:A:PHE:HZ	11	0.29	0.11	0.26
(2,406)	1:156:A:LEU:HD12	1:93:A:PHE:HZ	11	0.29	0.11	0.26
(2,1321)	1:23:A:THR:HG21	1:22:A:GLN:HB3	11	0.27	0.07	0.29
(2,1321)	1:23:A:THR:HG22	1:22:A:GLN:HB3	11	0.27	0.07	0.29
(2,1321)	1:23:A:THR:HG23	1:22:A:GLN:HB3	11	0.27	0.07	0.29
(2,1520)	1:76:A:LEU:HD11	1:29:A:ARG:H	11	0.27	0.08	0.28
(2,1520)	1:76:A:LEU:HD13	1:29:A:ARG:H	11	0.27	0.08	0.28
(2,1520)	1:76:A:LEU:HD12	1:29:A:ARG:H	11	0.27	0.08	0.28
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD23	11	0.26	0.11	0.21
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD21	11	0.26	0.11	0.21
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD22	11	0.26	0.11	0.21
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	11	0.25	0.12	0.24
(2,1318)	1:177:A:MET:HE1	1:173:A:GLY:H	11	0.24	0.12	0.19
(2,1318)	1:177:A:MET:HE3	1:173:A:GLY:H	11	0.24	0.12	0.19
(2,1318)	1:177:A:MET:HE2	1:173:A:GLY:H	11	0.24	0.12	0.19
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG21	11	0.24	0.09	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG23	11	0.24	0.09	0.23
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG22	11	0.24	0.09	0.23
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG13	11	0.23	0.08	0.22
(2,4356)	1:180:A:VAL:HG12	1:180:A:VAL:H	11	0.23	0.08	0.22
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG11	11	0.23	0.08	0.22
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG12	11	0.23	0.08	0.22
(2,2927)	1:156:A:LEU:HD22	1:173:A:GLY:H	11	0.21	0.08	0.21
(2,2927)	1:156:A:LEU:HD21	1:173:A:GLY:H	11	0.21	0.08	0.21
(2,2927)	1:156:A:LEU:HD23	1:173:A:GLY:H	11	0.21	0.08	0.21
(2,1279)	1:59:A:ILE:HG22	1:112:A:ASP:HB3	11	0.2	0.08	0.21
(2,1279)	1:59:A:ILE:HG23	1:112:A:ASP:HB3	11	0.2	0.08	0.21
(2,1279)	1:59:A:ILE:HG21	1:112:A:ASP:HB3	11	0.2	0.08	0.21
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	11	0.19	0.06	0.17
(2,3743)	1:97:A:ALA:HB1	1:97:A:ALA:H	11	0.19	0.06	0.17
(2,3743)	1:97:A:ALA:HB3	1:97:A:ALA:H	11	0.19	0.06	0.17
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG21	11	0.18	0.06	0.18
(2,4428)	1:42:A:MET:HG2	1:128:A:ILE:HD11	11	0.18	0.06	0.18
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG23	11	0.18	0.06	0.18
(2,4428)	1:42:A:MET:HG2	1:128:A:ILE:HD12	11	0.18	0.06	0.18
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG22	11	0.18	0.06	0.18
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG23	11	0.18	0.05	0.19
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG22	11	0.18	0.05	0.19
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG21	11	0.18	0.05	0.19
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	11	0.18	0.01	0.18
(2,3998)	1:49:A:ILE:HD11	1:54:A:LEU:H	11	0.17	0.03	0.17
(2,3998)	1:49:A:ILE:HD12	1:54:A:LEU:H	11	0.17	0.03	0.17
(2,3998)	1:49:A:ILE:HD13	1:54:A:LEU:H	11	0.17	0.03	0.17
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	11	0.17	0.05	0.17
(2,1510)	1:116:A:LEU:HD22	1:54:A:LEU:H	11	0.17	0.05	0.17
(2,1510)	1:116:A:LEU:HD23	1:54:A:LEU:H	11	0.17	0.05	0.17
(2,1510)	1:116:A:LEU:HD21	1:54:A:LEU:H	11	0.17	0.05	0.17
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	11	0.16	0.04	0.15
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	11	0.16	0.08	0.12
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	11	0.16	0.02	0.16
(2,2313)	1:54:A:LEU:HD23	1:55:A:ASN:HD22	11	0.14	0.03	0.14
(2,2313)	1:54:A:LEU:HD21	1:55:A:ASN:HD22	11	0.14	0.03	0.14
(2,2313)	1:54:A:LEU:HD22	1:55:A:ASN:HD22	11	0.14	0.03	0.14
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG22	11	0.13	0.02	0.13
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG21	11	0.13	0.02	0.13
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG23	11	0.13	0.02	0.13
(2,3671)	1:43:A:THR:HG23	1:43:A:THR:H	11	0.12	0.01	0.12
(2,3671)	1:43:A:THR:HG22	1:43:A:THR:H	11	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3671)	1:43:A:THR:HG21	1:43:A:THR:H	11	0.12	0.01	0.12
(2,1593)	1:135:A:ALA:HB3	1:129:A:GLN:HE21	10	0.74	0.3	0.76
(2,1593)	1:135:A:ALA:HB1	1:129:A:GLN:HE21	10	0.74	0.3	0.76
(2,1593)	1:135:A:ALA:HB2	1:129:A:GLN:HE21	10	0.74	0.3	0.76
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	10	0.72	0.36	0.64
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	10	0.52	0.51	0.26
(2,4594)	1:148:A:ARG:H	1:144:A:LYS:HD2	10	0.52	0.51	0.26
(2,4489)	1:184:A:ALA:HB2	1:108:A:LYS:HE3	10	0.48	0.3	0.34
(2,4489)	1:184:A:ALA:HB3	1:108:A:LYS:HE2	10	0.48	0.3	0.34
(2,4489)	1:184:A:ALA:HB2	1:108:A:LYS:HE2	10	0.48	0.3	0.34
(2,4489)	1:184:A:ALA:HB3	1:108:A:LYS:HE3	10	0.48	0.3	0.34
(2,4489)	1:184:A:ALA:HB1	1:108:A:LYS:HE3	10	0.48	0.3	0.34
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	10	0.47	0.17	0.45
(2,4587)	1:94:A:VAL:H	1:176:A:VAL:HB	10	0.47	0.17	0.45
(2,351)	1:188:A:MET:HE3	1:108:A:LYS:HA	10	0.46	0.17	0.54
(2,351)	1:188:A:MET:HE1	1:108:A:LYS:HA	10	0.46	0.17	0.54
(2,351)	1:188:A:MET:HE2	1:108:A:LYS:HA	10	0.46	0.17	0.54
(2,638)	1:150:A:THR:HG23	1:153:A:GLN:HE21	10	0.43	0.22	0.43
(2,638)	1:150:A:THR:HG22	1:153:A:GLN:HE21	10	0.43	0.22	0.43
(2,638)	1:150:A:THR:HG21	1:153:A:GLN:HE21	10	0.43	0.22	0.43
(2,601)	1:28:A:VAL:HG23	1:71:A:HIS:HB2	10	0.43	0.39	0.21
(2,601)	1:28:A:VAL:HG22	1:71:A:HIS:HB2	10	0.43	0.39	0.21
(2,601)	1:28:A:VAL:HG21	1:71:A:HIS:HB2	10	0.43	0.39	0.21
(2,4778)	1:11:A:ARG:HD3	1:12:A:LYS:H	10	0.4	0.13	0.4
(2,4778)	1:11:A:ARG:HD2	1:12:A:LYS:H	10	0.4	0.13	0.4
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	10	0.4	0.17	0.42
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG2	10	0.4	0.17	0.42
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	10	0.32	0.04	0.32
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD12	10	0.32	0.21	0.31
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD13	10	0.32	0.21	0.31
(2,3554)	1:152:A:TYR:HD2	1:155:A:LEU:HD11	10	0.32	0.21	0.31
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD11	10	0.32	0.21	0.31
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD1	10	0.32	0.2	0.26
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD2	10	0.32	0.2	0.26
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD2	10	0.26	0.09	0.27
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD3	10	0.26	0.09	0.27
(2,3481)	1:100:A:PHE:HD2	1:176:A:VAL:HG23	10	0.26	0.08	0.26
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG21	10	0.26	0.08	0.26
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG22	10	0.26	0.08	0.26
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG23	10	0.26	0.08	0.26
(2,3481)	1:100:A:PHE:HD2	1:176:A:VAL:HG22	10	0.26	0.08	0.26
(2,4329)	1:156:A:LEU:HD22	1:175:A:GLU:HG2	10	0.24	0.09	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4329)	1:156:A:LEU:HD21	1:175:A:GLU:HG3	10	0.24	0.09	0.23
(2,4329)	1:156:A:LEU:HD23	1:175:A:GLU:HG3	10	0.24	0.09	0.23
(2,4329)	1:156:A:LEU:HD22	1:175:A:GLU:HG3	10	0.24	0.09	0.23
(2,1343)	1:17:A:MET:HE3	1:86:A:PRO:HA	10	0.23	0.06	0.22
(2,1343)	1:17:A:MET:HE2	1:86:A:PRO:HA	10	0.23	0.06	0.22
(2,1343)	1:17:A:MET:HE1	1:86:A:PRO:HA	10	0.23	0.06	0.22
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG12	10	0.22	0.1	0.2
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG11	10	0.22	0.1	0.2
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG13	10	0.22	0.1	0.2
(2,134)	1:18:A:ALA:HB3	1:22:A:GLN:HB2	10	0.21	0.12	0.18
(2,134)	1:18:A:ALA:HB1	1:22:A:GLN:HB2	10	0.21	0.12	0.18
(2,134)	1:18:A:ALA:HB2	1:22:A:GLN:HB2	10	0.21	0.12	0.18
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	10	0.21	0.08	0.22
(2,632)	1:64:A:ILE:HG23	1:39:A:LEU:HB2	10	0.21	0.08	0.22
(2,632)	1:64:A:ILE:HG22	1:39:A:LEU:HB2	10	0.21	0.08	0.22
(2,3974)	1:161:A:THR:HG21	1:160:A:LEU:H	10	0.2	0.04	0.2
(2,3974)	1:161:A:THR:HG22	1:160:A:LEU:H	10	0.2	0.04	0.2
(2,3974)	1:161:A:THR:HG23	1:160:A:LEU:H	10	0.2	0.04	0.2
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG12	10	0.19	0.06	0.18
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG11	10	0.19	0.06	0.18
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG13	10	0.19	0.06	0.18
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	10	0.19	0.08	0.16
(2,4015)	1:39:A:LEU:HD21	1:61:A:PHE:H	10	0.18	0.04	0.18
(2,4015)	1:39:A:LEU:HD23	1:61:A:PHE:H	10	0.18	0.04	0.18
(2,4015)	1:39:A:LEU:HD22	1:61:A:PHE:H	10	0.18	0.04	0.18
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	10	0.18	0.02	0.18
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD23	10	0.16	0.04	0.15
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD21	10	0.16	0.04	0.15
(2,631)	1:64:A:ILE:HG21	1:35:A:LEU:HD23	10	0.16	0.04	0.15
(2,631)	1:64:A:ILE:HG21	1:35:A:LEU:HD21	10	0.16	0.04	0.15
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD22	10	0.16	0.04	0.15
(2,631)	1:64:A:ILE:HG23	1:35:A:LEU:HD23	10	0.16	0.04	0.15
(2,133)	1:23:A:THR:HG21	1:22:A:GLN:HB2	10	0.16	0.03	0.15
(2,133)	1:23:A:THR:HG22	1:22:A:GLN:HB2	10	0.16	0.03	0.15
(2,133)	1:23:A:THR:HG23	1:22:A:GLN:HB2	10	0.16	0.03	0.15
(2,1991)	1:35:A:LEU:HD22	1:68:A:TYR:H	10	0.15	0.04	0.15
(2,1991)	1:35:A:LEU:HD23	1:68:A:TYR:H	10	0.15	0.04	0.15
(2,1991)	1:35:A:LEU:HD21	1:68:A:TYR:H	10	0.15	0.04	0.15
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG22	10	0.15	0.03	0.15
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG21	10	0.15	0.03	0.15
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG23	10	0.15	0.03	0.15
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	10	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,401)	1:35:A:LEU:HD22	1:31:A:LEU:HB3	10	0.14	0.02	0.14
(2,401)	1:35:A:LEU:HD23	1:31:A:LEU:HB3	10	0.14	0.02	0.14
(2,401)	1:35:A:LEU:HD21	1:31:A:LEU:HB3	10	0.14	0.02	0.14
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	10	0.14	0.04	0.12
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD12	10	0.13	0.02	0.13
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD11	10	0.13	0.02	0.13
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD13	10	0.13	0.02	0.13
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	10	0.13	0.03	0.12
(2,3920)	1:42:A:MET:HE3	1:42:A:MET:H	10	0.12	0.02	0.12
(2,3920)	1:42:A:MET:HE2	1:42:A:MET:H	10	0.12	0.02	0.12
(2,3920)	1:42:A:MET:HE1	1:42:A:MET:H	10	0.12	0.02	0.12
(2,82)	1:76:A:LEU:HD13	1:77:A:LYS:HE2	9	0.78	0.57	0.61
(2,82)	1:76:A:LEU:HD12	1:77:A:LYS:HE2	9	0.78	0.57	0.61
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	9	0.65	0.36	0.62
(2,1442)	1:74:A:ILE:HD11	1:99:A:LYS:HE2	9	0.62	0.18	0.67
(2,1442)	1:74:A:ILE:HD13	1:99:A:LYS:HE2	9	0.62	0.18	0.67
(2,1442)	1:74:A:ILE:HD12	1:99:A:LYS:HE2	9	0.62	0.18	0.67
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	9	0.59	0.06	0.59
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	9	0.58	0.14	0.64
(2,4305)	1:56:A:LYS:HE2	1:55:A:ASN:HD21	9	0.58	0.14	0.64
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	9	0.57	0.26	0.75
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB2	9	0.54	0.21	0.52
(2,4755)	1:124:A:PHE:HE2	1:50:A:PRO:HG2	9	0.54	0.21	0.52
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB3	9	0.54	0.21	0.52
(2,444)	1:31:A:LEU:HD12	1:30:A:ASP:HB2	9	0.53	0.21	0.63
(2,444)	1:31:A:LEU:HD11	1:30:A:ASP:HB2	9	0.53	0.21	0.63
(2,444)	1:31:A:LEU:HD13	1:30:A:ASP:HB2	9	0.53	0.21	0.63
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD2	9	0.47	0.22	0.48
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD3	9	0.47	0.22	0.48
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	9	0.47	0.14	0.45
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	9	0.44	0.13	0.42
(2,1476)	1:134:A:LEU:HD22	1:34:A:CYS:HA	9	0.36	0.1	0.33
(2,1476)	1:134:A:LEU:HD23	1:34:A:CYS:HA	9	0.36	0.1	0.33
(2,1476)	1:134:A:LEU:HD21	1:34:A:CYS:HA	9	0.36	0.1	0.33
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD11	9	0.29	0.08	0.27
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD13	9	0.29	0.08	0.27
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD12	9	0.29	0.08	0.27
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	9	0.29	0.12	0.3
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	9	0.27	0.08	0.29
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG23	9	0.26	0.11	0.24
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG21	9	0.26	0.11	0.24
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG22	9	0.26	0.11	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD13	9	0.22	0.08	0.23
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD12	9	0.22	0.08	0.23
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD11	9	0.22	0.08	0.23
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	9	0.18	0.03	0.18
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	9	0.18	0.04	0.16
(2,4829)	1:77:A:LYS:HE3	1:78:A:GLU:H	9	0.18	0.04	0.16
(2,57)	1:142:A:LEU:HD12	1:61:A:PHE:HE1	9	0.18	0.05	0.15
(2,57)	1:142:A:LEU:HD11	1:61:A:PHE:HE1	9	0.18	0.05	0.15
(2,57)	1:142:A:LEU:HD13	1:61:A:PHE:HE1	9	0.18	0.05	0.15
(2,1994)	1:67:A:ILE:HG22	1:71:A:HIS:H	9	0.16	0.06	0.15
(2,1994)	1:67:A:ILE:HG21	1:71:A:HIS:H	9	0.16	0.06	0.15
(2,1994)	1:67:A:ILE:HG23	1:71:A:HIS:H	9	0.16	0.06	0.15
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	9	0.15	0.04	0.16
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	9	0.14	0.03	0.13
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	9	0.13	0.03	0.12
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	9	0.12	0.01	0.12
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	9	0.12	0.01	0.11
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	9	0.11	0.01	0.11
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	8	1.01	0.03	1.02
(2,876)	1:97:A:ALA:HB1	1:98:A:ASP:HB2	8	1.01	0.24	1.03
(2,876)	1:97:A:ALA:HB2	1:98:A:ASP:HB2	8	1.01	0.24	1.03
(2,876)	1:97:A:ALA:HB3	1:98:A:ASP:HB2	8	1.01	0.24	1.03
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	8	0.62	0.59	0.42
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	8	0.6	0.55	0.24
(2,4287)	1:13:A:LYS:HD3	1:15:A:PHE:HD1	8	0.53	0.16	0.47
(2,4287)	1:13:A:LYS:HD2	1:15:A:PHE:HD2	8	0.53	0.16	0.47
(2,4287)	1:13:A:LYS:HD2	1:15:A:PHE:HD1	8	0.53	0.16	0.47
(2,4457)	1:164:A:GLU:HG3	1:164:A:GLU:HA	8	0.43	0.26	0.43
(2,4457)	1:164:A:GLU:HG2	1:164:A:GLU:HA	8	0.43	0.26	0.43
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	8	0.39	0.18	0.42
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	8	0.37	0.22	0.36
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	8	0.37	0.22	0.36
(2,4299)	1:101:A:GLN:HG2	1:104:A:VAL:HG13	8	0.37	0.22	0.36
(2,4299)	1:101:A:GLN:HG2	1:104:A:VAL:HG11	8	0.37	0.22	0.36
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	8	0.37	0.1	0.37
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	8	0.36	0.27	0.25
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	8	0.33	0.1	0.34
(2,170)	1:37:A:THR:HG23	1:33:A:GLU:HG3	8	0.33	0.13	0.36
(2,170)	1:37:A:THR:HG22	1:33:A:GLU:HG3	8	0.33	0.13	0.36
(2,170)	1:37:A:THR:HG21	1:33:A:GLU:HG3	8	0.33	0.13	0.36
(2,4466)	1:98:A:ASP:HA	1:176:A:VAL:HB	8	0.31	0.33	0.2
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	8	0.31	0.33	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG21	8	0.29	0.12	0.24
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG23	8	0.29	0.12	0.24
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG22	8	0.29	0.12	0.24
(2,4687)	1:11:A:ARG:HG2	1:12:A:LYS:H	8	0.28	0.1	0.3
(2,4687)	1:11:A:ARG:HG3	1:12:A:LYS:H	8	0.28	0.1	0.3
(2,1037)	1:143:A:ILE:HG23	1:140:A:SER:HB2	8	0.28	0.13	0.32
(2,1037)	1:143:A:ILE:HG21	1:140:A:SER:HB2	8	0.28	0.13	0.32
(2,1037)	1:143:A:ILE:HG22	1:140:A:SER:HB2	8	0.28	0.13	0.32
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	8	0.27	0.09	0.26
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE3	8	0.27	0.09	0.26
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	8	0.27	0.08	0.27
(2,3557)	1:141:A:TYR:HD1	1:136:A:ASN:HB2	8	0.27	0.08	0.27
(2,18)	1:79:A:LEU:HD12	1:92:A:CYS:HB2	8	0.26	0.08	0.29
(2,18)	1:79:A:LEU:HD13	1:92:A:CYS:HB2	8	0.26	0.08	0.29
(2,18)	1:79:A:LEU:HD11	1:92:A:CYS:HB2	8	0.26	0.08	0.29
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD22	8	0.25	0.08	0.22
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD23	8	0.25	0.08	0.22
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD21	8	0.25	0.08	0.22
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	8	0.24	0.08	0.26
(2,4788)	1:99:A:LYS:H	1:98:A:ASP:HB3	8	0.23	0.08	0.24
(2,4788)	1:98:A:ASP:HB2	1:99:A:LYS:H	8	0.23	0.08	0.24
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	8	0.22	0.09	0.2
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	8	0.22	0.09	0.19
(2,643)	1:105:A:THR:HG23	1:106:A:TYR:HD2	8	0.21	0.07	0.22
(2,643)	1:105:A:THR:HG22	1:106:A:TYR:HD2	8	0.21	0.07	0.22
(2,643)	1:105:A:THR:HG21	1:106:A:TYR:HD2	8	0.21	0.07	0.22
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	8	0.21	0.08	0.18
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG23	8	0.21	0.04	0.2
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG22	8	0.21	0.04	0.2
(2,1300)	1:117:A:ILE:HG22	1:60:A:ILE:HG21	8	0.21	0.04	0.2
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG21	8	0.21	0.04	0.2
(2,1300)	1:117:A:ILE:HG21	1:60:A:ILE:HG21	8	0.21	0.04	0.2
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG11	8	0.2	0.03	0.2
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG12	8	0.2	0.03	0.2
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG13	8	0.2	0.03	0.2
(2,312)	1:3:A:LEU:HD22	1:3:A:LEU:HA	8	0.2	0.04	0.21
(2,312)	1:3:A:LEU:HD21	1:3:A:LEU:HA	8	0.2	0.04	0.21
(2,312)	1:3:A:LEU:HD23	1:3:A:LEU:HA	8	0.2	0.04	0.21
(2,3910)	1:156:A:LEU:HD23	1:153:A:GLN:H	8	0.2	0.07	0.2
(2,3910)	1:156:A:LEU:HD22	1:153:A:GLN:H	8	0.2	0.07	0.2
(2,3910)	1:156:A:LEU:HD21	1:153:A:GLN:H	8	0.2	0.07	0.2
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	8	0.19	0.04	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD13	8	0.19	0.04	0.18
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD11	8	0.19	0.04	0.18
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD12	8	0.19	0.04	0.18
(2,4267)	1:134:A:LEU:HD11	1:132:A:HIS:H	8	0.18	0.05	0.16
(2,4267)	1:134:A:LEU:HD13	1:132:A:HIS:H	8	0.18	0.05	0.16
(2,4267)	1:134:A:LEU:HD12	1:130:A:GLN:H	8	0.18	0.05	0.16
(2,4267)	1:134:A:LEU:HD11	1:130:A:GLN:H	8	0.18	0.05	0.16
(2,4267)	1:134:A:LEU:HD12	1:132:A:HIS:H	8	0.18	0.05	0.16
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	8	0.17	0.06	0.16
(2,92)	1:116:A:LEU:HD13	1:115:A:GLN:HB2	8	0.17	0.06	0.15
(2,92)	1:116:A:LEU:HD11	1:115:A:GLN:HB2	8	0.17	0.06	0.15
(2,92)	1:116:A:LEU:HD12	1:115:A:GLN:HB2	8	0.17	0.06	0.15
(2,1349)	1:20:A:LEU:HD11	1:23:A:THR:H	8	0.17	0.04	0.16
(2,1349)	1:20:A:LEU:HD12	1:23:A:THR:H	8	0.17	0.04	0.16
(2,1349)	1:20:A:LEU:HD13	1:23:A:THR:H	8	0.17	0.04	0.16
(2,1255)	1:17:A:MET:HE2	1:82:A:TYR:HE2	8	0.16	0.05	0.16
(2,1255)	1:17:A:MET:HE3	1:82:A:TYR:HE2	8	0.16	0.05	0.16
(2,1255)	1:17:A:MET:HE1	1:82:A:TYR:HE2	8	0.16	0.05	0.16
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	8	0.16	0.03	0.16
(2,4629)	1:126:A:ASP:H	1:129:A:GLN:HB3	8	0.16	0.03	0.16
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD11	8	0.16	0.02	0.16
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD12	8	0.16	0.02	0.16
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD13	8	0.16	0.02	0.16
(2,4599)	1:173:A:GLY:H	1:94:A:VAL:HB	8	0.14	0.02	0.14
(2,4599)	1:173:A:GLY:H	1:169:A:GLU:HB2	8	0.14	0.02	0.14
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	8	0.14	0.03	0.14
(2,1038)	1:49:A:ILE:HD11	1:54:A:LEU:HA	8	0.13	0.02	0.13
(2,1038)	1:49:A:ILE:HD12	1:54:A:LEU:HA	8	0.13	0.02	0.13
(2,1038)	1:49:A:ILE:HD13	1:54:A:LEU:HA	8	0.13	0.02	0.13
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	8	0.12	0.01	0.12
(2,4339)	1:134:A:LEU:HD22	1:129:A:GLN:HG3	7	0.97	0.72	0.69
(2,4339)	1:134:A:LEU:HD23	1:129:A:GLN:HG3	7	0.97	0.72	0.69
(2,4339)	1:134:A:LEU:HD21	1:129:A:GLN:HG3	7	0.97	0.72	0.69
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	7	0.87	0.34	0.74
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD3	7	0.54	0.13	0.5
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD2	7	0.54	0.13	0.5
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD13	7	0.53	0.14	0.5
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD11	7	0.53	0.14	0.5
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD12	7	0.53	0.14	0.5
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	7	0.52	0.3	0.73
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG23	7	0.49	0.21	0.52
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG22	7	0.49	0.21	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG21	7	0.49	0.21	0.52
(2,4325)	1:188:A:MET:HE1	1:108:A:LYS:HE3	7	0.43	0.27	0.35
(2,4325)	1:188:A:MET:HE2	1:108:A:LYS:HE3	7	0.43	0.27	0.35
(2,4325)	1:188:A:MET:HE3	1:108:A:LYS:HE3	7	0.43	0.27	0.35
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	7	0.4	0.09	0.38
(2,4271)	1:116:A:LEU:HD22	1:56:A:LYS:HE2	7	0.34	0.13	0.3
(2,4271)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	7	0.34	0.13	0.3
(2,4271)	1:116:A:LEU:HD23	1:56:A:LYS:HE2	7	0.34	0.13	0.3
(2,4304)	1:186:A:ASP:HB3	1:183:A:LYS:HG3	7	0.33	0.11	0.32
(2,4304)	1:186:A:ASP:HB2	1:183:A:LYS:HG3	7	0.33	0.11	0.32
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	7	0.31	0.11	0.29
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD22	7	0.3	0.12	0.26
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD21	7	0.3	0.12	0.26
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD23	7	0.3	0.12	0.26
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	7	0.28	0.16	0.23
(2,4715)	1:7:A:GLU:H	1:6:A:PRO:HD2	7	0.28	0.14	0.21
(2,4715)	1:7:A:GLU:H	1:9:A:PRO:HD3	7	0.28	0.14	0.21
(2,112)	1:177:A:MET:HE1	1:100:A:PHE:HE1	7	0.28	0.16	0.23
(2,112)	1:177:A:MET:HE2	1:100:A:PHE:HE2	7	0.28	0.16	0.23
(2,112)	1:177:A:MET:HE3	1:100:A:PHE:HE2	7	0.28	0.16	0.23
(2,112)	1:177:A:MET:HE3	1:100:A:PHE:HE1	7	0.28	0.16	0.23
(2,4841)	1:171:A:LYS:HG2	1:170:A:LEU:H	7	0.27	0.08	0.3
(2,4841)	1:171:A:LYS:HG3	1:170:A:LEU:H	7	0.27	0.08	0.3
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE2	7	0.25	0.14	0.23
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE1	7	0.25	0.14	0.23
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE3	7	0.25	0.14	0.23
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG21	7	0.24	0.1	0.24
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG22	7	0.24	0.1	0.24
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG23	7	0.24	0.1	0.24
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG21	7	0.24	0.05	0.24
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG23	7	0.24	0.05	0.24
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG22	7	0.24	0.05	0.24
(2,1245)	1:20:A:LEU:HD11	1:24:A:GLU:H	7	0.23	0.08	0.18
(2,1245)	1:20:A:LEU:HD12	1:24:A:GLU:H	7	0.23	0.08	0.18
(2,1245)	1:20:A:LEU:HD13	1:24:A:GLU:H	7	0.23	0.08	0.18
(2,4529)	1:60:A:ILE:HG23	1:113:A:SER:HB2	7	0.21	0.08	0.2
(2,4529)	1:60:A:ILE:HG21	1:113:A:SER:HB2	7	0.21	0.08	0.2
(2,4529)	1:60:A:ILE:HG22	1:113:A:SER:HB2	7	0.21	0.08	0.2
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	7	0.19	0.04	0.19
(2,4112)	1:76:A:LEU:HD23	1:25:A:LYS:H	7	0.18	0.05	0.18
(2,4112)	1:76:A:LEU:HD21	1:25:A:LYS:H	7	0.18	0.05	0.18
(2,4112)	1:76:A:LEU:HD22	1:25:A:LYS:H	7	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	7	0.18	0.08	0.16
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD13	7	0.17	0.05	0.17
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD11	7	0.17	0.05	0.17
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD12	7	0.17	0.05	0.17
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	7	0.17	0.04	0.17
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD23	7	0.17	0.06	0.13
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD21	7	0.17	0.06	0.13
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	7	0.17	0.05	0.19
(2,73)	1:76:A:LEU:HD21	1:80:A:GLU:H	7	0.16	0.08	0.13
(2,73)	1:76:A:LEU:HD22	1:80:A:GLU:H	7	0.16	0.08	0.13
(2,73)	1:76:A:LEU:HD23	1:80:A:GLU:H	7	0.16	0.08	0.13
(2,1534)	1:53:A:ILE:HG21	1:60:A:ILE:HA	7	0.16	0.05	0.17
(2,1534)	1:53:A:ILE:HG23	1:60:A:ILE:HA	7	0.16	0.05	0.17
(2,1534)	1:53:A:ILE:HG22	1:60:A:ILE:HA	7	0.16	0.05	0.17
(2,3992)	1:35:A:LEU:HD21	1:65:A:GLN:H	7	0.16	0.04	0.16
(2,3992)	1:35:A:LEU:HD23	1:65:A:GLN:H	7	0.16	0.04	0.16
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	7	0.16	0.03	0.16
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG22	7	0.16	0.05	0.15
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG21	7	0.16	0.05	0.15
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG23	7	0.16	0.05	0.15
(2,325)	1:17:A:MET:HE3	1:83:A:GLU:HA	7	0.15	0.03	0.16
(2,325)	1:17:A:MET:HE1	1:83:A:GLU:HA	7	0.15	0.03	0.16
(2,325)	1:17:A:MET:HE2	1:83:A:GLU:HA	7	0.15	0.03	0.16
(2,106)	1:43:A:THR:HG23	1:42:A:MET:HG2	7	0.15	0.03	0.14
(2,106)	1:43:A:THR:HG22	1:42:A:MET:HG2	7	0.15	0.03	0.14
(2,106)	1:43:A:THR:HG21	1:42:A:MET:HG2	7	0.15	0.03	0.14
(2,2577)	1:89:A:VAL:HG12	1:92:A:CYS:H	7	0.15	0.02	0.14
(2,2577)	1:89:A:VAL:HG11	1:92:A:CYS:H	7	0.15	0.02	0.14
(2,2577)	1:89:A:VAL:HG13	1:92:A:CYS:H	7	0.15	0.02	0.14
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	7	0.14	0.03	0.13
(2,3320)	1:143:A:ILE:HG23	1:142:A:LEU:H	7	0.14	0.03	0.12
(2,3320)	1:143:A:ILE:HG22	1:142:A:LEU:H	7	0.14	0.03	0.12
(2,3320)	1:143:A:ILE:HG21	1:142:A:LEU:H	7	0.14	0.03	0.12
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD23	7	0.14	0.01	0.13
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD21	7	0.14	0.01	0.13
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD22	7	0.14	0.01	0.13
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	7	0.13	0.02	0.13
(2,389)	1:39:A:LEU:HD22	1:41:A:GLU:H	7	0.13	0.02	0.13
(2,389)	1:39:A:LEU:HD21	1:41:A:GLU:H	7	0.13	0.02	0.13
(2,389)	1:39:A:LEU:HD23	1:41:A:GLU:H	7	0.13	0.02	0.13
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	7	0.13	0.01	0.14
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	7	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3745)	1:97:A:ALA:HB1	1:98:A:ASP:H	7	0.13	0.02	0.14
(2,3745)	1:97:A:ALA:HB3	1:98:A:ASP:H	7	0.13	0.02	0.14
(2,3745)	1:97:A:ALA:HB2	1:98:A:ASP:H	7	0.13	0.02	0.14
(2,4421)	1:56:A:LYS:HE3	1:56:A:LYS:HD2	7	0.11	0.01	0.11
(2,4421)	1:56:A:LYS:HE2	1:56:A:LYS:HD3	7	0.11	0.01	0.11
(2,1261)	1:17:A:MET:HE1	1:21:A:LEU:HD21	7	0.11	0.01	0.11
(2,1261)	1:17:A:MET:HE2	1:21:A:LEU:HD21	7	0.11	0.01	0.11
(2,1261)	1:17:A:MET:HE3	1:21:A:LEU:HD23	7	0.11	0.01	0.11
(2,1261)	1:17:A:MET:HE2	1:21:A:LEU:HD22	7	0.11	0.01	0.11
(2,1261)	1:17:A:MET:HE2	1:21:A:LEU:HD23	7	0.11	0.01	0.11
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	7	0.11	0.01	0.11
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	7	0.11	0.01	0.11
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG21	6	0.94	0.56	0.6
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG22	6	0.94	0.56	0.6
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG23	6	0.94	0.56	0.6
(2,703)	1:18:A:ALA:HB1	1:15:A:PHE:HD1	6	0.82	0.23	0.82
(2,703)	1:18:A:ALA:HB3	1:15:A:PHE:HD1	6	0.82	0.23	0.82
(2,703)	1:18:A:ALA:HB2	1:15:A:PHE:HD2	6	0.82	0.23	0.82
(2,703)	1:18:A:ALA:HB3	1:15:A:PHE:HD2	6	0.82	0.23	0.82
(2,703)	1:18:A:ALA:HB2	1:15:A:PHE:HD1	6	0.82	0.23	0.82
(2,712)	1:157:A:LYS:HG2	1:157:A:LYS:HE2	6	0.61	0.13	0.55
(2,4058)	1:16:A:ILE:HD12	1:15:A:PHE:H	6	0.6	0.27	0.76
(2,4058)	1:16:A:ILE:HD13	1:15:A:PHE:H	6	0.6	0.27	0.76
(2,4058)	1:16:A:ILE:HD11	1:15:A:PHE:H	6	0.6	0.27	0.76
(2,168)	1:33:A:GLU:HG3	1:37:A:THR:H	6	0.56	0.2	0.66
(2,1562)	1:13:A:LYS:HB3	1:13:A:LYS:H	6	0.55	0.23	0.42
(2,1833)	1:13:A:LYS:H	1:13:A:LYS:HB2	6	0.52	0.36	0.42
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG3	6	0.5	0.12	0.52
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG2	6	0.5	0.12	0.52
(2,4654)	1:83:A:GLU:HG2	1:84:A:GLN:HE21	6	0.45	0.14	0.52
(2,4654)	1:83:A:GLU:HG3	1:84:A:GLN:HE21	6	0.45	0.14	0.52
(2,2904)	1:166:A:GLY:H	1:167:A:LYS:H	6	0.41	0.29	0.3
(2,2643)	1:108:A:LYS:H	1:107:A:CYS:HB2	6	0.39	0.05	0.39
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD11	6	0.35	0.19	0.37
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD12	6	0.35	0.19	0.37
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD13	6	0.35	0.19	0.37
(2,4119)	1:7:A:GLU:HG2	1:7:A:GLU:H	6	0.3	0.13	0.31
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG23	6	0.29	0.09	0.31
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG21	6	0.29	0.09	0.31
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG22	6	0.29	0.09	0.31
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG12	6	0.27	0.07	0.25
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG13	6	0.27	0.07	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG11	6	0.27	0.07	0.25
(2,4812)	1:162:A:CYS:H	1:160:A:LEU:HB2	6	0.27	0.09	0.26
(2,918)	1:99:A:LYS:HD2	1:99:A:LYS:HE2	6	0.26	0.04	0.24
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD23	6	0.25	0.1	0.27
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD21	6	0.25	0.1	0.27
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD22	6	0.25	0.1	0.27
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD12	6	0.24	0.06	0.22
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD13	6	0.24	0.06	0.22
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD11	6	0.24	0.06	0.22
(2,1384)	1:33:A:GLU:HG2	1:141:A:TYR:HE2	6	0.24	0.09	0.23
(2,4084)	1:162:A:CYS:H	1:162:A:CYS:HB2	6	0.24	0.09	0.25
(2,3942)	1:102:A:MET:HE2	1:102:A:MET:H	6	0.24	0.11	0.22
(2,3942)	1:102:A:MET:HE3	1:102:A:MET:H	6	0.24	0.11	0.22
(2,1309)	1:134:A:LEU:HD23	1:132:A:HIS:HD2	6	0.22	0.05	0.22
(2,1309)	1:134:A:LEU:HD21	1:132:A:HIS:HD2	6	0.22	0.05	0.22
(2,1309)	1:134:A:LEU:HD22	1:132:A:HIS:HD2	6	0.22	0.05	0.22
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG11	6	0.22	0.05	0.22
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG13	6	0.22	0.05	0.22
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG12	6	0.22	0.05	0.22
(2,2556)	1:89:A:VAL:H	1:88:A:ASP:HB3	6	0.22	0.07	0.26
(2,868)	1:18:A:ALA:HB3	1:22:A:GLN:HG3	6	0.22	0.07	0.2
(2,868)	1:18:A:ALA:HB1	1:22:A:GLN:HG3	6	0.22	0.07	0.2
(2,868)	1:18:A:ALA:HB2	1:22:A:GLN:HG3	6	0.22	0.07	0.2
(2,3923)	1:49:A:ILE:HD13	1:42:A:MET:H	6	0.21	0.05	0.2
(2,3923)	1:49:A:ILE:HD11	1:42:A:MET:H	6	0.21	0.05	0.2
(2,3923)	1:49:A:ILE:HD12	1:42:A:MET:H	6	0.21	0.05	0.2
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG21	6	0.2	0.04	0.19
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG23	6	0.2	0.04	0.19
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG22	6	0.2	0.04	0.19
(2,4472)	1:20:A:LEU:HD23	1:155:A:LEU:HD13	6	0.19	0.05	0.22
(2,4472)	1:20:A:LEU:HD22	1:155:A:LEU:HD11	6	0.19	0.05	0.22
(2,4472)	1:20:A:LEU:HD21	1:155:A:LEU:HD11	6	0.19	0.05	0.22
(2,4422)	1:56:A:LYS:HE2	1:56:A:LYS:HG2	6	0.19	0.05	0.19
(2,529)	1:176:A:VAL:HG22	1:97:A:ALA:HB3	6	0.18	0.04	0.19
(2,529)	1:176:A:VAL:HG21	1:97:A:ALA:HB1	6	0.18	0.04	0.19
(2,529)	1:176:A:VAL:HG23	1:97:A:ALA:HB2	6	0.18	0.04	0.19
(2,529)	1:176:A:VAL:HG22	1:97:A:ALA:HB1	6	0.18	0.04	0.19
(2,529)	1:176:A:VAL:HG23	1:97:A:ALA:HB1	6	0.18	0.04	0.19
(2,4309)	1:182:A:LYS:HE2	1:183:A:LYS:H	6	0.18	0.03	0.18
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD11	6	0.17	0.04	0.19
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD13	6	0.17	0.04	0.19
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD12	6	0.17	0.04	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1422)	1:116:A:LEU:HD23	1:60:A:ILE:HA	6	0.17	0.06	0.15
(2,1422)	1:116:A:LEU:HD22	1:60:A:ILE:HA	6	0.17	0.06	0.15
(2,1422)	1:116:A:LEU:HD21	1:60:A:ILE:HA	6	0.17	0.06	0.15
(2,4601)	1:186:A:ASP:HB3	1:186:A:ASP:H	6	0.17	0.04	0.17
(2,4601)	1:186:A:ASP:HB2	1:186:A:ASP:H	6	0.17	0.04	0.17
(2,4624)	1:98:A:ASP:HB2	1:100:A:PHE:H	6	0.17	0.05	0.16
(2,2484)	1:17:A:MET:H	1:15:A:PHE:HB3	6	0.16	0.1	0.12
(2,3657)	1:33:A:GLU:HB3	1:33:A:GLU:H	6	0.16	0.06	0.14
(2,4332)	1:31:A:LEU:HD22	1:32:A:HIS:H	6	0.15	0.04	0.15
(2,4332)	1:31:A:LEU:HD21	1:32:A:HIS:H	6	0.15	0.04	0.15
(2,4332)	1:31:A:LEU:HD23	1:32:A:HIS:H	6	0.15	0.04	0.15
(2,4056)	1:163:A:CYS:H	1:163:A:CYS:HB3	6	0.15	0.03	0.17
(2,4732)	1:121:A:ALA:H	1:118:A:LEU:HA	6	0.15	0.05	0.14
(2,4732)	1:121:A:ALA:H	1:119:A:GLU:HA	6	0.15	0.05	0.14
(2,4043)	1:12:A:LYS:HB3	1:12:A:LYS:H	6	0.14	0.05	0.12
(2,1094)	1:150:A:THR:HG23	1:151:A:LYS:HA	6	0.14	0.02	0.14
(2,1094)	1:150:A:THR:HG21	1:151:A:LYS:HA	6	0.14	0.02	0.14
(2,3895)	1:143:A:ILE:HD12	1:146:A:VAL:H	6	0.14	0.02	0.14
(2,3895)	1:143:A:ILE:HD11	1:146:A:VAL:H	6	0.14	0.02	0.14
(2,3895)	1:143:A:ILE:HD13	1:146:A:VAL:H	6	0.14	0.02	0.14
(2,2264)	1:142:A:LEU:H	1:141:A:TYR:HB3	6	0.14	0.02	0.14
(2,139)	1:36:A:GLU:HG3	1:32:A:HIS:HE1	6	0.12	0.02	0.11
(2,2893)	1:161:A:THR:H	1:162:A:CYS:HB3	5	0.97	0.33	1.09
(2,201)	1:99:A:LYS:HE2	1:96:A:TRP:HZ3	5	0.92	0.04	0.92
(2,3928)	1:162:A:CYS:H	1:162:A:CYS:HB3	5	0.9	0.19	0.92
(2,4120)	1:7:A:GLU:HG3	1:7:A:GLU:H	5	0.87	0.38	1.13
(2,1887)	1:152:A:TYR:H	1:177:A:MET:HG2	5	0.66	0.56	0.31
(2,291)	1:172:A:ASP:HA	1:171:A:LYS:HG2	5	0.6	0.21	0.66
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG21	5	0.59	0.14	0.62
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG23	5	0.59	0.14	0.62
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG22	5	0.59	0.14	0.62
(2,2614)	1:99:A:LYS:H	1:99:A:LYS:HE2	5	0.54	0.05	0.5
(2,3622)	1:4:A:GLY:HA2	1:5:A:SER:H	5	0.52	0.31	0.41
(2,2274)	1:189:A:HIS:H	1:188:A:MET:HB3	5	0.47	0.34	0.43
(2,3832)	1:179:A:SER:HB2	1:179:A:SER:H	5	0.47	0.03	0.46
(2,913)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	5	0.42	0.33	0.44
(2,4802)	1:167:A:LYS:HD3	1:167:A:LYS:H	5	0.41	0.18	0.5
(2,4802)	1:167:A:LYS:HD2	1:167:A:LYS:H	5	0.41	0.18	0.5
(2,666)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	5	0.4	0.28	0.31
(2,3260)	1:161:A:THR:HG21	1:158:A:GLU:H	5	0.35	0.23	0.25
(2,3260)	1:161:A:THR:HG23	1:158:A:GLU:H	5	0.35	0.23	0.25
(2,3260)	1:161:A:THR:HG22	1:158:A:GLU:H	5	0.35	0.23	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4803)	1:167:A:LYS:H	1:167:A:LYS:HE2	5	0.34	0.1	0.34
(2,4803)	1:167:A:LYS:H	1:167:A:LYS:HE3	5	0.34	0.1	0.34
(2,337)	1:102:A:MET:HE3	1:66:A:GLU:HA	5	0.31	0.23	0.15
(2,337)	1:102:A:MET:HE1	1:66:A:GLU:HA	5	0.31	0.23	0.15
(2,337)	1:102:A:MET:HE2	1:66:A:GLU:HA	5	0.31	0.23	0.15
(2,3886)	1:161:A:THR:H	1:162:A:CYS:HB2	5	0.31	0.08	0.27
(2,3012)	1:12:A:LYS:H	1:12:A:LYS:HB2	5	0.29	0.08	0.32
(2,1399)	1:7:A:GLU:HG3	1:8:A:PHE:HD2	5	0.29	0.08	0.27
(2,1399)	1:7:A:GLU:HG3	1:8:A:PHE:HD1	5	0.29	0.08	0.27
(2,3569)	1:141:A:TYR:HE2	1:136:A:ASN:HB3	5	0.28	0.06	0.3
(2,114)	1:177:A:MET:HE2	1:93:A:PHE:HE1	5	0.27	0.1	0.29
(2,114)	1:177:A:MET:HE3	1:93:A:PHE:HE1	5	0.27	0.1	0.29
(2,603)	1:28:A:VAL:HG22	1:72:A:ASN:HB3	5	0.27	0.18	0.18
(2,603)	1:28:A:VAL:HG21	1:72:A:ASN:HB3	5	0.27	0.18	0.18
(2,730)	1:97:A:ALA:HB3	1:93:A:PHE:HB3	5	0.26	0.03	0.25
(2,730)	1:97:A:ALA:HB1	1:93:A:PHE:HB3	5	0.26	0.03	0.25
(2,730)	1:97:A:ALA:HB2	1:93:A:PHE:HB3	5	0.26	0.03	0.25
(2,3200)	1:5:A:SER:H	1:6:A:PRO:HA	5	0.26	0.04	0.27
(2,4800)	1:164:A:GLU:HG3	1:164:A:GLU:H	5	0.26	0.17	0.18
(2,4800)	1:164:A:GLU:HG2	1:164:A:GLU:H	5	0.26	0.17	0.18
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG21	5	0.26	0.06	0.27
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG22	5	0.26	0.06	0.27
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG23	5	0.26	0.06	0.27
(2,86)	1:67:A:ILE:HG23	1:106:A:TYR:HD2	5	0.25	0.1	0.25
(2,86)	1:67:A:ILE:HG22	1:106:A:TYR:HD2	5	0.25	0.1	0.25
(2,4603)	1:10:A:GLY:H	1:9:A:PRO:HG2	5	0.23	0.1	0.2
(2,4603)	1:10:A:GLY:H	1:9:A:PRO:HG3	5	0.23	0.1	0.2
(2,4816)	1:98:A:ASP:HB3	1:101:A:GLN:H	5	0.22	0.06	0.22
(2,3856)	1:135:A:ALA:HB3	1:136:A:ASN:HD21	5	0.21	0.01	0.21
(2,3856)	1:135:A:ALA:HB1	1:136:A:ASN:HD21	5	0.21	0.01	0.21
(2,3856)	1:135:A:ALA:HB2	1:136:A:ASN:HD21	5	0.21	0.01	0.21
(2,4409)	1:172:A:ASP:HB2	1:94:A:VAL:HB	5	0.21	0.08	0.16
(2,4409)	1:172:A:ASP:HB3	1:94:A:VAL:HB	5	0.21	0.08	0.16
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD23	5	0.21	0.08	0.18
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD21	5	0.21	0.08	0.18
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD22	5	0.21	0.08	0.18
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG22	5	0.2	0.1	0.16
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG21	5	0.2	0.1	0.16
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG23	5	0.2	0.1	0.16
(2,530)	1:49:A:ILE:HD13	1:124:A:PHE:HZ	5	0.19	0.06	0.18
(2,530)	1:49:A:ILE:HD11	1:124:A:PHE:HZ	5	0.19	0.06	0.18
(2,63)	1:174:A:LEU:HD23	1:175:A:GLU:HA	5	0.18	0.06	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,63)	1:174:A:LEU:HD21	1:175:A:GLU:HA	5	0.18	0.06	0.15
(2,63)	1:174:A:LEU:HD22	1:175:A:GLU:HA	5	0.18	0.06	0.15
(2,3830)	1:177:A:MET:HE1	1:178:A:LEU:H	5	0.18	0.05	0.2
(2,3830)	1:177:A:MET:HE3	1:178:A:LEU:H	5	0.18	0.05	0.2
(2,3830)	1:177:A:MET:HE2	1:178:A:LEU:H	5	0.18	0.05	0.2
(2,2922)	1:170:A:LEU:H	1:159:A:LEU:HD13	5	0.18	0.08	0.14
(2,2922)	1:170:A:LEU:H	1:159:A:LEU:HD12	5	0.18	0.08	0.14
(2,1570)	1:156:A:LEU:HD22	1:178:A:LEU:H	5	0.16	0.03	0.17
(2,1570)	1:156:A:LEU:HD21	1:178:A:LEU:H	5	0.16	0.03	0.17
(2,1570)	1:156:A:LEU:HD23	1:178:A:LEU:H	5	0.16	0.03	0.17
(2,3875)	1:39:A:LEU:HD22	1:43:A:THR:H	5	0.16	0.04	0.16
(2,3875)	1:39:A:LEU:HD21	1:43:A:THR:H	5	0.16	0.04	0.16
(2,3875)	1:39:A:LEU:HD23	1:43:A:THR:H	5	0.16	0.04	0.16
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG23	5	0.16	0.05	0.13
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG22	5	0.16	0.05	0.13
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG21	5	0.16	0.05	0.13
(2,4767)	1:8:A:PHE:HD2	1:9:A:PRO:HG3	5	0.16	0.05	0.17
(2,4767)	1:8:A:PHE:HD1	1:9:A:PRO:HG2	5	0.16	0.05	0.17
(2,1152)	1:104:A:VAL:HG13	1:101:A:GLN:HA	5	0.16	0.02	0.15
(2,1152)	1:104:A:VAL:HG11	1:101:A:GLN:HA	5	0.16	0.02	0.15
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD12	5	0.15	0.04	0.15
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD11	5	0.15	0.04	0.15
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD13	5	0.15	0.04	0.15
(2,3808)	1:143:A:ILE:HG23	1:144:A:LYS:H	5	0.14	0.03	0.15
(2,3808)	1:143:A:ILE:HG21	1:144:A:LYS:H	5	0.14	0.03	0.15
(2,3808)	1:143:A:ILE:HG22	1:144:A:LYS:H	5	0.14	0.03	0.15
(2,2287)	1:22:A:GLN:H	1:20:A:LEU:HB2	5	0.14	0.04	0.12
(2,3837)	1:182:A:LYS:HD2	1:182:A:LYS:H	5	0.14	0.03	0.12
(2,2943)	1:138:A:ILE:H	1:137:A:SER:HA	5	0.12	0.01	0.12
(2,682)	1:171:A:LYS:HG2	1:175:A:GLU:HG3	4	1.7	0.26	1.56
(2,1882)	1:149:A:VAL:H	1:151:A:LYS:HB3	4	1.68	0.07	1.68
(2,4018)	1:190:A:VAL:HG11	1:190:A:VAL:H	4	1.2	0.57	1.52
(2,1335)	1:157:A:LYS:HA	1:157:A:LYS:HD3	4	1.19	0.11	1.21
(2,3307)	1:31:A:LEU:H	1:29:A:ARG:HD3	4	1.13	0.47	1.36
(2,916)	1:183:A:LYS:HE2	1:183:A:LYS:HA	4	1.09	0.09	1.08
(2,1885)	1:150:A:THR:H	1:151:A:LYS:HB3	4	0.94	0.02	0.93
(2,828)	1:128:A:ILE:HD11	1:47:A:GLU:HG2	4	0.72	0.16	0.78
(2,828)	1:128:A:ILE:HD13	1:47:A:GLU:HG2	4	0.72	0.16	0.78
(2,828)	1:128:A:ILE:HD12	1:47:A:GLU:HG2	4	0.72	0.16	0.78
(2,2166)	1:151:A:LYS:H	1:151:A:LYS:HB3	4	0.7	0.04	0.72
(2,1860)	1:136:A:ASN:H	1:129:A:GLN:HE22	4	0.68	0.34	0.67
(2,4091)	1:36:A:GLU:H	1:36:A:GLU:HG3	4	0.66	0.54	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4502)	1:14:A:GLU:HB3	1:15:A:PHE:HE2	4	0.66	0.25	0.64
(2,4502)	1:14:A:GLU:HB2	1:15:A:PHE:HE1	4	0.66	0.25	0.64
(2,4502)	1:14:A:GLU:HB2	1:15:A:PHE:HE2	4	0.66	0.25	0.64
(2,933)	1:15:A:PHE:HB3	1:18:A:ALA:HB1	4	0.6	0.09	0.57
(2,933)	1:15:A:PHE:HB3	1:18:A:ALA:HB2	4	0.6	0.09	0.57
(2,933)	1:15:A:PHE:HB3	1:18:A:ALA:HB3	4	0.6	0.09	0.57
(2,30)	1:32:A:HIS:HD2	1:35:A:LEU:HD13	4	0.58	0.04	0.57
(2,30)	1:32:A:HIS:HD2	1:35:A:LEU:HD12	4	0.58	0.04	0.57
(2,1828)	1:131:A:ARG:HE	1:47:A:GLU:HG3	4	0.58	0.29	0.58
(2,1932)	1:10:A:GLY:H	1:11:A:ARG:HB3	4	0.54	0.27	0.57
(2,3862)	1:101:A:GLN:HE21	1:104:A:VAL:HG12	4	0.5	0.05	0.51
(2,3862)	1:101:A:GLN:HE21	1:104:A:VAL:HG13	4	0.5	0.05	0.51
(2,3862)	1:101:A:GLN:HE21	1:104:A:VAL:HG11	4	0.5	0.05	0.51
(2,1783)	1:94:A:VAL:H	1:169:A:GLU:HB3	4	0.49	0.56	0.18
(2,124)	1:187:A:ALA:HB2	1:183:A:LYS:HE2	4	0.48	0.29	0.48
(2,124)	1:187:A:ALA:HB3	1:183:A:LYS:HE2	4	0.48	0.29	0.48
(2,1395)	1:188:A:MET:HE2	1:188:A:MET:HG3	4	0.44	0.02	0.43
(2,1395)	1:188:A:MET:HE1	1:188:A:MET:HG3	4	0.44	0.02	0.43
(2,1395)	1:188:A:MET:HE3	1:188:A:MET:HG3	4	0.44	0.02	0.43
(2,2901)	1:166:A:GLY:HA2	1:167:A:LYS:H	4	0.43	0.15	0.51
(2,346)	1:102:A:MET:HE1	1:67:A:ILE:HD11	4	0.4	0.05	0.39
(2,346)	1:102:A:MET:HE2	1:67:A:ILE:HD13	4	0.4	0.05	0.39
(2,346)	1:102:A:MET:HE1	1:67:A:ILE:HD13	4	0.4	0.05	0.39
(2,346)	1:102:A:MET:HE2	1:67:A:ILE:HD11	4	0.4	0.05	0.39
(2,2165)	1:151:A:LYS:H	1:151:A:LYS:HB2	4	0.4	0.08	0.39
(2,2275)	1:190:A:VAL:H	1:189:A:HIS:HB3	4	0.4	0.04	0.41
(2,4320)	1:188:A:MET:HA	1:108:A:LYS:HE2	4	0.39	0.17	0.32
(2,4320)	1:188:A:MET:HA	1:108:A:LYS:HE3	4	0.39	0.17	0.32
(2,874)	1:188:A:MET:HG3	1:108:A:LYS:HG2	4	0.36	0.34	0.18
(2,1088)	1:161:A:THR:HG23	1:158:A:GLU:HA	4	0.34	0.1	0.29
(2,1088)	1:161:A:THR:HG22	1:158:A:GLU:HA	4	0.34	0.1	0.29
(2,3624)	1:3:A:LEU:H	1:3:A:LEU:HB3	4	0.33	0.03	0.34
(2,3961)	1:155:A:LEU:HD12	1:155:A:LEU:H	4	0.32	0.15	0.32
(2,3961)	1:155:A:LEU:HD11	1:155:A:LEU:H	4	0.32	0.15	0.32
(2,2273)	1:189:A:HIS:H	1:189:A:HIS:HB2	4	0.31	0.17	0.3
(2,3728)	1:87:A:GLU:HG3	1:87:A:GLU:H	4	0.3	0.1	0.3
(2,2896)	1:164:A:GLU:H	1:163:A:CYS:H	4	0.29	0.17	0.24
(2,4284)	1:171:A:LYS:HG2	1:172:A:ASP:H	4	0.29	0.14	0.29
(2,4284)	1:171:A:LYS:HG3	1:172:A:ASP:H	4	0.29	0.14	0.29
(2,3014)	1:16:A:ILE:H	1:14:A:GLU:HB3	4	0.29	0.19	0.22
(2,25)	1:37:A:THR:HG22	1:33:A:GLU:HG2	4	0.26	0.14	0.2
(2,25)	1:37:A:THR:HG23	1:33:A:GLU:HG2	4	0.26	0.14	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2527)	1:87:A:GLU:H	1:88:A:ASP:HB3	4	0.25	0.04	0.26
(2,4236)	1:33:A:GLU:HG3	1:34:A:CYS:H	4	0.24	0.02	0.24
(2,619)	1:40:A:TRP:HD1	1:43:A:THR:HG22	4	0.23	0.04	0.22
(2,619)	1:40:A:TRP:HD1	1:43:A:THR:HG21	4	0.23	0.04	0.22
(2,619)	1:40:A:TRP:HD1	1:43:A:THR:HG23	4	0.23	0.04	0.22
(2,267)	1:183:A:LYS:HA	1:186:A:ASP:HB2	4	0.21	0.06	0.23
(2,3585)	1:100:A:PHE:HD1	1:97:A:ALA:HB3	4	0.21	0.08	0.18
(2,3585)	1:100:A:PHE:HD1	1:97:A:ALA:HB1	4	0.21	0.08	0.18
(2,3905)	1:28:A:VAL:HG12	1:72:A:ASN:H	4	0.21	0.06	0.2
(2,3905)	1:28:A:VAL:HG13	1:72:A:ASN:H	4	0.21	0.06	0.2
(2,2128)	1:163:A:CYS:H	1:163:A:CYS:HA	4	0.2	0.06	0.2
(2,4047)	1:156:A:LEU:HD13	1:159:A:LEU:H	4	0.18	0.06	0.19
(2,4047)	1:156:A:LEU:HD12	1:159:A:LEU:H	4	0.18	0.06	0.19
(2,3635)	1:12:A:LYS:HA	1:13:A:LYS:H	4	0.18	0.11	0.13
(2,4756)	1:32:A:HIS:HD2	1:35:A:LEU:H	4	0.18	0.02	0.18
(2,3636)	1:13:A:LYS:HA	1:14:A:GLU:H	4	0.18	0.05	0.18
(1,3)	1:15:A:PHE:O	1:19:A:GLU:H	4	0.16	0.02	0.16
(2,4385)	1:48:A:GLU:HB3	1:48:A:GLU:H	4	0.16	0.02	0.16
(2,4385)	1:48:A:GLU:HB2	1:48:A:GLU:H	4	0.16	0.02	0.16
(2,1028)	1:105:A:THR:HA	1:104:A:VAL:HG21	4	0.16	0.02	0.16
(2,1028)	1:105:A:THR:HA	1:104:A:VAL:HG22	4	0.16	0.02	0.16
(2,1028)	1:105:A:THR:HA	1:104:A:VAL:HG23	4	0.16	0.02	0.16
(2,3581)	1:96:A:TRP:HH2	1:74:A:ILE:HD11	4	0.16	0.01	0.16
(2,3581)	1:96:A:TRP:HH2	1:74:A:ILE:HD13	4	0.16	0.01	0.16
(2,2120)	1:153:A:GLN:HG2	1:153:A:GLN:H	4	0.15	0.03	0.15
(2,3188)	1:72:A:ASN:H	1:68:A:TYR:H	4	0.13	0.01	0.13
(2,554)	1:67:A:ILE:HG22	1:31:A:LEU:HD21	4	0.12	0.01	0.12
(2,554)	1:67:A:ILE:HG21	1:31:A:LEU:HD22	4	0.12	0.01	0.12
(2,554)	1:67:A:ILE:HG22	1:31:A:LEU:HD23	4	0.12	0.01	0.12
(2,4658)	1:87:A:GLU:HG3	1:88:A:ASP:H	4	0.12	0.03	0.11
(2,14)	1:75:A:PHE:HD1	1:79:A:LEU:HD12	4	0.12	0.02	0.11
(2,14)	1:75:A:PHE:HD2	1:79:A:LEU:HD13	4	0.12	0.02	0.11
(2,14)	1:75:A:PHE:HD2	1:79:A:LEU:HD12	4	0.12	0.02	0.11
(2,14)	1:75:A:PHE:HD1	1:79:A:LEU:HD13	4	0.12	0.02	0.11
(2,3094)	1:39:A:LEU:H	1:38:A:TYR:HB3	4	0.12	0.01	0.12
(2,3543)	1:68:A:TYR:HD1	1:28:A:VAL:HG23	4	0.12	0.01	0.11
(2,3543)	1:68:A:TYR:HD1	1:28:A:VAL:HG22	4	0.12	0.01	0.11
(2,1645)	1:174:A:LEU:H	1:178:A:LEU:HG	4	0.12	0.02	0.11
(2,2686)	1:114:A:ASN:H	1:112:A:ASP:HB2	4	0.11	0.02	0.11
(2,2906)	1:168:A:GLY:HA3	1:168:A:GLY:H	4	0.11	0.0	0.11
(2,3089)	1:36:A:GLU:HG2	1:37:A:THR:H	4	0.11	0.01	0.11
(2,4082)	1:130:A:GLN:H	1:130:A:GLN:HG3	3	1.42	0.01	1.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2624)	1:102:A:MET:HG2	1:102:A:MET:H	3	1.33	0.05	1.3
(2,896)	1:81:A:LYS:HE3	1:78:A:GLU:HA	3	1.19	0.06	1.21
(2,3233)	1:166:A:GLY:H	1:165:A:GLU:HB3	3	1.0	0.58	1.35
(2,2528)	1:87:A:GLU:HG2	1:87:A:GLU:H	3	0.91	0.38	0.84
(2,1909)	1:177:A:MET:H	1:153:A:GLN:HG2	3	0.84	0.47	1.13
(2,2435)	1:73:A:ASN:HB2	1:73:A:ASN:H	3	0.78	0.0	0.78
(2,343)	1:99:A:LYS:HD2	1:102:A:MET:HE1	3	0.75	0.57	0.37
(2,343)	1:99:A:LYS:HD2	1:102:A:MET:HE3	3	0.75	0.57	0.37
(2,1852)	1:130:A:GLN:HG2	1:130:A:GLN:H	3	0.73	0.0	0.73
(2,2296)	1:29:A:ARG:HD3	1:29:A:ARG:H	3	0.65	0.01	0.66
(2,3063)	1:29:A:ARG:HD3	1:30:A:ASP:H	3	0.65	0.06	0.62
(2,3199)	1:5:A:SER:H	1:4:A:GLY:HA3	3	0.63	0.22	0.77
(2,4083)	1:163:A:CYS:HB2	1:162:A:CYS:H	3	0.6	0.2	0.69
(2,830)	1:174:A:LEU:HD23	1:175:A:GLU:HG3	3	0.56	0.61	0.14
(2,830)	1:174:A:LEU:HD21	1:175:A:GLU:HG3	3	0.56	0.61	0.14
(2,335)	1:102:A:MET:HE2	1:71:A:HIS:HE1	3	0.54	0.4	0.39
(2,335)	1:102:A:MET:HE1	1:71:A:HIS:HE1	3	0.54	0.4	0.39
(2,2853)	1:150:A:THR:H	1:153:A:GLN:HE21	3	0.53	0.14	0.47
(2,1953)	1:141:A:TYR:HE1	1:30:A:ASP:H	3	0.53	0.31	0.41
(2,1144)	1:164:A:GLU:HA	1:163:A:CYS:HB3	3	0.53	0.29	0.55
(2,2895)	1:164:A:GLU:H	1:163:A:CYS:HB2	3	0.52	0.3	0.43
(2,2902)	1:166:A:GLY:HA3	1:167:A:LYS:H	3	0.51	0.15	0.51
(2,4818)	1:7:A:GLU:H	1:5:A:SER:HB2	3	0.5	0.12	0.57
(2,894)	1:99:A:LYS:HE3	1:75:A:PHE:H	3	0.46	0.24	0.6
(2,1508)	1:105:A:THR:HG23	1:63:A:ASN:HB3	3	0.45	0.25	0.33
(2,1508)	1:105:A:THR:HG22	1:63:A:ASN:HB3	3	0.45	0.25	0.33
(2,302)	1:136:A:ASN:HA	1:129:A:GLN:HE22	3	0.45	0.18	0.44
(2,4699)	1:7:A:GLU:H	1:5:A:SER:HB2	3	0.44	0.12	0.51
(2,4699)	1:7:A:GLU:H	1:6:A:PRO:HD3	3	0.44	0.12	0.51
(2,140)	1:36:A:GLU:HG3	1:37:A:THR:H	3	0.44	0.24	0.6
(2,2908)	1:169:A:GLU:H	1:168:A:GLY:HA2	3	0.44	0.21	0.45
(2,1190)	1:19:A:GLU:HA	1:22:A:GLN:HG2	3	0.41	0.27	0.25
(2,1525)	1:143:A:ILE:HG21	1:144:A:LYS:HE3	3	0.41	0.27	0.3
(2,535)	1:76:A:LEU:HD22	1:71:A:HIS:HB3	3	0.41	0.13	0.35
(2,535)	1:76:A:LEU:HD23	1:71:A:HIS:HB3	3	0.41	0.13	0.35
(2,535)	1:76:A:LEU:HD21	1:71:A:HIS:HB3	3	0.41	0.13	0.35
(2,156)	1:7:A:GLU:HG2	1:8:A:PHE:H	3	0.4	0.21	0.52
(2,3719)	1:81:A:LYS:HE2	1:81:A:LYS:H	3	0.4	0.13	0.31
(2,1095)	1:190:A:VAL:HA	1:190:A:VAL:HB	3	0.39	0.0	0.39
(2,2644)	1:108:A:LYS:H	1:109:A:ASN:HB2	3	0.38	0.05	0.35
(2,1594)	1:135:A:ALA:HA	1:129:A:GLN:HE22	3	0.35	0.17	0.37
(2,132)	1:23:A:THR:HG22	1:148:A:ARG:HD2	3	0.33	0.17	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,132)	1:23:A:THR:HG21	1:148:A:ARG:HD2	3	0.33	0.17	0.32
(2,132)	1:23:A:THR:HG23	1:148:A:ARG:HD2	3	0.33	0.17	0.32
(2,131)	1:23:A:THR:HG22	1:148:A:ARG:HD3	3	0.32	0.04	0.34
(2,131)	1:23:A:THR:HG21	1:148:A:ARG:HD3	3	0.32	0.04	0.34
(2,131)	1:23:A:THR:HG23	1:148:A:ARG:HD3	3	0.32	0.04	0.34
(2,935)	1:29:A:ARG:HG2	1:29:A:ARG:HD3	3	0.32	0.03	0.3
(2,1386)	1:33:A:GLU:HG2	1:29:A:ARG:HD3	3	0.31	0.18	0.29
(2,1805)	1:185:A:ASN:HD21	1:182:A:LYS:HA	3	0.3	0.12	0.37
(2,3182)	1:15:A:PHE:HB2	1:15:A:PHE:H	3	0.3	0.14	0.39
(2,1122)	1:7:A:GLU:HG2	1:7:A:GLU:HA	3	0.3	0.19	0.23
(2,338)	1:102:A:MET:HE2	1:70:A:PHE:HB3	3	0.29	0.08	0.3
(2,338)	1:102:A:MET:HE3	1:70:A:PHE:HB3	3	0.29	0.08	0.3
(2,1861)	1:141:A:TYR:HE2	1:136:A:ASN:H	3	0.28	0.19	0.16
(2,3041)	1:22:A:GLN:HG2	1:23:A:THR:H	3	0.27	0.19	0.15
(2,2455)	1:73:A:ASN:HB2	1:74:A:ILE:H	3	0.27	0.13	0.28
(2,2247)	1:132:A:HIS:H	1:130:A:GLN:HG3	3	0.26	0.02	0.27
(2,859)	1:130:A:GLN:HG2	1:131:A:ARG:H	3	0.25	0.04	0.25
(1,11)	1:19:A:GLU:O	1:23:A:THR:H	3	0.24	0.09	0.3
(2,4353)	1:146:A:VAL:HG22	1:145:A:PRO:HG2	3	0.23	0.07	0.19
(2,4353)	1:146:A:VAL:HG23	1:145:A:PRO:HG2	3	0.23	0.07	0.19
(2,4353)	1:43:A:THR:HG23	1:39:A:LEU:HB3	3	0.23	0.07	0.19
(2,4780)	1:47:A:GLU:HG2	1:47:A:GLU:H	3	0.23	0.09	0.22
(2,4780)	1:47:A:GLU:HG3	1:47:A:GLU:H	3	0.23	0.09	0.22
(2,4460)	1:19:A:GLU:HA	1:23:A:THR:HG23	3	0.22	0.08	0.22
(2,4460)	1:19:A:GLU:HA	1:23:A:THR:HG21	3	0.22	0.08	0.22
(2,4460)	1:19:A:GLU:HA	1:23:A:THR:HG22	3	0.22	0.08	0.22
(2,4038)	1:29:A:ARG:HG2	1:29:A:ARG:H	3	0.22	0.03	0.23
(2,102)	1:28:A:VAL:HG13	1:72:A:ASN:HB3	3	0.21	0.12	0.14
(2,102)	1:28:A:VAL:HG11	1:72:A:ASN:HB3	3	0.21	0.12	0.14
(2,2056)	1:72:A:ASN:H	1:73:A:ASN:HB3	3	0.21	0.08	0.22
(2,4243)	1:94:A:VAL:HG22	1:92:A:CYS:H	3	0.2	0.05	0.17
(2,4243)	1:94:A:VAL:HG23	1:92:A:CYS:H	3	0.2	0.05	0.17
(2,3447)	1:40:A:TRP:HZ3	1:46:A:VAL:HG21	3	0.2	0.08	0.21
(2,3447)	1:40:A:TRP:HZ3	1:46:A:VAL:HG23	3	0.2	0.08	0.21
(2,4073)	1:131:A:ARG:HE	1:131:A:ARG:HG2	3	0.2	0.03	0.21
(2,597)	1:28:A:VAL:HG22	1:72:A:ASN:HD22	3	0.2	0.05	0.2
(2,3536)	1:32:A:HIS:HD2	1:32:A:HIS:HA	3	0.2	0.03	0.2
(2,4642)	1:62:A:GLY:H	1:64:A:ILE:HB	3	0.2	0.08	0.16
(2,2583)	1:94:A:VAL:H	1:177:A:MET:HE1	3	0.2	0.07	0.15
(2,2583)	1:94:A:VAL:H	1:177:A:MET:HE2	3	0.2	0.07	0.15
(2,2583)	1:94:A:VAL:H	1:177:A:MET:HE3	3	0.2	0.07	0.15
(2,3011)	1:12:A:LYS:HA	1:12:A:LYS:H	3	0.19	0.01	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2718)	1:11:A:ARG:H	1:11:A:ARG:HB3	3	0.19	0.06	0.17
(2,2899)	1:165:A:GLU:H	1:164:A:GLU:H	3	0.18	0.06	0.14
(2,1930)	1:11:A:ARG:H	1:11:A:ARG:HB2	3	0.18	0.09	0.12
(2,3555)	1:96:A:TRP:HD1	1:95:A:THR:HG23	3	0.18	0.04	0.18
(2,3555)	1:96:A:TRP:HD1	1:95:A:THR:HG21	3	0.18	0.04	0.18
(2,3555)	1:96:A:TRP:HD1	1:95:A:THR:HG22	3	0.18	0.04	0.18
(2,1308)	1:142:A:LEU:HD22	1:61:A:PHE:HD2	3	0.17	0.08	0.12
(2,1308)	1:142:A:LEU:HD21	1:61:A:PHE:HD2	3	0.17	0.08	0.12
(2,1308)	1:142:A:LEU:HD23	1:61:A:PHE:HD1	3	0.17	0.08	0.12
(2,199)	1:134:A:LEU:HD22	1:37:A:THR:HB	3	0.17	0.01	0.16
(2,951)	1:15:A:PHE:HB2	1:18:A:ALA:HB1	3	0.17	0.03	0.18
(2,951)	1:15:A:PHE:HB2	1:18:A:ALA:HB2	3	0.17	0.03	0.18
(2,4200)	1:22:A:GLN:HE21	1:18:A:ALA:HB3	3	0.17	0.03	0.19
(2,4200)	1:22:A:GLN:HE21	1:18:A:ALA:HB1	3	0.17	0.03	0.19
(2,477)	1:59:A:ILE:HG21	1:60:A:ILE:HD11	3	0.16	0.04	0.18
(2,477)	1:59:A:ILE:HG21	1:60:A:ILE:HD12	3	0.16	0.04	0.18
(2,477)	1:59:A:ILE:HG22	1:60:A:ILE:HD12	3	0.16	0.04	0.18
(2,4393)	1:130:A:GLN:HB2	1:131:A:ARG:HG2	3	0.16	0.04	0.18
(2,3326)	1:46:A:VAL:HB	1:46:A:VAL:H	3	0.16	0.02	0.15
(2,4214)	1:156:A:LEU:HD11	1:173:A:GLY:H	3	0.16	0.03	0.17
(2,4214)	1:156:A:LEU:HD13	1:173:A:GLY:H	3	0.16	0.03	0.17
(2,928)	1:29:A:ARG:HD2	1:29:A:ARG:H	3	0.15	0.05	0.12
(2,1394)	1:156:A:LEU:HD21	1:152:A:TYR:HA	3	0.15	0.04	0.13
(2,1394)	1:156:A:LEU:HD23	1:152:A:TYR:HA	3	0.15	0.04	0.13
(2,4057)	1:163:A:CYS:HB2	1:163:A:CYS:H	3	0.15	0.02	0.14
(2,2500)	1:81:A:LYS:H	1:79:A:LEU:HB3	3	0.15	0.05	0.12
(2,690)	1:184:A:ALA:HB1	1:185:A:ASN:HB3	3	0.14	0.03	0.16
(2,3953)	1:183:A:LYS:HB2	1:183:A:LYS:H	3	0.14	0.02	0.15
(2,4300)	1:92:A:CYS:HB2	1:75:A:PHE:HE2	3	0.14	0.02	0.15
(2,4300)	1:92:A:CYS:HB2	1:75:A:PHE:HE1	3	0.14	0.02	0.15
(2,4294)	1:164:A:GLU:HB2	1:164:A:GLU:HG2	3	0.14	0.04	0.13
(2,4294)	1:164:A:GLU:HB2	1:164:A:GLU:HG3	3	0.14	0.04	0.13
(2,4813)	1:188:A:MET:H	1:186:A:ASP:HB3	3	0.14	0.01	0.14
(2,4813)	1:188:A:MET:H	1:186:A:ASP:HB2	3	0.14	0.01	0.14
(2,1939)	1:20:A:LEU:H	1:16:A:ILE:HA	3	0.14	0.03	0.13
(2,4595)	1:152:A:TYR:H	1:154:A:LEU:HB2	3	0.14	0.04	0.12
(2,3898)	1:46:A:VAL:HG21	1:46:A:VAL:H	3	0.13	0.02	0.14
(2,3898)	1:46:A:VAL:HG23	1:46:A:VAL:H	3	0.13	0.02	0.14
(2,3898)	1:46:A:VAL:HG22	1:46:A:VAL:H	3	0.13	0.02	0.14
(2,3887)	1:94:A:VAL:HG23	1:173:A:GLY:H	3	0.13	0.01	0.13
(2,3887)	1:94:A:VAL:HG21	1:173:A:GLY:H	3	0.13	0.01	0.13
(2,447)	1:31:A:LEU:HD12	1:31:A:LEU:HB3	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,447)	1:31:A:LEU:HD13	1:31:A:LEU:HB3	3	0.12	0.0	0.12
(2,447)	1:31:A:LEU:HD11	1:31:A:LEU:HB3	3	0.12	0.0	0.12
(2,2903)	1:167:A:LYS:HA	1:167:A:LYS:H	3	0.12	0.01	0.12
(2,1732)	1:69:A:ASP:H	1:72:A:ASN:HB3	3	0.12	0.02	0.12
(2,3806)	1:143:A:ILE:H	1:143:A:ILE:HG21	3	0.12	0.01	0.12
(2,3806)	1:143:A:ILE:H	1:143:A:ILE:HG23	3	0.12	0.01	0.12
(2,3806)	1:143:A:ILE:H	1:143:A:ILE:HG22	3	0.12	0.01	0.12
(2,3538)	1:32:A:HIS:HD2	1:36:A:GLU:H	3	0.12	0.01	0.11
(2,3546)	1:68:A:TYR:HE1	1:29:A:ARG:HA	3	0.11	0.01	0.11
(2,3218)	1:125:A:PHE:H	1:123:A:THR:H	3	0.11	0.0	0.11
(2,2270)	1:141:A:TYR:H	1:138:A:ILE:HG13	3	0.11	0.0	0.11
(2,1693)	1:38:A:TYR:H	1:38:A:TYR:HB2	3	0.11	0.01	0.11
(2,3446)	1:40:A:TRP:HZ3	1:41:A:GLU:HA	3	0.11	0.0	0.11
(2,65)	1:117:A:ILE:HG23	1:117:A:ILE:HB	3	0.1	0.0	0.1
(2,65)	1:117:A:ILE:HG22	1:117:A:ILE:HB	3	0.1	0.0	0.1
(2,1056)	1:157:A:LYS:HG3	1:157:A:LYS:HA	2	1.26	0.0	1.26
(2,3117)	1:44:A:SER:H	1:44:A:SER:HB2	2	1.04	0.03	1.04
(2,196)	1:41:A:GLU:HG2	1:128:A:ILE:HD13	2	0.93	0.07	0.93
(2,196)	1:41:A:GLU:HG2	1:128:A:ILE:HD11	2	0.93	0.07	0.93
(2,4100)	1:44:A:SER:HB2	1:43:A:THR:H	2	0.86	0.06	0.86
(2,1036)	1:140:A:SER:HB2	1:136:A:ASN:HB3	2	0.83	0.59	0.83
(2,3722)	1:84:A:GLN:HG3	1:84:A:GLN:H	2	0.78	0.66	0.78
(2,3379)	1:173:A:GLY:H	1:169:A:GLU:HB3	2	0.77	0.62	0.77
(2,2878)	1:157:A:LYS:HG2	1:157:A:LYS:H	2	0.74	0.02	0.74
(2,4052)	1:185:A:ASN:HB2	1:186:A:ASP:H	2	0.73	0.61	0.73
(2,1483)	1:36:A:GLU:HG2	1:33:A:GLU:H	2	0.64	0.03	0.64
(2,154)	1:181:A:PRO:HG3	1:153:A:GLN:HE21	2	0.62	0.5	0.62
(2,2575)	1:36:A:GLU:HG2	1:35:A:LEU:H	2	0.61	0.03	0.61
(2,4417)	1:153:A:GLN:HG2	1:149:A:VAL:HG11	2	0.61	0.04	0.61
(2,3860)	1:149:A:VAL:HG11	1:153:A:GLN:HE21	2	0.58	0.36	0.58
(2,3860)	1:149:A:VAL:HG13	1:153:A:GLN:HE21	2	0.58	0.36	0.58
(2,734)	1:36:A:GLU:HG3	1:35:A:LEU:H	2	0.56	0.03	0.56
(2,4815)	1:165:A:GLU:HG3	1:167:A:LYS:H	2	0.56	0.23	0.56
(2,4815)	1:165:A:GLU:HG2	1:167:A:LYS:H	2	0.56	0.23	0.56
(2,1385)	1:33:A:GLU:HG3	1:29:A:ARG:HD3	2	0.5	0.12	0.5
(2,4823)	1:13:A:LYS:H	1:13:A:LYS:HE2	2	0.48	0.21	0.48
(2,4823)	1:13:A:LYS:H	1:13:A:LYS:HE3	2	0.48	0.21	0.48
(2,2948)	1:178:A:LEU:H	1:177:A:MET:HB3	2	0.48	0.01	0.48
(2,4429)	1:11:A:ARG:HB3	1:11:A:ARG:HD2	2	0.47	0.13	0.47
(2,4429)	1:11:A:ARG:HB3	1:11:A:ARG:HD3	2	0.47	0.13	0.47
(2,2303)	1:41:A:GLU:HG2	1:41:A:GLU:H	2	0.46	0.0	0.46
(2,1463)	1:16:A:ILE:HG22	1:158:A:GLU:HG3	2	0.46	0.11	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1826)	1:131:A:ARG:HE	1:128:A:ILE:HG21	2	0.45	0.03	0.45
(2,336)	1:102:A:MET:HE1	1:100:A:PHE:HA	2	0.44	0.04	0.44
(2,336)	1:102:A:MET:HE2	1:100:A:PHE:HA	2	0.44	0.04	0.44
(2,4558)	1:99:A:LYS:HD2	1:98:A:ASP:HB2	2	0.42	0.1	0.42
(2,160)	1:177:A:MET:HB3	1:156:A:LEU:HD23	2	0.4	0.05	0.4
(2,160)	1:177:A:MET:HB3	1:156:A:LEU:HD22	2	0.4	0.05	0.4
(2,654)	1:177:A:MET:HE3	1:174:A:LEU:HA	2	0.38	0.03	0.38
(2,654)	1:177:A:MET:HE1	1:174:A:LEU:HA	2	0.38	0.03	0.38
(2,1202)	1:38:A:TYR:HA	1:128:A:ILE:HD12	2	0.36	0.02	0.36
(2,1202)	1:38:A:TYR:HA	1:128:A:ILE:HD11	2	0.36	0.02	0.36
(2,533)	1:49:A:ILE:HD13	1:42:A:MET:HE2	2	0.34	0.08	0.34
(2,533)	1:49:A:ILE:HD12	1:42:A:MET:HE1	2	0.34	0.08	0.34
(2,3106)	1:43:A:THR:H	1:44:A:SER:HB3	2	0.34	0.03	0.34
(2,3042)	1:22:A:GLN:HB2	1:23:A:THR:H	2	0.32	0.01	0.32
(2,2028)	1:8:A:PHE:H	1:8:A:PHE:HB3	2	0.32	0.12	0.32
(2,4282)	1:146:A:VAL:HG12	1:103:A:TYR:HE1	2	0.32	0.03	0.32
(2,3646)	1:22:A:GLN:HB3	1:23:A:THR:H	2	0.3	0.02	0.3
(2,4596)	1:166:A:GLY:H	1:167:A:LYS:HD2	2	0.3	0.2	0.3
(2,2148)	1:42:A:MET:H	1:41:A:GLU:HG3	2	0.3	0.01	0.3
(2,4347)	1:76:A:LEU:HD21	1:77:A:LYS:HE3	2	0.29	0.12	0.29
(2,4347)	1:174:A:LEU:HD12	1:157:A:LYS:HE2	2	0.29	0.12	0.29
(2,4545)	1:67:A:ILE:HD12	1:145:A:PRO:HG3	2	0.26	0.02	0.26
(2,4545)	1:67:A:ILE:HD11	1:145:A:PRO:HG3	2	0.26	0.02	0.26
(2,1322)	1:74:A:ILE:HG23	1:78:A:GLU:HG2	2	0.26	0.04	0.26
(2,121)	1:161:A:THR:HG23	1:158:A:GLU:HB3	2	0.24	0.01	0.24
(2,121)	1:161:A:THR:HG21	1:158:A:GLU:HB3	2	0.24	0.01	0.24
(2,285)	1:19:A:GLU:HA	1:22:A:GLN:HB3	2	0.24	0.04	0.24
(2,2963)	1:179:A:SER:H	1:177:A:MET:HB3	2	0.24	0.02	0.24
(2,3119)	1:45:A:GLY:H	1:44:A:SER:HB2	2	0.24	0.01	0.24
(2,2907)	1:169:A:GLU:H	1:169:A:GLU:HA	2	0.24	0.03	0.24
(2,1097)	1:78:A:GLU:HA	1:81:A:LYS:HG3	2	0.23	0.05	0.23
(2,4277)	1:16:A:ILE:HG22	1:158:A:GLU:HB2	2	0.23	0.09	0.23
(2,2004)	1:162:A:CYS:H	1:163:A:CYS:HA	2	0.22	0.05	0.22
(2,4543)	1:157:A:LYS:HB2	1:156:A:LEU:HD21	2	0.22	0.08	0.22
(2,3464)	1:152:A:TYR:HE1	1:20:A:LEU:HD12	2	0.22	0.02	0.22
(2,3464)	1:152:A:TYR:HE1	1:20:A:LEU:HD11	2	0.22	0.02	0.22
(2,1099)	1:22:A:GLN:HA	1:22:A:GLN:HG2	2	0.22	0.1	0.22
(2,195)	1:41:A:GLU:HG2	1:40:A:TRP:HE3	2	0.2	0.0	0.2
(2,1278)	1:54:A:LEU:HA	1:42:A:MET:HE1	2	0.2	0.08	0.2
(2,3436)	1:82:A:TYR:HD1	1:85:A:LEU:HD22	2	0.2	0.03	0.2
(2,3436)	1:82:A:TYR:HD1	1:85:A:LEU:HD21	2	0.2	0.03	0.2
(2,236)	1:25:A:LYS:HA	1:76:A:LEU:HD12	2	0.2	0.08	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,236)	1:25:A:LYS:HA	1:76:A:LEU:HD13	2	0.2	0.08	0.2
(2,2882)	1:158:A:GLU:H	1:157:A:LYS:HG3	2	0.2	0.04	0.2
(2,4781)	1:48:A:GLU:HG2	1:49:A:ILE:H	2	0.2	0.02	0.2
(2,4395)	1:48:A:GLU:HB3	1:48:A:GLU:HG3	2	0.19	0.06	0.19
(2,157)	1:80:A:GLU:HG2	1:21:A:LEU:HD23	2	0.18	0.02	0.18
(2,157)	1:80:A:GLU:HG2	1:21:A:LEU:HD22	2	0.18	0.02	0.18
(2,3100)	1:40:A:TRP:H	1:41:A:GLU:HB2	2	0.18	0.01	0.18
(2,2276)	1:190:A:VAL:H	1:188:A:MET:HA	2	0.18	0.05	0.18
(2,2279)	1:153:A:GLN:HE21	1:178:A:LEU:HA	2	0.18	0.03	0.18
(2,3983)	1:177:A:MET:HB2	1:178:A:LEU:H	2	0.18	0.0	0.18
(2,4427)	1:8:A:PHE:HB2	1:7:A:GLU:HB2	2	0.18	0.03	0.18
(2,4427)	1:8:A:PHE:HB2	1:7:A:GLU:HB3	2	0.18	0.03	0.18
(1,20)	1:23:A:THR:O	1:27:A:TYR:N	2	0.18	0.0	0.18
(2,886)	1:153:A:GLN:HB3	1:150:A:THR:HG23	2	0.18	0.03	0.18
(2,1427)	1:19:A:GLU:HA	1:22:A:GLN:HG3	2	0.18	0.04	0.18
(2,3492)	1:100:A:PHE:HE1	1:71:A:HIS:HE1	2	0.18	0.03	0.18
(2,4608)	1:28:A:VAL:H	1:29:A:ARG:HB3	2	0.16	0.04	0.16
(2,848)	1:143:A:ILE:HD12	1:146:A:VAL:HB	2	0.16	0.05	0.16
(2,1841)	1:158:A:GLU:H	1:158:A:GLU:HB3	2	0.16	0.01	0.16
(2,2468)	1:71:A:HIS:HA	1:76:A:LEU:H	2	0.16	0.01	0.16
(2,3975)	1:7:A:GLU:H	1:8:A:PHE:HA	2	0.15	0.02	0.15
(2,3006)	1:10:A:GLY:H	1:8:A:PHE:HA	2	0.15	0.0	0.15
(2,3376)	1:153:A:GLN:HE22	1:149:A:VAL:HG22	2	0.15	0.04	0.15
(2,3376)	1:153:A:GLN:HE22	1:149:A:VAL:HG23	2	0.15	0.04	0.15
(2,3391)	1:153:A:GLN:H	1:153:A:GLN:HB3	2	0.15	0.0	0.15
(2,4771)	1:124:A:PHE:HE2	1:43:A:THR:H	2	0.15	0.0	0.15
(2,1586)	1:154:A:LEU:HD12	1:150:A:THR:HA	2	0.14	0.03	0.14
(1,123)	1:154:A:LEU:O	1:158:A:GLU:H	2	0.14	0.02	0.14
(2,616)	1:28:A:VAL:HG11	1:72:A:ASN:HB2	2	0.14	0.02	0.14
(2,616)	1:28:A:VAL:HG13	1:72:A:ASN:HB2	2	0.14	0.02	0.14
(2,1355)	1:131:A:ARG:HG2	1:131:A:ARG:HD3	2	0.14	0.03	0.14
(2,2766)	1:131:A:ARG:HG2	1:131:A:ARG:H	2	0.14	0.03	0.14
(2,4419)	1:103:A:TYR:HB2	1:104:A:VAL:HG11	2	0.14	0.04	0.14
(2,4419)	1:103:A:TYR:HB2	1:104:A:VAL:HG13	2	0.14	0.04	0.14
(2,4579)	1:69:A:ASP:H	1:67:A:ILE:HG12	2	0.14	0.0	0.14
(1,12)	1:19:A:GLU:O	1:23:A:THR:N	2	0.14	0.02	0.14
(2,1341)	1:140:A:SER:HB3	1:140:A:SER:H	2	0.14	0.02	0.14
(2,3584)	1:40:A:TRP:HZ2	1:41:A:GLU:HA	2	0.14	0.02	0.14
(2,3812)	1:154:A:LEU:HB3	1:154:A:LEU:H	2	0.14	0.04	0.14
(2,465)	1:134:A:LEU:HD23	1:37:A:THR:HG23	2	0.13	0.01	0.13
(2,465)	1:134:A:LEU:HD22	1:37:A:THR:HG22	2	0.13	0.01	0.13
(2,1110)	1:184:A:ALA:HA	1:104:A:VAL:HG23	2	0.13	0.01	0.13

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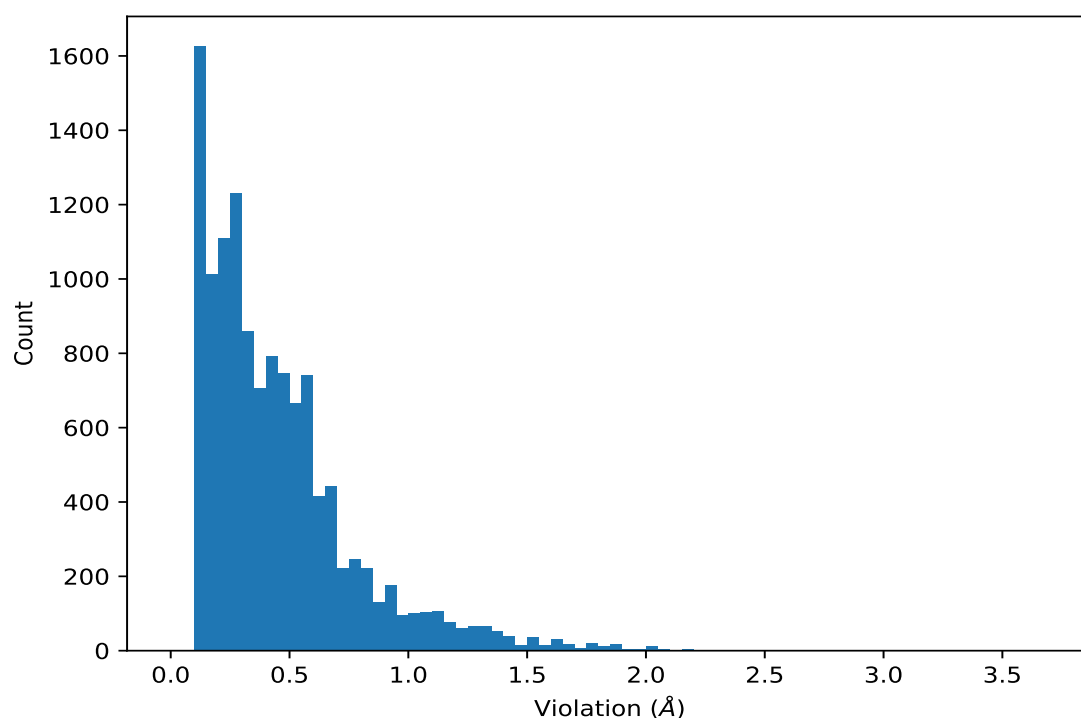
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1110)	1:184:A:ALA:HA	1:104:A:VAL:HG21	2	0.13	0.01	0.13
(2,1842)	1:158:A:GLU:H	1:158:A:GLU:HG3	2	0.13	0.01	0.13
(2,4198)	1:189:A:HIS:HD2	1:189:A:HIS:H	2	0.13	0.02	0.13
(2,206)	1:60:A:ILE:HA	1:113:A:SER:HG	2	0.12	0.02	0.12
(2,1486)	1:41:A:GLU:HG3	1:40:A:TRP:HZ3	2	0.12	0.01	0.12
(2,1829)	1:131:A:ARG:HE	1:131:A:ARG:HD2	2	0.12	0.02	0.12
(2,3058)	1:30:A:ASP:H	1:32:A:HIS:H	2	0.12	0.02	0.12
(2,1151)	1:43:A:THR:HA	1:39:A:LEU:HD22	2	0.12	0.02	0.12
(2,1672)	1:133:A:GLY:H	1:130:A:GLN:HG3	2	0.12	0.02	0.12
(2,1185)	1:97:A:ALA:HA	1:97:A:ALA:HB3	2	0.12	0.01	0.12
(2,1185)	1:97:A:ALA:HA	1:97:A:ALA:HB2	2	0.12	0.01	0.12
(2,2879)	1:157:A:LYS:HG3	1:157:A:LYS:H	2	0.12	0.01	0.12
(2,1638)	1:42:A:MET:H	1:124:A:PHE:HZ	2	0.12	0.02	0.12
(2,3341)	1:188:A:MET:H	1:185:A:ASN:HB2	2	0.12	0.02	0.12
(2,1830)	1:131:A:ARG:HE	1:128:A:ILE:HA	2	0.12	0.0	0.12
(2,4138)	1:100:A:PHE:HD1	1:97:A:ALA:H	2	0.12	0.0	0.12
(2,4344)	1:21:A:LEU:HD12	1:83:A:GLU:H	2	0.12	0.0	0.12
(2,4344)	1:21:A:LEU:HD11	1:83:A:GLU:H	2	0.12	0.0	0.12
(2,760)	1:36:A:GLU:HG2	1:32:A:HIS:HD2	2	0.11	0.0	0.11
(2,1579)	1:124:A:PHE:HB2	1:50:A:PRO:HG2	2	0.11	0.0	0.11
(2,1815)	1:139:A:SER:H	1:140:A:SER:HA	2	0.11	0.0	0.11
(2,2545)	1:89:A:VAL:HG21	1:88:A:ASP:H	2	0.11	0.0	0.11
(2,2545)	1:89:A:VAL:HG22	1:88:A:ASP:H	2	0.11	0.0	0.11
(2,4748)	1:106:A:TYR:HD1	1:110:A:LYS:HB2	2	0.11	0.01	0.11
(2,1461)	1:71:A:HIS:HA	1:67:A:ILE:HG21	2	0.11	0.0	0.11
(2,1461)	1:71:A:HIS:HA	1:67:A:ILE:HG22	2	0.11	0.0	0.11
(2,2366)	1:63:A:ASN:HA	1:64:A:ILE:H	2	0.11	0.0	0.11
(2,2005)	1:15:A:PHE:H	1:15:A:PHE:HA	2	0.1	0.0	0.1
(2,2752)	1:129:A:GLN:H	1:126:A:ASP:HA	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)
(2,1397)	1:188:A:MET:HE3	1:190:A:VAL:HG12	12	3.7
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG13	9	3.48
(2,1397)	1:188:A:MET:HE3	1:190:A:VAL:HG13	5	2.88
(2,505)	1:174:A:LEU:HD23	1:157:A:LYS:HE3	14	2.21
(2,505)	1:174:A:LEU:HD22	1:157:A:LYS:HE3	6	2.16
(2,682)	1:171:A:LYS:HG2	1:175:A:GLU:HG3	2	2.15
(2,505)	1:174:A:LEU:HD22	1:157:A:LYS:HE3	15	2.15
(2,505)	1:174:A:LEU:HD21	1:157:A:LYS:HE3	10	2.14
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD11	15	2.09
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD12	15	2.09
(2,707)	1:18:A:ALA:HB3	1:21:A:LEU:HD21	3	2.06
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD12	14	2.05
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG21	7	2.05
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG21	6	2.03
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG22	10	2.02
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD12	1	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD13	5	2.02
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD12	6	2.02
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD11	12	2.02
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD13	10	2.01
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD13	11	2.01
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG21	15	2.01
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD11	4	2.0
(2,4339)	1:134:A:LEU:HD23	1:129:A:GLN:HG3	12	1.99
(2,1569)	1:16:A:ILE:HD13	1:161:A:THR:HG21	2	1.98
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD12	13	1.96
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG23	10	1.96
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	3	1.95
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG23	12	1.94
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG21	14	1.94
(2,4549)	1:178:A:LEU:HD22	1:152:A:TYR:H	12	1.91
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG23	9	1.91
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	15	1.9
(2,707)	1:18:A:ALA:HB2	1:21:A:LEU:HD23	1	1.9
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD23	15	1.9
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD21	6	1.89
(2,4259)	1:31:A:LEU:HD21	1:106:A:TYR:HD2	13	1.88
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG22	4	1.87
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	1	1.87
(2,4259)	1:31:A:LEU:HD22	1:106:A:TYR:HD2	14	1.87
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG23	6	1.87
(2,707)	1:18:A:ALA:HB2	1:21:A:LEU:HD23	10	1.87
(2,707)	1:18:A:ALA:HB3	1:21:A:LEU:HD23	11	1.87
(2,4549)	1:178:A:LEU:HD21	1:152:A:TYR:H	10	1.86
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG22	11	1.86
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	9	1.86
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG23	9	1.86
(2,707)	1:18:A:ALA:HB3	1:21:A:LEU:HD23	7	1.86
(2,707)	1:18:A:ALA:HB2	1:21:A:LEU:HD22	12	1.85
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD21	14	1.85
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	6	1.84
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD23	5	1.84
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD21	13	1.84
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG21	11	1.83
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD22	8	1.83
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	4	1.82
(2,4259)	1:31:A:LEU:HD22	1:106:A:TYR:HD2	11	1.82
(2,586)	1:180:A:VAL:HG22	1:183:A:LYS:HG2	7	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	8	1.8
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD11	8	1.8
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG22	3	1.8
(2,586)	1:180:A:VAL:HG21	1:183:A:LYS:HG2	4	1.79
(2,4359)	1:104:A:VAL:HG11	1:103:A:TYR:HD2	12	1.78
(2,4259)	1:31:A:LEU:HD22	1:106:A:TYR:HD2	7	1.78
(2,4259)	1:31:A:LEU:HD23	1:106:A:TYR:HD2	10	1.78
(2,4259)	1:31:A:LEU:HD22	1:106:A:TYR:HD2	12	1.78
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	11	1.78
(2,82)	1:76:A:LEU:HD13	1:77:A:LYS:HE2	3	1.78
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	5	1.77
(2,4339)	1:134:A:LEU:HD22	1:129:A:GLN:HG3	3	1.77
(2,4259)	1:31:A:LEU:HD21	1:106:A:TYR:HD2	6	1.77
(2,707)	1:18:A:ALA:HB2	1:21:A:LEU:HD22	2	1.77
(2,707)	1:18:A:ALA:HB1	1:21:A:LEU:HD22	9	1.77
(2,586)	1:180:A:VAL:HG22	1:183:A:LYS:HG2	10	1.76
(2,586)	1:180:A:VAL:HG21	1:183:A:LYS:HG2	13	1.76
(2,4549)	1:178:A:LEU:HD23	1:152:A:TYR:H	7	1.75
(2,4549)	1:178:A:LEU:HD23	1:152:A:TYR:H	11	1.75
(2,4259)	1:31:A:LEU:HD22	1:106:A:TYR:HD2	5	1.75
(2,1882)	1:149:A:VAL:H	1:151:A:LYS:HB3	10	1.75
(2,1569)	1:16:A:ILE:HD13	1:161:A:THR:HG22	13	1.75
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD13	2	1.74
(2,1882)	1:149:A:VAL:H	1:151:A:LYS:HB3	9	1.74
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG22	6	1.74
(2,707)	1:18:A:ALA:HB3	1:21:A:LEU:HD21	4	1.74
(2,4359)	1:104:A:VAL:HG11	1:103:A:TYR:HD2	2	1.73
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG21	9	1.73
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD11	7	1.71
(2,421)	1:53:A:ILE:HD11	1:138:A:ILE:HD11	5	1.7
(2,96)	1:180:A:VAL:HG23	1:181:A:PRO:HB2	11	1.7
(2,96)	1:180:A:VAL:HG21	1:181:A:PRO:HB2	14	1.7
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	3	1.69
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	7	1.69
(2,96)	1:180:A:VAL:HG22	1:181:A:PRO:HB2	3	1.69
(2,96)	1:180:A:VAL:HG22	1:181:A:PRO:HB2	12	1.69
(2,96)	1:180:A:VAL:HG21	1:181:A:PRO:HB2	15	1.69
(2,421)	1:53:A:ILE:HD13	1:138:A:ILE:HD12	4	1.68
(2,96)	1:180:A:VAL:HG22	1:181:A:PRO:HB2	9	1.68
(2,52)	1:159:A:LEU:HD23	1:158:A:GLU:HB2	1	1.67
(2,4549)	1:178:A:LEU:HD21	1:152:A:TYR:H	6	1.66
(2,4549)	1:178:A:LEU:HD21	1:152:A:TYR:H	15	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	7	1.66
(2,1569)	1:16:A:ILE:HD13	1:161:A:THR:HG23	5	1.66
(2,96)	1:180:A:VAL:HG23	1:181:A:PRO:HB2	4	1.66
(2,96)	1:180:A:VAL:HG23	1:181:A:PRO:HB2	6	1.66
(2,96)	1:180:A:VAL:HG21	1:181:A:PRO:HB2	8	1.66
(2,4594)	1:148:A:ARG:H	1:144:A:LYS:HD2	10	1.65
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	1	1.65
(2,4328)	1:156:A:LEU:HD22	1:152:A:TYR:H	13	1.65
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD13	2	1.65
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	6	1.65
(2,4549)	1:178:A:LEU:HD23	1:152:A:TYR:H	14	1.64
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	9	1.64
(2,421)	1:53:A:ILE:HD13	1:138:A:ILE:HD12	10	1.64
(2,421)	1:53:A:ILE:HD13	1:138:A:ILE:HD12	11	1.64
(2,96)	1:180:A:VAL:HG23	1:181:A:PRO:HB2	5	1.64
(2,4549)	1:178:A:LEU:HD21	1:152:A:TYR:H	13	1.63
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD12	9	1.63
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	5	1.63
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG21	1	1.63
(2,1553)	1:63:A:ASN:HB2	1:66:A:GLU:H	5	1.63
(2,421)	1:53:A:ILE:HD11	1:138:A:ILE:HD13	8	1.63
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD13	12	1.63
(2,96)	1:180:A:VAL:HG21	1:181:A:PRO:HB2	10	1.63
(2,96)	1:180:A:VAL:HG23	1:181:A:PRO:HB2	13	1.63
(2,1882)	1:149:A:VAL:H	1:151:A:LYS:HB3	13	1.62
(2,505)	1:174:A:LEU:HD21	1:157:A:LYS:HE3	9	1.62
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	4	1.61
(2,4259)	1:31:A:LEU:HD22	1:106:A:TYR:HD2	2	1.61
(2,1882)	1:149:A:VAL:H	1:151:A:LYS:HB3	3	1.61
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD12	9	1.61
(2,96)	1:180:A:VAL:HG21	1:181:A:PRO:HB2	1	1.61
(2,96)	1:180:A:VAL:HG21	1:181:A:PRO:HB2	7	1.61
(2,4549)	1:178:A:LEU:HD21	1:152:A:TYR:H	1	1.6
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD11	7	1.6
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG21	14	1.6
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD12	14	1.6
(2,4359)	1:104:A:VAL:HG11	1:103:A:TYR:HD2	15	1.59
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD11	1	1.59
(2,421)	1:53:A:ILE:HD13	1:138:A:ILE:HD11	3	1.59
(2,52)	1:159:A:LEU:HD21	1:158:A:GLU:HB2	10	1.59
(2,4549)	1:178:A:LEU:HD22	1:152:A:TYR:H	2	1.58
(2,682)	1:171:A:LYS:HG2	1:175:A:GLU:HG3	11	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	6	1.58
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	7	1.58
(2,52)	1:159:A:LEU:HD21	1:158:A:GLU:HB2	15	1.58
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	7	1.57
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	10	1.57
(2,4359)	1:104:A:VAL:HG11	1:103:A:TYR:HD2	8	1.56
(2,4308)	1:106:A:TYR:HB3	1:184:A:ALA:HB3	15	1.56
(2,4260)	1:156:A:LEU:HD11	1:172:A:ASP:HB2	12	1.55
(2,682)	1:171:A:LYS:HG2	1:175:A:GLU:HG3	13	1.55
(2,343)	1:99:A:LYS:HD2	1:102:A:MET:HE3	10	1.55
(2,4260)	1:156:A:LEU:HD12	1:172:A:ASP:HB3	3	1.54
(2,4260)	1:156:A:LEU:HD11	1:172:A:ASP:HB2	8	1.54
(2,4018)	1:190:A:VAL:HG11	1:190:A:VAL:H	5	1.54
(2,4018)	1:190:A:VAL:HG11	1:190:A:VAL:H	12	1.54
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	2	1.54
(2,421)	1:53:A:ILE:HD11	1:138:A:ILE:HD12	13	1.54
(2,421)	1:53:A:ILE:HD12	1:138:A:ILE:HD13	15	1.54
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	13	1.53
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	10	1.53
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	1	1.53
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG21	4	1.53
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG23	15	1.53
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	4	1.53
(2,682)	1:171:A:LYS:HG2	1:175:A:GLU:HG3	5	1.53
(2,96)	1:180:A:VAL:HG23	1:181:A:PRO:HB2	2	1.53
(2,52)	1:159:A:LEU:HD21	1:158:A:GLU:HB2	3	1.53
(2,52)	1:159:A:LEU:HD21	1:158:A:GLU:HB2	4	1.53
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	8	1.53
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	12	1.53
(2,4339)	1:134:A:LEU:HD21	1:129:A:GLN:HG3	13	1.52
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	8	1.52
(2,586)	1:180:A:VAL:HG22	1:183:A:LYS:HG2	1	1.52
(2,4359)	1:104:A:VAL:HG12	1:103:A:TYR:HD2	10	1.51
(2,4260)	1:156:A:LEU:HD12	1:172:A:ASP:HB2	2	1.51
(2,4018)	1:190:A:VAL:HG11	1:190:A:VAL:H	9	1.51
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	7	1.51
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG22	11	1.51
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	4	1.51
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD22	2	1.5
(2,4689)	1:18:A:ALA:H	1:16:A:ILE:HD11	15	1.5
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	15	1.5
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	8	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,238)	1:69:A:ASP:HA	1:72:A:ASN:HD21	5	1.5
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	11	1.5
(2,52)	1:159:A:LEU:HD21	1:158:A:GLU:HB2	14	1.5
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	6	1.49
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	13	1.49
(2,4260)	1:156:A:LEU:HD13	1:172:A:ASP:HB2	4	1.49
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD23	7	1.48
(2,4447)	1:179:A:SER:HB3	1:182:A:LYS:HD3	14	1.48
(2,4359)	1:104:A:VAL:HG13	1:103:A:TYR:HD2	11	1.48
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	11	1.48
(2,421)	1:53:A:ILE:HD11	1:138:A:ILE:HD12	6	1.48
(2,3307)	1:31:A:LEU:H	1:29:A:ARG:HD3	12	1.47
(2,3233)	1:166:A:GLY:H	1:165:A:GLU:HB3	13	1.47
(2,1783)	1:94:A:VAL:H	1:169:A:GLU:HB3	3	1.47
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	13	1.46
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	9	1.46
(2,1569)	1:16:A:ILE:HD12	1:161:A:THR:HG23	8	1.46
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG21	11	1.46
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	7	1.46
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD21	3	1.45
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	1	1.45
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG22	8	1.45
(2,52)	1:159:A:LEU:HD21	1:158:A:GLU:HB2	9	1.45
(2,4695)	1:23:A:THR:H	1:21:A:LEU:HD13	2	1.44
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	11	1.44
(2,4308)	1:106:A:TYR:HB3	1:184:A:ALA:HB1	1	1.44
(2,4082)	1:130:A:GLN:H	1:130:A:GLN:HG3	12	1.44
(2,3722)	1:84:A:GLN:HG3	1:84:A:GLN:H	1	1.44
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	3	1.44
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	11	1.44
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	8	1.44
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	13	1.44
(2,4689)	1:18:A:ALA:H	1:16:A:ILE:HD12	12	1.43
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	9	1.43
(2,4262)	1:31:A:LEU:HD11	1:103:A:TYR:HE1	11	1.43
(2,4129)	1:84:A:GLN:HG3	1:83:A:GLU:H	1	1.43
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	9	1.43
(2,2990)	1:184:A:ALA:H	1:185:A:ASN:HB3	3	1.43
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	3	1.43
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	3	1.43
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	6	1.43
(2,393)	1:39:A:LEU:HD22	1:57:A:GLU:HB3	14	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	3	1.42
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD23	5	1.42
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	1	1.42
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG21	2	1.42
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	5	1.42
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	14	1.42
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	15	1.42
(2,1036)	1:140:A:SER:HB2	1:136:A:ASN:HB3	10	1.42
(2,830)	1:174:A:LEU:HD23	1:175:A:GLU:HG3	2	1.42
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG22	15	1.41
(2,4082)	1:130:A:GLN:H	1:130:A:GLN:HG3	1	1.41
(2,4082)	1:130:A:GLN:H	1:130:A:GLN:HG3	6	1.41
(2,2528)	1:87:A:GLU:HG2	1:87:A:GLU:H	6	1.41
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	2	1.41
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	11	1.41
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	12	1.41
(2,1569)	1:16:A:ILE:HD11	1:161:A:THR:HG22	4	1.41
(2,4749)	1:15:A:PHE:HD2	1:14:A:GLU:HG2	12	1.4
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	15	1.4
(2,3861)	1:143:A:ILE:HG22	1:147:A:GLN:HE22	1	1.4
(2,3307)	1:31:A:LEU:H	1:29:A:ARG:HD3	10	1.4
(2,2624)	1:102:A:MET:HG2	1:102:A:MET:H	11	1.4
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	7	1.4
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	14	1.4
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	2	1.4
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	5	1.39
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	12	1.39
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD21	14	1.39
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	6	1.39
(2,3379)	1:173:A:GLY:H	1:169:A:GLU:HB3	3	1.39
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	4	1.39
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	5	1.39
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	10	1.39
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	15	1.39
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	3	1.39
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG23	5	1.39
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	5	1.39
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	3	1.39
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	9	1.39
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	2	1.39
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	13	1.39
(2,4695)	1:23:A:THR:H	1:21:A:LEU:HD11	7	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	13	1.38
(2,4262)	1:31:A:LEU:HD13	1:103:A:TYR:HE1	9	1.38
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	4	1.38
(2,1887)	1:152:A:TYR:H	1:177:A:MET:HG2	14	1.38
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	8	1.38
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG23	14	1.38
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD21	14	1.37
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD23	10	1.37
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	13	1.37
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG21	2	1.37
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD23	1	1.36
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD21	4	1.36
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD21	6	1.36
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD21	13	1.36
(2,4549)	1:178:A:LEU:HD22	1:152:A:TYR:H	8	1.36
(2,4549)	1:178:A:LEU:HD22	1:152:A:TYR:H	9	1.36
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	6	1.36
(2,4260)	1:156:A:LEU:HD13	1:172:A:ASP:HB2	15	1.36
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG21	7	1.36
(2,1053)	1:140:A:SER:HB3	1:136:A:ASN:HB3	10	1.36
(2,340)	1:102:A:MET:HE2	1:99:A:LYS:HE3	6	1.36
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD22	8	1.35
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD22	9	1.35
(2,4549)	1:178:A:LEU:HD23	1:152:A:TYR:H	3	1.35
(2,3233)	1:166:A:GLY:H	1:165:A:GLU:HB3	4	1.35
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	5	1.35
(2,1438)	1:95:A:THR:HG22	1:97:A:ALA:HB2	7	1.35
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	1	1.35
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	6	1.34
(2,4052)	1:185:A:ASN:HB2	1:186:A:ASP:H	3	1.34
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	1	1.34
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG23	9	1.34
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	6	1.34
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	1	1.34
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	5	1.34
(2,340)	1:102:A:MET:HE2	1:99:A:LYS:HE3	5	1.34
(2,52)	1:159:A:LEU:HD22	1:158:A:GLU:HB2	5	1.34
(2,4534)	1:76:A:LEU:HD11	1:24:A:GLU:H	12	1.33
(2,4308)	1:106:A:TYR:HB3	1:184:A:ALA:HB2	11	1.33
(2,4260)	1:156:A:LEU:HD12	1:172:A:ASP:HB2	5	1.33
(2,4260)	1:156:A:LEU:HD13	1:172:A:ASP:HB2	14	1.33
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	15	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	10	1.33
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG21	10	1.33
(2,876)	1:97:A:ALA:HB2	1:98:A:ASP:HB2	10	1.33
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	2	1.33
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	6	1.33
(2,82)	1:76:A:LEU:HD13	1:77:A:LYS:HE2	2	1.33
(2,4549)	1:178:A:LEU:HD22	1:152:A:TYR:H	5	1.32
(2,4494)	1:35:A:LEU:HD13	1:67:A:ILE:H	10	1.32
(2,4494)	1:35:A:LEU:HD11	1:67:A:ILE:H	12	1.32
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG2	5	1.32
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG13	14	1.32
(2,4260)	1:156:A:LEU:HD13	1:172:A:ASP:HB2	7	1.32
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG23	2	1.32
(2,3307)	1:31:A:LEU:H	1:29:A:ARG:HD3	13	1.32
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	13	1.32
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	13	1.32
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	12	1.32
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	13	1.32
(2,4494)	1:35:A:LEU:HD11	1:67:A:ILE:H	8	1.31
(2,4494)	1:35:A:LEU:HD13	1:66:A:GLU:H	15	1.31
(2,4281)	1:177:A:MET:HE2	1:175:A:GLU:HA	14	1.31
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	2	1.31
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	3	1.31
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	9	1.31
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	10	1.31
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	11	1.31
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	6	1.31
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	10	1.31
(2,1887)	1:152:A:TYR:H	1:177:A:MET:HG2	1	1.31
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	2	1.31
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	2	1.31
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	9	1.31
(2,393)	1:39:A:LEU:HD23	1:57:A:GLU:HB3	3	1.31
(2,393)	1:39:A:LEU:HD22	1:57:A:GLU:HB3	15	1.31
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	12	1.3
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD23	3	1.3
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	5	1.3
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG2	3	1.3
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG11	13	1.3
(2,4260)	1:156:A:LEU:HD11	1:172:A:ASP:HB2	10	1.3
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	7	1.3
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	11	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	15	1.3
(2,2624)	1:102:A:MET:HG2	1:102:A:MET:H	4	1.3
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	14	1.3
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	15	1.3
(2,1335)	1:157:A:LYS:HA	1:157:A:LYS:HD3	11	1.3
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	3	1.3
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	11	1.3
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	12	1.3
(2,82)	1:76:A:LEU:HD13	1:77:A:LYS:HE2	5	1.3
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	1	1.29
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	10	1.29
(2,4281)	1:177:A:MET:HE1	1:175:A:GLU:HA	1	1.29
(2,4260)	1:156:A:LEU:HD12	1:172:A:ASP:HB2	11	1.29
(2,3861)	1:143:A:ILE:HG21	1:147:A:GLN:HE22	7	1.29
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	5	1.29
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	13	1.29
(2,2624)	1:102:A:MET:HG2	1:102:A:MET:H	14	1.29
(2,2310)	1:55:A:ASN:HB3	1:55:A:ASN:HD21	4	1.29
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG22	3	1.29
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG23	6	1.29
(2,1335)	1:157:A:LYS:HA	1:157:A:LYS:HD3	2	1.29
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	3	1.29
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	8	1.29
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	10	1.29
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD11	15	1.29
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD22	10	1.28
(2,4547)	1:102:A:MET:HE2	1:64:A:ILE:HA	3	1.28
(2,4336)	1:35:A:LEU:HD11	1:39:A:LEU:HB2	10	1.28
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	4	1.28
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	5	1.28
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	4	1.28
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	6	1.28
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	12	1.28
(2,2893)	1:161:A:THR:H	1:162:A:CYS:HB3	9	1.28
(2,1918)	1:182:A:LYS:HB2	1:183:A:LYS:H	13	1.28
(2,1781)	1:140:A:SER:H	1:136:A:ASN:HB3	10	1.28
(2,1438)	1:95:A:THR:HG21	1:97:A:ALA:HB2	6	1.28
(2,1438)	1:95:A:THR:HG22	1:97:A:ALA:HB2	14	1.28
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	7	1.28
(2,4594)	1:148:A:ARG:H	1:144:A:LYS:HD2	9	1.27
(2,4547)	1:102:A:MET:HE2	1:64:A:ILE:HA	14	1.27
(2,4507)	1:85:A:LEU:HD21	1:82:A:TYR:H	7	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	8	1.27
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	8	1.27
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	14	1.27
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG23	3	1.27
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	12	1.27
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	5	1.27
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	15	1.27
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	15	1.27
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD11	2	1.26
(2,4494)	1:35:A:LEU:HD13	1:67:A:ILE:H	14	1.26
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	2	1.26
(2,1438)	1:95:A:THR:HG21	1:97:A:ALA:HB2	12	1.26
(2,1056)	1:157:A:LYS:HG3	1:157:A:LYS:HA	2	1.26
(2,1056)	1:157:A:LYS:HG3	1:157:A:LYS:HA	11	1.26
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	10	1.26
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	2	1.26
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	4	1.26
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	13	1.26
(2,586)	1:180:A:VAL:HG21	1:183:A:LYS:HG2	2	1.26
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	11	1.26
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD21	15	1.25
(2,4552)	1:21:A:LEU:HD21	1:82:A:TYR:HE2	13	1.25
(2,4549)	1:178:A:LEU:HD23	1:152:A:TYR:H	4	1.25
(2,4494)	1:35:A:LEU:HD11	1:67:A:ILE:H	13	1.25
(2,3861)	1:143:A:ILE:HG21	1:147:A:GLN:HE22	12	1.25
(2,1456)	1:147:A:GLN:HG3	1:143:A:ILE:HG13	13	1.25
(2,896)	1:81:A:LYS:HE3	1:78:A:GLU:HA	5	1.25
(2,393)	1:39:A:LEU:HD22	1:57:A:GLU:HB3	1	1.25
(2,393)	1:39:A:LEU:HD23	1:57:A:GLU:HB3	8	1.25
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	2	1.25
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	8	1.25
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	9	1.25
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	10	1.25
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	13	1.25
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD21	7	1.24
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD12	9	1.24
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	9	1.24
(2,4507)	1:85:A:LEU:HD22	1:82:A:TYR:H	13	1.24
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG12	7	1.24
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD11	4	1.24
(2,3861)	1:143:A:ILE:HG23	1:147:A:GLN:HE22	9	1.24
(2,3141)	1:51:A:PRO:HG3	1:52:A:GLY:H	7	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	8	1.24
(2,1438)	1:95:A:THR:HG21	1:97:A:ALA:HB2	11	1.24
(2,850)	1:22:A:GLN:HG2	1:22:A:GLN:H	3	1.24
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	5	1.24
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD22	5	1.23
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD11	13	1.23
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	14	1.23
(2,4689)	1:18:A:ALA:H	1:21:A:LEU:HD23	11	1.23
(2,4552)	1:21:A:LEU:HD23	1:82:A:TYR:HE2	1	1.23
(2,4552)	1:21:A:LEU:HD23	1:82:A:TYR:HE2	10	1.23
(2,4507)	1:85:A:LEU:HD23	1:82:A:TYR:H	8	1.23
(2,4507)	1:85:A:LEU:HD21	1:88:A:ASP:H	11	1.23
(2,4494)	1:35:A:LEU:HD12	1:67:A:ILE:H	3	1.23
(2,4494)	1:35:A:LEU:HD12	1:66:A:GLU:H	11	1.23
(2,4359)	1:104:A:VAL:HG12	1:103:A:TYR:HD2	14	1.23
(2,4336)	1:35:A:LEU:HD12	1:39:A:LEU:HB2	12	1.23
(2,4260)	1:156:A:LEU:HD13	1:172:A:ASP:HB2	13	1.23
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	6	1.23
(2,876)	1:97:A:ALA:HB2	1:98:A:ASP:HB2	11	1.23
(2,795)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	14	1.23
(2,575)	1:89:A:VAL:HG13	1:93:A:PHE:HD2	10	1.23
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	1	1.23
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	3	1.23
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	7	1.23
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	4	1.22
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	5	1.22
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	3	1.22
(2,4507)	1:85:A:LEU:HD21	1:88:A:ASP:H	3	1.22
(2,4336)	1:35:A:LEU:HD12	1:39:A:LEU:HB2	13	1.22
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG13	5	1.22
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG13	15	1.22
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	1	1.22
(2,1593)	1:135:A:ALA:HB1	1:129:A:GLN:HE21	8	1.22
(2,1439)	1:102:A:MET:HE3	1:106:A:TYR:HD2	3	1.22
(2,1438)	1:95:A:THR:HG22	1:97:A:ALA:HB2	13	1.22
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	7	1.22
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	12	1.22
(2,916)	1:183:A:LYS:HE2	1:183:A:LYS:HA	6	1.22
(2,575)	1:89:A:VAL:HG12	1:93:A:PHE:HD2	12	1.22
(2,393)	1:39:A:LEU:HD21	1:57:A:GLU:HB3	2	1.22
(2,4552)	1:21:A:LEU:HD23	1:82:A:TYR:HE2	11	1.21
(2,4507)	1:85:A:LEU:HD22	1:88:A:ASP:H	1	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4507)	1:85:A:LEU:HD22	1:88:A:ASP:H	2	1.21
(2,4490)	1:152:A:TYR:HE1	1:79:A:LEU:HD23	6	1.21
(2,4336)	1:35:A:LEU:HD12	1:39:A:LEU:HB2	11	1.21
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	4	1.21
(2,4091)	1:36:A:GLU:H	1:36:A:GLU:HG3	6	1.21
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG22	9	1.21
(2,896)	1:81:A:LYS:HE3	1:78:A:GLU:HA	15	1.21
(2,876)	1:97:A:ALA:HB2	1:98:A:ASP:HB2	14	1.21
(2,575)	1:89:A:VAL:HG13	1:93:A:PHE:HD2	11	1.21
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	12	1.21
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	9	1.2
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD22	1	1.2
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	8	1.2
(2,4552)	1:21:A:LEU:HD23	1:82:A:TYR:HE2	5	1.2
(2,4494)	1:35:A:LEU:HD12	1:67:A:ILE:H	4	1.2
(2,4494)	1:35:A:LEU:HD11	1:66:A:GLU:H	5	1.2
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	6	1.2
(2,4091)	1:36:A:GLU:H	1:36:A:GLU:HG3	11	1.2
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD13	13	1.2
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	14	1.2
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	6	1.2
(2,1909)	1:177:A:MET:H	1:153:A:GLN:HG2	3	1.2
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG22	6	1.2
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB1	3	1.2
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG21	13	1.2
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	6	1.2
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD12	11	1.19
(2,4535)	1:174:A:LEU:HD23	1:173:A:GLY:HA3	2	1.19
(2,4515)	1:142:A:LEU:HD23	1:60:A:ILE:H	4	1.19
(2,4494)	1:35:A:LEU:HD13	1:66:A:GLU:H	2	1.19
(2,4336)	1:35:A:LEU:HD12	1:39:A:LEU:HB2	8	1.19
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	1	1.19
(2,1866)	1:146:A:VAL:HG12	1:143:A:ILE:H	13	1.19
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	6	1.19
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	9	1.19
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	11	1.19
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	6	1.19
(2,876)	1:97:A:ALA:HB2	1:98:A:ASP:HB2	6	1.19
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	14	1.19
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	3	1.18
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	13	1.18
(2,4535)	1:174:A:LEU:HD23	1:173:A:GLY:HA3	9	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4515)	1:142:A:LEU:HD22	1:60:A:ILE:H	5	1.18
(2,4494)	1:35:A:LEU:HD13	1:66:A:GLU:H	6	1.18
(2,4466)	1:98:A:ASP:HA	1:176:A:VAL:HB	2	1.18
(2,4260)	1:156:A:LEU:HD11	1:172:A:ASP:HB2	9	1.18
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	9	1.18
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG12	2	1.18
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	13	1.18
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB3	9	1.18
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB2	10	1.18
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	6	1.18
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD21	13	1.18
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	1	1.18
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	11	1.17
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD13	4	1.17
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	4	1.17
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	11	1.17
(2,4535)	1:174:A:LEU:HD22	1:173:A:GLY:HA3	11	1.17
(2,4507)	1:85:A:LEU:HD22	1:82:A:TYR:H	10	1.17
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG13	10	1.17
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	2	1.17
(2,4285)	1:97:A:ALA:HB2	1:172:A:ASP:HB3	3	1.17
(2,4280)	1:177:A:MET:HE3	1:174:A:LEU:H	5	1.17
(2,4280)	1:177:A:MET:HE2	1:174:A:LEU:H	11	1.17
(2,4172)	1:18:A:ALA:HB1	1:22:A:GLN:HE22	3	1.17
(2,1431)	1:95:A:THR:HG23	1:74:A:ILE:HG22	1	1.17
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG22	4	1.17
(2,1370)	1:176:A:VAL:HG21	1:100:A:PHE:HE1	13	1.17
(2,703)	1:18:A:ALA:HB1	1:15:A:PHE:HD1	1	1.17
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD13	9	1.17
(2,4705)	1:173:A:GLY:H	1:160:A:LEU:HD21	6	1.16
(2,4552)	1:21:A:LEU:HD21	1:82:A:TYR:HE2	4	1.16
(2,4515)	1:142:A:LEU:HD22	1:60:A:ILE:H	11	1.16
(2,4507)	1:85:A:LEU:HD21	1:82:A:TYR:H	14	1.16
(2,4494)	1:35:A:LEU:HD12	1:67:A:ILE:H	9	1.16
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	4	1.16
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	4	1.16
(2,4120)	1:7:A:GLU:HG3	1:7:A:GLU:H	15	1.16
(2,4022)	1:143:A:ILE:HD13	1:147:A:GLN:HE22	13	1.16
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	13	1.16
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	1	1.16
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG22	8	1.16
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG23	12	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1438)	1:95:A:THR:HG21	1:97:A:ALA:HB2	2	1.16
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	7	1.16
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	9	1.16
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	15	1.15
(2,4552)	1:21:A:LEU:HD23	1:82:A:TYR:HE2	15	1.15
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	13	1.15
(2,4522)	1:149:A:VAL:HG22	1:147:A:GLN:HA	1	1.15
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG11	15	1.15
(2,4281)	1:177:A:MET:HE1	1:175:A:GLU:HA	6	1.15
(2,4281)	1:177:A:MET:HE1	1:175:A:GLU:HA	12	1.15
(2,4120)	1:7:A:GLU:HG3	1:7:A:GLU:H	7	1.15
(2,2995)	1:185:A:ASN:HB3	1:185:A:ASN:H	3	1.15
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	3	1.15
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	4	1.15
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	2	1.15
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	10	1.15
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	4	1.15
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG23	3	1.15
(2,575)	1:89:A:VAL:HG12	1:93:A:PHE:HD2	3	1.15
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	9	1.15
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	4	1.15
(2,340)	1:102:A:MET:HE1	1:99:A:LYS:HE3	12	1.15
(2,4695)	1:23:A:THR:H	1:76:A:LEU:HG	6	1.14
(2,4552)	1:21:A:LEU:HD22	1:82:A:TYR:HE2	12	1.14
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	6	1.14
(2,4535)	1:174:A:LEU:HD23	1:173:A:GLY:HA3	1	1.14
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	6	1.14
(2,4535)	1:174:A:LEU:HD22	1:173:A:GLY:HA3	7	1.14
(2,4535)	1:174:A:LEU:HD22	1:173:A:GLY:HA3	10	1.14
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	12	1.14
(2,4507)	1:85:A:LEU:HD23	1:82:A:TYR:H	5	1.14
(2,4494)	1:35:A:LEU:HD12	1:67:A:ILE:H	7	1.14
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	7	1.14
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	9	1.14
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	6	1.14
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	7	1.14
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	7	1.14
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG22	15	1.14
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	14	1.14
(2,1335)	1:157:A:LYS:HA	1:157:A:LYS:HD3	13	1.14
(2,290)	1:172:A:ASP:HA	1:171:A:LYS:HB2	4	1.14
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	10	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	4	1.13
(2,4535)	1:174:A:LEU:HD22	1:173:A:GLY:HA3	14	1.13
(2,4515)	1:142:A:LEU:HD21	1:60:A:ILE:H	13	1.13
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG2	9	1.13
(2,4120)	1:7:A:GLU:HG3	1:7:A:GLU:H	1	1.13
(2,3861)	1:143:A:ILE:HG23	1:147:A:GLN:HE22	10	1.13
(2,3826)	1:175:A:GLU:H	1:175:A:GLU:HG3	2	1.13
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	9	1.13
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	11	1.13
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	11	1.13
(2,1909)	1:177:A:MET:H	1:153:A:GLN:HG2	7	1.13
(2,1431)	1:95:A:THR:HG22	1:74:A:ILE:HG21	7	1.13
(2,916)	1:183:A:LYS:HE2	1:183:A:LYS:HA	10	1.13
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD12	2	1.13
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	1	1.12
(2,4534)	1:76:A:LEU:HD13	1:73:A:ASN:H	3	1.12
(2,4515)	1:142:A:LEU:HD21	1:60:A:ILE:H	12	1.12
(2,4281)	1:177:A:MET:HE3	1:175:A:GLU:HA	3	1.12
(2,4263)	1:178:A:LEU:HD22	1:175:A:GLU:HG2	7	1.12
(2,4260)	1:156:A:LEU:HD13	1:172:A:ASP:HB2	6	1.12
(2,3928)	1:162:A:CYS:H	1:162:A:CYS:HB3	10	1.12
(2,2893)	1:161:A:THR:H	1:162:A:CYS:HB3	2	1.12
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	8	1.12
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	1	1.12
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	9	1.12
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG22	6	1.12
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG13	14	1.12
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	13	1.12
(2,601)	1:28:A:VAL:HG22	1:71:A:HIS:HB2	7	1.12
(2,154)	1:181:A:PRO:HG3	1:153:A:GLN:HE21	13	1.12
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD11	15	1.12
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD13	8	1.11
(2,4522)	1:149:A:VAL:HG23	1:147:A:GLN:HA	6	1.11
(2,4507)	1:85:A:LEU:HD23	1:82:A:TYR:H	15	1.11
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	2	1.11
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	3	1.11
(2,3861)	1:143:A:ILE:HG22	1:147:A:GLN:HE22	6	1.11
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	5	1.11
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	10	1.11
(2,1593)	1:135:A:ALA:HB3	1:129:A:GLN:HE21	14	1.11
(2,1370)	1:176:A:VAL:HG22	1:100:A:PHE:HE1	8	1.11
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD11	12	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,575)	1:89:A:VAL:HG12	1:93:A:PHE:HD2	2	1.11
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	4	1.11
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	14	1.11
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD21	5	1.11
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	8	1.1
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	14	1.1
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	15	1.1
(2,4534)	1:76:A:LEU:HD12	1:24:A:GLU:H	15	1.1
(2,4515)	1:142:A:LEU:HD22	1:60:A:ILE:H	10	1.1
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	14	1.1
(2,4291)	1:121:A:ALA:HB3	1:120:A:HIS:HD2	1	1.1
(2,4281)	1:177:A:MET:HE2	1:175:A:GLU:HA	11	1.1
(2,4171)	1:134:A:LEU:HD22	1:129:A:GLN:H	6	1.1
(2,3928)	1:162:A:CYS:H	1:162:A:CYS:HB3	9	1.1
(2,2996)	1:185:A:ASN:H	1:182:A:LYS:HD2	12	1.1
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	2	1.1
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	15	1.1
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	7	1.1
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	15	1.1
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	12	1.1
(2,896)	1:81:A:LYS:HE3	1:78:A:GLU:HA	2	1.1
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	15	1.1
(2,318)	1:20:A:LEU:HD21	1:152:A:TYR:HD1	1	1.1
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD11	1	1.1
(2,4552)	1:21:A:LEU:HD21	1:82:A:TYR:HE2	6	1.09
(2,4515)	1:142:A:LEU:HD21	1:60:A:ILE:H	8	1.09
(2,4515)	1:142:A:LEU:HD21	1:60:A:ILE:H	14	1.09
(2,4507)	1:85:A:LEU:HD21	1:82:A:TYR:H	9	1.09
(2,4308)	1:106:A:TYR:HB3	1:110:A:LYS:HG3	12	1.09
(2,4281)	1:177:A:MET:HE3	1:175:A:GLU:HA	7	1.09
(2,4263)	1:178:A:LEU:HD22	1:175:A:GLU:HG2	14	1.09
(2,3634)	1:12:A:LYS:H	1:11:A:ARG:HA	12	1.09
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	10	1.09
(2,2893)	1:161:A:THR:H	1:162:A:CYS:HB3	10	1.09
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	12	1.09
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	13	1.09
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	5	1.09
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	6	1.09
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	6	1.09
(2,1558)	1:20:A:LEU:HD21	1:89:A:VAL:HA	12	1.09
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG13	7	1.09
(2,1454)	1:103:A:TYR:HD1	1:149:A:VAL:HG11	13	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG23	8	1.09
(2,1397)	1:188:A:MET:HE3	1:190:A:VAL:HG13	15	1.09
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD23	2	1.09
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	10	1.09
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD22	10	1.09
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	6	1.08
(2,4552)	1:21:A:LEU:HD23	1:82:A:TYR:HE2	7	1.08
(2,4535)	1:174:A:LEU:HD21	1:173:A:GLY:HA3	8	1.08
(2,4494)	1:35:A:LEU:HD12	1:67:A:ILE:H	1	1.08
(2,4336)	1:35:A:LEU:HD11	1:39:A:LEU:HB2	14	1.08
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG12	10	1.08
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	14	1.08
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	13	1.08
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	1	1.08
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	8	1.08
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	7	1.08
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	9	1.08
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	15	1.08
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	12	1.08
(2,1370)	1:176:A:VAL:HG21	1:100:A:PHE:HE1	6	1.08
(2,1130)	1:183:A:LYS:HA	1:182:A:LYS:HD2	12	1.08
(2,335)	1:102:A:MET:HE2	1:71:A:HIS:HE1	3	1.08
(2,41)	1:31:A:LEU:HD13	1:67:A:ILE:HD13	9	1.08
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD11	13	1.08
(2,4692)	1:18:A:ALA:HB1	1:20:A:LEU:H	12	1.07
(2,4554)	1:146:A:VAL:HG22	1:110:A:LYS:HD3	4	1.07
(2,4552)	1:21:A:LEU:HD21	1:82:A:TYR:HE2	14	1.07
(2,4515)	1:142:A:LEU:HD23	1:60:A:ILE:H	2	1.07
(2,4490)	1:79:A:LEU:HD23	1:93:A:PHE:HZ	5	1.07
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	10	1.07
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG11	4	1.07
(2,4263)	1:178:A:LEU:HD21	1:175:A:GLU:HG2	2	1.07
(2,3117)	1:44:A:SER:H	1:44:A:SER:HB2	5	1.07
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	12	1.07
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	3	1.07
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG12	12	1.07
(2,1431)	1:95:A:THR:HG21	1:74:A:ILE:HG21	12	1.07
(2,1370)	1:176:A:VAL:HG23	1:100:A:PHE:HE2	4	1.07
(2,1370)	1:176:A:VAL:HG23	1:100:A:PHE:HE1	9	1.07
(2,776)	1:121:A:ALA:HB2	1:138:A:ILE:HD12	12	1.07
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD11	13	1.07
(2,575)	1:89:A:VAL:HG13	1:93:A:PHE:HD2	1	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,575)	1:89:A:VAL:HG13	1:93:A:PHE:HD2	5	1.07
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	9	1.07
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	13	1.07
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD23	6	1.07
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD21	11	1.07
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	13	1.07
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD23	13	1.07
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG3	5	1.06
(2,4552)	1:21:A:LEU:HD21	1:82:A:TYR:HE2	3	1.06
(2,4552)	1:21:A:LEU:HD22	1:82:A:TYR:HE2	9	1.06
(2,4515)	1:142:A:LEU:HD21	1:60:A:ILE:H	15	1.06
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	1	1.06
(2,4325)	1:188:A:MET:HE2	1:108:A:LYS:HE3	15	1.06
(2,4280)	1:177:A:MET:HE3	1:174:A:LEU:H	1	1.06
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD12	10	1.06
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	3	1.06
(2,2274)	1:189:A:HIS:H	1:188:A:MET:HB3	1	1.06
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	10	1.06
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	3	1.06
(2,1866)	1:146:A:VAL:HG13	1:143:A:ILE:H	6	1.06
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD12	8	1.06
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD23	12	1.06
(2,41)	1:31:A:LEU:HD12	1:67:A:ILE:HD12	4	1.06
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD12	10	1.06
(2,4522)	1:149:A:VAL:HG21	1:147:A:GLN:HA	15	1.05
(2,4490)	1:152:A:TYR:HE1	1:79:A:LEU:HD22	11	1.05
(2,4336)	1:35:A:LEU:HD11	1:39:A:LEU:HB2	5	1.05
(2,4291)	1:121:A:ALA:HB1	1:120:A:HIS:HD2	7	1.05
(2,4281)	1:177:A:MET:HE3	1:175:A:GLU:HA	5	1.05
(2,4260)	1:156:A:LEU:HD11	1:172:A:ASP:HB2	1	1.05
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD11	1	1.05
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	6	1.05
(2,2904)	1:166:A:GLY:H	1:167:A:LYS:H	9	1.05
(2,2717)	1:172:A:ASP:H	1:171:A:LYS:HB2	14	1.05
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	7	1.05
(2,1454)	1:103:A:TYR:HD1	1:149:A:VAL:HG11	9	1.05
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG13	11	1.05
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG23	7	1.05
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	13	1.05
(2,1335)	1:157:A:LYS:HA	1:157:A:LYS:HD3	1	1.05
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	15	1.05
(2,575)	1:89:A:VAL:HG11	1:93:A:PHE:HD2	8	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,575)	1:89:A:VAL:HG13	1:93:A:PHE:HD2	14	1.05
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD21	7	1.05
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	5	1.04
(2,4552)	1:21:A:LEU:HD22	1:82:A:TYR:HE2	8	1.04
(2,4535)	1:174:A:LEU:HD23	1:173:A:GLY:HA3	5	1.04
(2,4534)	1:76:A:LEU:HD11	1:24:A:GLU:H	11	1.04
(2,4291)	1:121:A:ALA:HB2	1:120:A:HIS:HD2	2	1.04
(2,4291)	1:121:A:ALA:HB2	1:120:A:HIS:HD2	4	1.04
(2,4285)	1:97:A:ALA:HB1	1:172:A:ASP:HB3	8	1.04
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD13	3	1.04
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	8	1.04
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	9	1.04
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	11	1.04
(2,1860)	1:136:A:ASN:H	1:129:A:GLN:HE22	12	1.04
(2,1370)	1:176:A:VAL:HG21	1:100:A:PHE:HE1	10	1.04
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD22	10	1.04
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	14	1.04
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD11	1	1.04
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	1	1.04
(2,436)	1:39:A:LEU:HD11	1:61:A:PHE:HD2	11	1.04
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD23	14	1.04
(2,4719)	1:78:A:GLU:H	1:74:A:ILE:HG13	2	1.03
(2,4554)	1:146:A:VAL:HG21	1:143:A:ILE:HG12	9	1.03
(2,4548)	1:49:A:ILE:HG22	1:55:A:ASN:HB3	9	1.03
(2,4515)	1:142:A:LEU:HD23	1:60:A:ILE:H	3	1.03
(2,4502)	1:14:A:GLU:HB3	1:15:A:PHE:HE2	1	1.03
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	3	1.03
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	8	1.03
(2,4336)	1:35:A:LEU:HD13	1:39:A:LEU:HB2	15	1.03
(2,4291)	1:121:A:ALA:HB2	1:120:A:HIS:HD2	5	1.03
(2,4291)	1:121:A:ALA:HB2	1:120:A:HIS:HD2	8	1.03
(2,4291)	1:121:A:ALA:HB1	1:120:A:HIS:HD2	12	1.03
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	2	1.03
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	11	1.03
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	14	1.03
(2,1438)	1:95:A:THR:HG22	1:97:A:ALA:HB2	5	1.03
(2,1438)	1:95:A:THR:HG22	1:97:A:ALA:HB1	15	1.03
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	4	1.03
(2,1370)	1:176:A:VAL:HG22	1:100:A:PHE:HE1	11	1.03
(2,916)	1:183:A:LYS:HE2	1:183:A:LYS:HA	2	1.03
(2,776)	1:121:A:ALA:HB2	1:138:A:ILE:HD13	7	1.03
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	8	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD23	12	1.03
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD22	8	1.03
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD12	8	1.03
(2,4692)	1:18:A:ALA:HB2	1:20:A:LEU:H	4	1.02
(2,4548)	1:49:A:ILE:HG21	1:55:A:ASN:HB3	14	1.02
(2,4534)	1:76:A:LEU:HD11	1:73:A:ASN:H	13	1.02
(2,4291)	1:121:A:ALA:HB3	1:120:A:HIS:HD2	3	1.02
(2,4280)	1:177:A:MET:HE3	1:174:A:LEU:H	3	1.02
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	12	1.02
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD13	14	1.02
(2,2893)	1:161:A:THR:H	1:162:A:CYS:HB3	14	1.02
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	6	1.02
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	10	1.02
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	4	1.02
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	14	1.02
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG22	1	1.02
(2,1370)	1:176:A:VAL:HG23	1:100:A:PHE:HE2	1	1.02
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	3	1.02
(2,4692)	1:18:A:ALA:HB2	1:20:A:LEU:H	11	1.01
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	13	1.01
(2,4548)	1:49:A:ILE:HG23	1:55:A:ASN:HB3	8	1.01
(2,4548)	1:49:A:ILE:HG21	1:55:A:ASN:HB3	10	1.01
(2,4534)	1:76:A:LEU:HD12	1:24:A:GLU:H	8	1.01
(2,4515)	1:142:A:LEU:HD23	1:60:A:ILE:H	7	1.01
(2,4291)	1:121:A:ALA:HB1	1:120:A:HIS:HD2	15	1.01
(2,4280)	1:177:A:MET:HE3	1:174:A:LEU:H	7	1.01
(2,3117)	1:44:A:SER:H	1:44:A:SER:HB2	15	1.01
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	6	1.01
(2,1651)	1:120:A:HIS:H	1:52:A:GLY:HA3	7	1.01
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	10	1.01
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	12	1.01
(2,913)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	2	1.01
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD11	4	1.01
(2,601)	1:28:A:VAL:HG21	1:71:A:HIS:HB2	15	1.01
(2,82)	1:76:A:LEU:HD13	1:77:A:LYS:HE2	6	1.01
(2,4705)	1:173:A:GLY:H	1:170:A:LEU:HD11	12	1.0
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	8	1.0
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD13	12	1.0
(2,4548)	1:49:A:ILE:HG23	1:55:A:ASN:HB3	13	1.0
(2,4515)	1:142:A:LEU:HD22	1:60:A:ILE:H	1	1.0
(2,4515)	1:142:A:LEU:HD22	1:60:A:ILE:H	9	1.0
(2,4507)	1:85:A:LEU:HD23	1:88:A:ASP:H	12	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4281)	1:177:A:MET:HE1	1:175:A:GLU:HA	4	1.0
(2,4281)	1:177:A:MET:HE2	1:175:A:GLU:HA	8	1.0
(2,4281)	1:177:A:MET:HE1	1:175:A:GLU:HA	15	1.0
(2,3962)	1:135:A:ALA:HB1	1:137:A:SER:H	10	1.0
(2,3618)	1:93:A:PHE:HE2	1:79:A:LEU:HD11	5	1.0
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD13	6	1.0
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	5	1.0
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	1	1.0
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	10	1.0
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	4	1.0
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	13	1.0
(2,1860)	1:136:A:ASN:H	1:129:A:GLN:HE22	3	1.0
(2,1833)	1:13:A:LYS:H	1:13:A:LYS:HB2	6	1.0
(2,393)	1:39:A:LEU:HD23	1:57:A:GLU:HB3	7	1.0
(2,196)	1:41:A:GLU:HG2	1:128:A:ILE:HD13	9	1.0
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD23	1	1.0
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD21	4	1.0
(2,41)	1:31:A:LEU:HD11	1:67:A:ILE:HD12	11	1.0
(2,4692)	1:18:A:ALA:HB2	1:20:A:LEU:H	3	0.99
(2,4692)	1:18:A:ALA:HB1	1:20:A:LEU:H	10	0.99
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	9	0.99
(2,4548)	1:49:A:ILE:HG22	1:55:A:ASN:HB3	3	0.99
(2,4548)	1:49:A:ILE:HG23	1:55:A:ASN:HB3	12	0.99
(2,4534)	1:76:A:LEU:HD13	1:24:A:GLU:H	9	0.99
(2,4522)	1:149:A:VAL:HG22	1:147:A:GLN:HA	3	0.99
(2,4522)	1:149:A:VAL:HG22	1:147:A:GLN:HA	9	0.99
(2,4490)	1:79:A:LEU:HD23	1:93:A:PHE:HZ	9	0.99
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG13	11	0.99
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG12	12	0.99
(2,4291)	1:121:A:ALA:HB3	1:120:A:HIS:HD2	10	0.99
(2,4263)	1:178:A:LEU:HD22	1:175:A:GLU:HG2	3	0.99
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD23	5	0.99
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	7	0.99
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	3	0.99
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	9	0.99
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	2	0.99
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	5	0.99
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	5	0.99
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD11	3	0.99
(2,539)	1:54:A:LEU:HD23	1:55:A:ASN:HB2	4	0.99
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD23	13	0.99
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	14	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4554)	1:146:A:VAL:HG23	1:110:A:LYS:HD3	14	0.98
(2,4534)	1:76:A:LEU:HD11	1:24:A:GLU:H	1	0.98
(2,4515)	1:142:A:LEU:HD23	1:60:A:ILE:H	6	0.98
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	14	0.98
(2,4295)	1:87:A:GLU:HB2	1:85:A:LEU:HD13	1	0.98
(2,4291)	1:121:A:ALA:HB2	1:120:A:HIS:HD2	13	0.98
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	12	0.98
(2,4281)	1:177:A:MET:HE2	1:181:A:PRO:HD3	9	0.98
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	15	0.98
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD12	15	0.98
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD13	3	0.98
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD11	4	0.98
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD11	10	0.98
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	11	0.98
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	4	0.98
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	9	0.98
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG12	1	0.98
(2,1370)	1:176:A:VAL:HG23	1:100:A:PHE:HE1	15	0.98
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	2	0.98
(2,916)	1:183:A:LYS:HE2	1:183:A:LYS:HA	7	0.98
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD12	10	0.98
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD12	13	0.98
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD21	2	0.98
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD22	9	0.98
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	6	0.97
(2,4692)	1:18:A:ALA:HB2	1:20:A:LEU:H	7	0.97
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	15	0.97
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	2	0.97
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD11	3	0.97
(2,4534)	1:76:A:LEU:HD13	1:24:A:GLU:H	10	0.97
(2,4530)	1:60:A:ILE:HG22	1:57:A:GLU:HG2	7	0.97
(2,4489)	1:184:A:ALA:HB3	1:108:A:LYS:HE3	11	0.97
(2,3618)	1:93:A:PHE:HE2	1:79:A:LEU:HD11	8	0.97
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	14	0.97
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	10	0.97
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	15	0.97
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	12	0.97
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG12	15	0.97
(2,1885)	1:150:A:THR:H	1:151:A:LYS:HB3	13	0.97
(2,1455)	1:147:A:GLN:HG3	1:143:A:ILE:HG12	13	0.97
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG21	11	0.97
(2,1370)	1:176:A:VAL:HG22	1:100:A:PHE:HE1	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	1	0.97
(2,776)	1:121:A:ALA:HB2	1:138:A:ILE:HD12	11	0.97
(2,436)	1:39:A:LEU:HD11	1:61:A:PHE:HD2	4	0.97
(2,201)	1:99:A:LYS:HE2	1:96:A:TRP:HZ3	9	0.97
(2,137)	1:81:A:LYS:HD2	1:81:A:LYS:HA	2	0.97
(2,4692)	1:18:A:ALA:HB1	1:20:A:LEU:H	1	0.96
(2,4534)	1:76:A:LEU:HD11	1:24:A:GLU:H	4	0.96
(2,4516)	1:138:A:ILE:HD13	1:39:A:LEU:H	11	0.96
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	7	0.96
(2,4291)	1:121:A:ALA:HB3	1:120:A:HIS:HD2	9	0.96
(2,4280)	1:177:A:MET:HE2	1:174:A:LEU:H	8	0.96
(2,4280)	1:177:A:MET:HE2	1:174:A:LEU:H	13	0.96
(2,4263)	1:178:A:LEU:HD21	1:175:A:GLU:HG2	8	0.96
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	13	0.96
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	2	0.96
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	12	0.96
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	8	0.96
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	9	0.96
(2,1833)	1:13:A:LYS:H	1:13:A:LYS:HB2	2	0.96
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG23	2	0.96
(2,1397)	1:188:A:MET:HE1	1:190:A:VAL:HG12	11	0.96
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	3	0.96
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	11	0.96
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	6	0.96
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	10	0.96
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD13	5	0.96
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD12	4	0.96
(2,586)	1:180:A:VAL:HG21	1:183:A:LYS:HG2	6	0.96
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	9	0.96
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD13	6	0.95
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD13	14	0.95
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD13	15	0.95
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	11	0.95
(2,4522)	1:149:A:VAL:HG22	1:147:A:GLN:HA	8	0.95
(2,4490)	1:79:A:LEU:HD23	1:93:A:PHE:HZ	2	0.95
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	4	0.95
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG12	1	0.95
(2,4322)	1:20:A:LEU:HD13	1:152:A:TYR:H	10	0.95
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	8	0.95
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	14	0.95
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	9	0.95
(2,3860)	1:149:A:VAL:HG13	1:153:A:GLN:HE21	13	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD12	9	0.95
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG21	3	0.95
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	8	0.95
(2,2604)	1:98:A:ASP:HB2	1:98:A:ASP:H	15	0.95
(2,2492)	1:80:A:GLU:H	1:77:A:LYS:HA	7	0.95
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	1	0.95
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	8	0.95
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	14	0.95
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	2	0.95
(2,1953)	1:141:A:TYR:HE1	1:30:A:ASP:H	11	0.95
(2,1828)	1:131:A:ARG:HE	1:47:A:GLU:HG3	3	0.95
(2,1454)	1:103:A:TYR:HD1	1:149:A:VAL:HG12	3	0.95
(2,1438)	1:95:A:THR:HG21	1:97:A:ALA:HB3	4	0.95
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD11	14	0.95
(2,874)	1:188:A:MET:HG3	1:108:A:LYS:HG2	12	0.95
(2,601)	1:28:A:VAL:HG22	1:71:A:HIS:HB2	12	0.95
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD12	10	0.95
(2,509)	1:174:A:LEU:HD21	1:156:A:LEU:HD23	5	0.95
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD12	13	0.95
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	2	0.95
(2,201)	1:99:A:LYS:HE2	1:96:A:TRP:HZ3	13	0.95
(2,4692)	1:18:A:ALA:HB1	1:20:A:LEU:H	2	0.94
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD23	13	0.94
(2,4552)	1:21:A:LEU:HD22	1:82:A:TYR:HE2	2	0.94
(2,4489)	1:184:A:ALA:HB2	1:108:A:LYS:HE3	9	0.94
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG11	9	0.94
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	15	0.94
(2,4171)	1:134:A:LEU:HD22	1:129:A:GLN:H	7	0.94
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	10	0.94
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD12	11	0.94
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD12	15	0.94
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	15	0.94
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	7	0.94
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	2	0.94
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	14	0.94
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB2	1	0.94
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	9	0.94
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	5	0.94
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	3	0.94
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD12	8	0.94
(2,703)	1:18:A:ALA:HB1	1:15:A:PHE:HD1	12	0.94
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD23	12	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD22	15	0.94
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	5	0.93
(2,4522)	1:149:A:VAL:HG21	1:147:A:GLN:HA	4	0.93
(2,4507)	1:85:A:LEU:HD22	1:82:A:TYR:H	4	0.93
(2,4507)	1:85:A:LEU:HD23	1:82:A:TYR:H	6	0.93
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG13	6	0.93
(2,4285)	1:97:A:ALA:HB1	1:172:A:ASP:HB3	15	0.93
(2,4281)	1:177:A:MET:HE2	1:175:A:GLU:HA	13	0.93
(2,4280)	1:177:A:MET:HE3	1:174:A:LEU:H	10	0.93
(2,4263)	1:178:A:LEU:HD21	1:175:A:GLU:HG2	9	0.93
(2,4263)	1:178:A:LEU:HD22	1:175:A:GLU:HG2	11	0.93
(2,3962)	1:135:A:ALA:HB3	1:137:A:SER:H	14	0.93
(2,2895)	1:164:A:GLU:H	1:163:A:CYS:HB2	5	0.93
(2,2506)	1:83:A:GLU:H	1:83:A:GLU:HG3	12	0.93
(2,1885)	1:150:A:THR:H	1:151:A:LYS:HB3	9	0.93
(2,1885)	1:150:A:THR:H	1:151:A:LYS:HB3	10	0.93
(2,1682)	1:153:A:GLN:HE21	1:181:A:PRO:HD3	13	0.93
(2,1558)	1:20:A:LEU:HD23	1:89:A:VAL:HA	8	0.93
(2,1438)	1:95:A:THR:HG23	1:97:A:ALA:HB1	8	0.93
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD21	6	0.93
(2,666)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	3	0.93
(2,436)	1:39:A:LEU:HD11	1:61:A:PHE:HD2	6	0.93
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	8	0.93
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	15	0.93
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	8	0.93
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD23	3	0.93
(2,41)	1:31:A:LEU:HD12	1:67:A:ILE:HD11	7	0.93
(2,4554)	1:146:A:VAL:HG22	1:110:A:LYS:HD3	13	0.92
(2,4548)	1:49:A:ILE:HG22	1:38:A:TYR:HB3	11	0.92
(2,4534)	1:76:A:LEU:HD13	1:73:A:ASN:H	2	0.92
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG3	4	0.92
(2,4522)	1:149:A:VAL:HG21	1:147:A:GLN:HA	2	0.92
(2,4522)	1:149:A:VAL:HG21	1:147:A:GLN:HA	11	0.92
(2,4522)	1:149:A:VAL:HG22	1:147:A:GLN:HA	14	0.92
(2,4490)	1:79:A:LEU:HD22	1:93:A:PHE:HZ	14	0.92
(2,4322)	1:20:A:LEU:HD11	1:152:A:TYR:H	1	0.92
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	11	0.92
(2,4291)	1:121:A:ALA:HB3	1:120:A:HIS:HD2	14	0.92
(2,4285)	1:97:A:ALA:HB2	1:172:A:ASP:HB3	5	0.92
(2,4285)	1:97:A:ALA:HB2	1:172:A:ASP:HB3	7	0.92
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	2	0.92
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	9	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4100)	1:44:A:SER:HB2	1:43:A:THR:H	5	0.92
(2,3962)	1:135:A:ALA:HB1	1:137:A:SER:H	3	0.92
(2,3962)	1:135:A:ALA:HB1	1:137:A:SER:H	4	0.92
(2,3928)	1:162:A:CYS:H	1:162:A:CYS:HB3	8	0.92
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD13	6	0.92
(2,3622)	1:4:A:GLY:HA2	1:5:A:SER:H	2	0.92
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	4	0.92
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	5	0.92
(2,1592)	1:135:A:ALA:HB3	1:129:A:GLN:HE22	8	0.92
(2,1420)	1:117:A:ILE:HG13	1:60:A:ILE:HG23	13	0.92
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	6	0.92
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	13	0.92
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG21	2	0.92
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	10	0.92
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	5	0.92
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	14	0.92
(2,201)	1:99:A:LYS:HE2	1:96:A:TRP:HZ3	6	0.92
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD11	11	0.91
(2,4548)	1:49:A:ILE:HG21	1:55:A:ASN:HB3	5	0.91
(2,4548)	1:49:A:ILE:HG21	1:38:A:TYR:HB3	6	0.91
(2,4522)	1:149:A:VAL:HG21	1:147:A:GLN:HA	7	0.91
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	12	0.91
(2,4490)	1:79:A:LEU:HD22	1:93:A:PHE:HZ	1	0.91
(2,4285)	1:97:A:ALA:HB2	1:172:A:ASP:HB3	2	0.91
(2,4281)	1:177:A:MET:HE1	1:181:A:PRO:HD3	10	0.91
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	4	0.91
(2,3962)	1:135:A:ALA:HB2	1:137:A:SER:H	6	0.91
(2,3962)	1:135:A:ALA:HB1	1:137:A:SER:H	11	0.91
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG21	15	0.91
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG21	14	0.91
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	8	0.91
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	13	0.91
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD11	15	0.91
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	3	0.91
(2,1885)	1:150:A:THR:H	1:151:A:LYS:HB3	3	0.91
(2,1866)	1:146:A:VAL:HG13	1:143:A:ILE:H	5	0.91
(2,1866)	1:146:A:VAL:HG13	1:143:A:ILE:H	9	0.91
(2,1593)	1:135:A:ALA:HB1	1:129:A:GLN:HE21	15	0.91
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	14	0.91
(2,1397)	1:188:A:MET:HE1	1:190:A:VAL:HG13	13	0.91
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD12	9	0.91
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD11	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,509)	1:174:A:LEU:HD21	1:156:A:LEU:HD22	1	0.91
(2,509)	1:174:A:LEU:HD23	1:156:A:LEU:HD23	7	0.91
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	14	0.91
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD21	5	0.91
(2,41)	1:31:A:LEU:HD13	1:67:A:ILE:HD11	12	0.91
(2,4749)	1:15:A:PHE:HD2	1:14:A:GLU:HG2	1	0.9
(2,4692)	1:18:A:ALA:HB3	1:20:A:LEU:H	9	0.9
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD11	1	0.9
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	3	0.9
(2,4522)	1:149:A:VAL:HG22	1:147:A:GLN:HA	5	0.9
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG12	3	0.9
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG13	8	0.9
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG12	11	0.9
(2,4291)	1:121:A:ALA:HB1	1:120:A:HIS:HD2	11	0.9
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	10	0.9
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	13	0.9
(2,4171)	1:134:A:LEU:HD22	1:129:A:GLN:H	11	0.9
(2,3962)	1:135:A:ALA:HB1	1:137:A:SER:H	5	0.9
(2,3962)	1:135:A:ALA:HB1	1:137:A:SER:H	8	0.9
(2,3962)	1:135:A:ALA:HB2	1:137:A:SER:H	12	0.9
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	6	0.9
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	8	0.9
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	1	0.9
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	3	0.9
(2,3285)	1:167:A:LYS:H	1:170:A:LEU:HD21	8	0.9
(2,1866)	1:146:A:VAL:HG13	1:143:A:ILE:H	10	0.9
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG21	1	0.9
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	13	0.9
(2,1592)	1:135:A:ALA:HB3	1:129:A:GLN:HE22	4	0.9
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG11	14	0.9
(2,1370)	1:176:A:VAL:HG21	1:100:A:PHE:HE1	12	0.9
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	4	0.9
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD22	9	0.9
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	4	0.9
(2,436)	1:39:A:LEU:HD12	1:61:A:PHE:HD2	13	0.9
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	4	0.9
(2,41)	1:31:A:LEU:HD12	1:67:A:ILE:HD11	3	0.9
(2,4548)	1:49:A:ILE:HG23	1:55:A:ASN:HB3	7	0.89
(2,4547)	1:102:A:MET:HE2	1:64:A:ILE:HA	9	0.89
(2,4534)	1:76:A:LEU:HD11	1:24:A:GLU:H	5	0.89
(2,4490)	1:79:A:LEU:HD23	1:93:A:PHE:HZ	8	0.89
(2,4328)	1:156:A:LEU:HD22	1:155:A:LEU:H	4	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4195)	1:18:A:ALA:HB1	1:21:A:LEU:H	11	0.89
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	12	0.89
(2,3962)	1:135:A:ALA:HB3	1:137:A:SER:H	2	0.89
(2,3962)	1:135:A:ALA:HB2	1:137:A:SER:H	13	0.89
(2,3618)	1:93:A:PHE:HE2	1:79:A:LEU:HD11	2	0.89
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG22	8	0.89
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG21	15	0.89
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	10	0.89
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	15	0.89
(2,2373)	1:99:A:LYS:HD2	1:99:A:LYS:H	10	0.89
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	5	0.89
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG13	14	0.89
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	2	0.89
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG23	2	0.89
(2,1593)	1:135:A:ALA:HB1	1:129:A:GLN:HE21	13	0.89
(2,1558)	1:20:A:LEU:HD21	1:89:A:VAL:HA	9	0.89
(2,1370)	1:176:A:VAL:HG22	1:100:A:PHE:HE1	3	0.89
(2,1370)	1:176:A:VAL:HG23	1:100:A:PHE:HE1	7	0.89
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD21	13	0.89
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD13	6	0.89
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD12	9	0.89
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD12	11	0.89
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG23	7	0.89
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	7	0.89
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	5	0.89
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	7	0.89
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	12	0.89
(2,201)	1:99:A:LYS:HE2	1:96:A:TRP:HZ3	5	0.89
(2,4755)	1:124:A:PHE:HE2	1:50:A:PRO:HG2	8	0.88
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	4	0.88
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	10	0.88
(2,4456)	1:43:A:THR:HB	1:57:A:GLU:HG3	7	0.88
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	2	0.88
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	6	0.88
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	14	0.88
(2,3962)	1:135:A:ALA:HB3	1:137:A:SER:H	1	0.88
(2,3962)	1:135:A:ALA:HB3	1:137:A:SER:H	7	0.88
(2,3618)	1:93:A:PHE:HE2	1:79:A:LEU:HD11	12	0.88
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	2	0.88
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	14	0.88
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	4	0.88
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	13	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	3	0.88
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	13	0.88
(2,1866)	1:146:A:VAL:HG13	1:143:A:ILE:H	7	0.88
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	4	0.88
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	8	0.88
(2,1562)	1:13:A:LYS:HB3	1:13:A:LYS:H	11	0.88
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG11	15	0.88
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG23	5	0.88
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	6	0.88
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	9	0.88
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD13	2	0.88
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD13	10	0.88
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	10	0.88
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	15	0.88
(2,4548)	1:49:A:ILE:HG23	1:55:A:ASN:HB3	2	0.87
(2,4534)	1:76:A:LEU:HD11	1:24:A:GLU:H	6	0.87
(2,4522)	1:149:A:VAL:HG23	1:147:A:GLN:HA	13	0.87
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG22	2	0.87
(2,4291)	1:121:A:ALA:HB2	1:120:A:HIS:HD2	6	0.87
(2,4171)	1:134:A:LEU:HD22	1:129:A:GLN:H	14	0.87
(2,3962)	1:135:A:ALA:HB2	1:137:A:SER:H	9	0.87
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG23	12	0.87
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	3	0.87
(2,2939)	1:178:A:LEU:HD13	1:177:A:MET:H	3	0.87
(2,2939)	1:178:A:LEU:HD13	1:177:A:MET:H	5	0.87
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	2	0.87
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	11	0.87
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG11	13	0.87
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG23	4	0.87
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG21	9	0.87
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG22	15	0.87
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	15	0.87
(2,1263)	1:42:A:MET:HE1	1:39:A:LEU:HD22	14	0.87
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD22	15	0.87
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG22	3	0.87
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG23	6	0.87
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG21	9	0.87
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG22	11	0.87
(2,1144)	1:164:A:GLU:HA	1:163:A:CYS:HB3	5	0.87
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD11	5	0.87
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD11	8	0.87
(2,876)	1:97:A:ALA:HB2	1:98:A:ASP:HB2	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD12	14	0.87
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	5	0.87
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	12	0.87
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	13	0.87
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD12	6	0.87
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	6	0.87
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	13	0.87
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD22	7	0.87
(2,41)	1:31:A:LEU:HD13	1:67:A:ILE:HD11	6	0.87
(2,29)	1:35:A:LEU:HD13	1:33:A:GLU:H	11	0.87
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	12	0.86
(2,4548)	1:49:A:ILE:HG22	1:38:A:TYR:HB3	1	0.86
(2,4548)	1:49:A:ILE:HG22	1:38:A:TYR:HB3	15	0.86
(2,4492)	1:79:A:LEU:HD21	1:25:A:LYS:HG3	2	0.86
(2,4489)	1:184:A:ALA:HB1	1:108:A:LYS:HE3	15	0.86
(2,4423)	1:54:A:LEU:HD13	1:56:A:LYS:HE3	13	0.86
(2,4171)	1:134:A:LEU:HD23	1:129:A:GLN:H	13	0.86
(2,3962)	1:135:A:ALA:HB2	1:137:A:SER:H	15	0.86
(2,3622)	1:4:A:GLY:HA2	1:5:A:SER:H	14	0.86
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD23	2	0.86
(2,3602)	1:96:A:TRP:HZ3	1:99:A:LYS:HD2	10	0.86
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD11	9	0.86
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	6	0.86
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG13	10	0.86
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	12	0.86
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	14	0.86
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG21	11	0.86
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG23	14	0.86
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	1	0.86
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	9	0.86
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	2	0.86
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD11	4	0.86
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD11	7	0.86
(2,876)	1:97:A:ALA:HB3	1:98:A:ASP:HB2	8	0.86
(2,828)	1:128:A:ILE:HD11	1:47:A:GLU:HG2	6	0.86
(2,509)	1:174:A:LEU:HD23	1:156:A:LEU:HD23	10	0.86
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	7	0.86
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	3	0.86
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	6	0.86
(2,201)	1:99:A:LYS:HE2	1:96:A:TRP:HZ3	12	0.86
(2,196)	1:41:A:GLU:HG2	1:128:A:ILE:HD11	6	0.86
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	12	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	7	0.85
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	12	0.85
(2,4281)	1:177:A:MET:HE1	1:175:A:GLU:HA	2	0.85
(2,4171)	1:134:A:LEU:HD22	1:129:A:GLN:H	9	0.85
(2,4171)	1:134:A:LEU:HD22	1:129:A:GLN:H	12	0.85
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	2	0.85
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	7	0.85
(2,3618)	1:93:A:PHE:HE2	1:79:A:LEU:HD11	7	0.85
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG23	10	0.85
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	14	0.85
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	7	0.85
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	7	0.85
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	9	0.85
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	10	0.85
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	11	0.85
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG22	10	0.85
(2,1454)	1:103:A:TYR:HD1	1:149:A:VAL:HG13	8	0.85
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG13	2	0.85
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	5	0.85
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	14	0.85
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD12	11	0.85
(2,824)	1:134:A:LEU:HD23	1:33:A:GLU:HG3	7	0.85
(2,703)	1:18:A:ALA:HB3	1:15:A:PHE:HD1	5	0.85
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD12	5	0.85
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	15	0.85
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG23	6	0.85
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	8	0.85
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	10	0.85
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	14	0.85
(2,41)	1:31:A:LEU:HD13	1:67:A:ILE:HD12	2	0.85
(2,41)	1:31:A:LEU:HD12	1:67:A:ILE:HD12	5	0.85
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	1	0.85
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	15	0.85
(2,4766)	1:8:A:PHE:HD2	1:7:A:GLU:HB3	7	0.84
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB2	1	0.84
(2,4287)	1:13:A:LYS:HD2	1:15:A:PHE:HD1	12	0.84
(2,4280)	1:177:A:MET:HE1	1:174:A:LEU:H	12	0.84
(2,4195)	1:18:A:ALA:HB3	1:21:A:LEU:H	1	0.84
(2,4171)	1:134:A:LEU:HD23	1:129:A:GLN:H	1	0.84
(2,4171)	1:134:A:LEU:HD23	1:129:A:GLN:H	2	0.84
(2,4171)	1:134:A:LEU:HD23	1:129:A:GLN:H	4	0.84
(2,4171)	1:134:A:LEU:HD21	1:129:A:GLN:H	5	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG22	3	0.84
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG23	4	0.84
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	10	0.84
(2,2939)	1:178:A:LEU:HD12	1:177:A:MET:H	2	0.84
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	8	0.84
(2,2528)	1:87:A:GLU:HG2	1:87:A:GLU:H	2	0.84
(2,1932)	1:10:A:GLY:H	1:11:A:ARG:HB3	6	0.84
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	3	0.84
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	4	0.84
(2,1838)	1:16:A:ILE:HD12	1:158:A:GLU:H	2	0.84
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG23	5	0.84
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	3	0.84
(2,1562)	1:13:A:LYS:HB3	1:13:A:LYS:H	12	0.84
(2,1558)	1:20:A:LEU:HD22	1:89:A:VAL:HA	2	0.84
(2,1558)	1:20:A:LEU:HD21	1:89:A:VAL:HA	15	0.84
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	1	0.84
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	10	0.84
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD12	3	0.84
(2,776)	1:121:A:ALA:HB2	1:138:A:ILE:HD13	15	0.84
(2,593)	1:64:A:ILE:HD12	1:67:A:ILE:HD12	14	0.84
(2,581)	1:180:A:VAL:HG22	1:183:A:LYS:H	7	0.84
(2,405)	1:117:A:ILE:HD12	1:138:A:ILE:HD12	9	0.84
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD22	9	0.84
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	2	0.84
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	4	0.84
(2,291)	1:172:A:ASP:HA	1:171:A:LYS:HG2	2	0.84
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	1	0.84
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	7	0.84
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	13	0.83
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD12	2	0.83
(2,4576)	1:62:A:GLY:H	1:106:A:TYR:HD2	9	0.83
(2,4554)	1:146:A:VAL:HG22	1:143:A:ILE:HG12	2	0.83
(2,4522)	1:149:A:VAL:HG23	1:147:A:GLN:HA	10	0.83
(2,4475)	1:17:A:MET:HE3	1:17:A:MET:HB2	10	0.83
(2,4475)	1:17:A:MET:HE3	1:17:A:MET:HB2	11	0.83
(2,4423)	1:174:A:LEU:HD13	1:157:A:LYS:HE2	5	0.83
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	4	0.83
(2,4322)	1:20:A:LEU:HD12	1:152:A:TYR:H	5	0.83
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	8	0.83
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	5	0.83
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	3	0.83
(2,3618)	1:93:A:PHE:HE1	1:79:A:LEU:HD13	14	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG21	4	0.83
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG23	13	0.83
(2,2939)	1:178:A:LEU:HD11	1:177:A:MET:H	1	0.83
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	14	0.83
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	5	0.83
(2,1592)	1:135:A:ALA:HB3	1:129:A:GLN:HE22	10	0.83
(2,1558)	1:20:A:LEU:HD22	1:89:A:VAL:HA	4	0.83
(2,1442)	1:74:A:ILE:HD11	1:99:A:LYS:HE2	3	0.83
(2,1368)	1:79:A:LEU:HD23	1:17:A:MET:HE2	1	0.83
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE2	10	0.83
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	4	0.83
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	13	0.83
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD12	1	0.83
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD13	3	0.83
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	1	0.83
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	8	0.83
(2,638)	1:150:A:THR:HG22	1:153:A:GLN:HE21	2	0.83
(2,586)	1:180:A:VAL:HG21	1:183:A:LYS:HG2	11	0.83
(2,509)	1:174:A:LEU:HD21	1:156:A:LEU:HD23	9	0.83
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	1	0.83
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	9	0.83
(2,299)	1:84:A:GLN:HA	1:83:A:GLU:HB3	11	0.83
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD12	4	0.83
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	11	0.83
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD3	9	0.82
(2,4766)	1:8:A:PHE:HD2	1:7:A:GLU:HB3	8	0.82
(2,4719)	1:78:A:GLU:H	1:21:A:LEU:HD21	7	0.82
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	13	0.82
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	6	0.82
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	14	0.82
(2,4539)	1:95:A:THR:HG21	1:91:A:HIS:HB2	1	0.82
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG3	9	0.82
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG22	4	0.82
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	14	0.82
(2,4058)	1:16:A:ILE:HD13	1:15:A:PHE:H	11	0.82
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	15	0.82
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG21	15	0.82
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	11	0.82
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	10	0.82
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	11	0.82
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG22	3	0.82
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG21	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	9	0.82
(2,1370)	1:176:A:VAL:HG22	1:100:A:PHE:HE2	14	0.82
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE1	13	0.82
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	1	0.82
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	6	0.82
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD13	13	0.82
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD11	7	0.82
(2,776)	1:121:A:ALA:HB1	1:138:A:ILE:HD11	1	0.82
(2,393)	1:39:A:LEU:HD22	1:57:A:GLU:HB3	9	0.82
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD11	2	0.82
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD13	7	0.82
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD13	8	0.82
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD13	9	0.82
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD12	15	0.82
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	4	0.82
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	8	0.81
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG13	14	0.81
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	4	0.81
(2,4522)	1:149:A:VAL:HG21	1:147:A:GLN:HA	12	0.81
(2,4486)	1:104:A:VAL:HG13	1:108:A:LYS:HD3	8	0.81
(2,4475)	1:17:A:MET:HE3	1:17:A:MET:HB2	6	0.81
(2,4475)	1:17:A:MET:HE1	1:17:A:MET:HB2	12	0.81
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD22	2	0.81
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	6	0.81
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG12	2	0.81
(2,4265)	1:142:A:LEU:HD12	1:110:A:LYS:HB2	1	0.81
(2,4195)	1:18:A:ALA:HB3	1:21:A:LEU:H	10	0.81
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	14	0.81
(2,3618)	1:93:A:PHE:HE2	1:79:A:LEU:HD11	13	0.81
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	15	0.81
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD11	13	0.81
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG23	13	0.81
(2,2939)	1:178:A:LEU:HD12	1:177:A:MET:H	14	0.81
(2,2795)	1:140:A:SER:HB2	1:137:A:SER:H	10	0.81
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	3	0.81
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	5	0.81
(2,2615)	1:99:A:LYS:H	1:96:A:TRP:HB3	6	0.81
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	5	0.81
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG21	13	0.81
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	12	0.81
(2,1558)	1:20:A:LEU:HD22	1:89:A:VAL:HA	5	0.81
(2,1558)	1:20:A:LEU:HD21	1:89:A:VAL:HA	13	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1555)	1:18:A:ALA:HB1	1:22:A:GLN:HB3	4	0.81
(2,1439)	1:102:A:MET:HE1	1:106:A:TYR:HD2	6	0.81
(2,1368)	1:79:A:LEU:HD23	1:17:A:MET:HE2	5	0.81
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	9	0.81
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD22	1	0.81
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD21	11	0.81
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	9	0.81
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	9	0.81
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD11	12	0.81
(2,1017)	1:129:A:GLN:HA	1:128:A:ILE:HD12	15	0.81
(2,581)	1:180:A:VAL:HG21	1:183:A:LYS:H	4	0.81
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD21	4	0.81
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	3	0.81
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	10	0.81
(2,124)	1:187:A:ALA:HB2	1:183:A:LYS:HE2	6	0.81
(2,29)	1:35:A:LEU:HD12	1:33:A:GLU:H	14	0.81
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD2	12	0.8
(2,4766)	1:8:A:PHE:HD2	1:7:A:GLU:HB3	2	0.8
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG3	6	0.8
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	7	0.8
(2,4570)	1:128:A:ILE:HG22	1:38:A:TYR:H	13	0.8
(2,4570)	1:128:A:ILE:HG21	1:38:A:TYR:H	14	0.8
(2,4554)	1:146:A:VAL:HG21	1:110:A:LYS:HD2	3	0.8
(2,4554)	1:146:A:VAL:HG21	1:110:A:LYS:HD3	15	0.8
(2,4547)	1:102:A:MET:HE3	1:64:A:ILE:HA	1	0.8
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	15	0.8
(2,4475)	1:17:A:MET:HE2	1:17:A:MET:HB2	3	0.8
(2,4475)	1:17:A:MET:HE2	1:17:A:MET:HB2	13	0.8
(2,4322)	1:20:A:LEU:HD11	1:152:A:TYR:H	6	0.8
(2,4263)	1:178:A:LEU:HD21	1:175:A:GLU:HG2	12	0.8
(2,4195)	1:18:A:ALA:HB3	1:21:A:LEU:H	12	0.8
(2,4171)	1:134:A:LEU:HD21	1:129:A:GLN:H	3	0.8
(2,4100)	1:44:A:SER:HB2	1:43:A:THR:H	15	0.8
(2,4058)	1:16:A:ILE:HD12	1:15:A:PHE:H	1	0.8
(2,3770)	1:117:A:ILE:HD12	1:118:A:LEU:H	1	0.8
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG22	5	0.8
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG22	1	0.8
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD11	1	0.8
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	5	0.8
(2,1866)	1:146:A:VAL:HG12	1:143:A:ILE:H	8	0.8
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	11	0.8
(2,1593)	1:135:A:ALA:HB1	1:129:A:GLN:HE21	3	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1558)	1:20:A:LEU:HD21	1:89:A:VAL:HA	7	0.8
(2,1508)	1:105:A:THR:HG23	1:63:A:ASN:HB3	10	0.8
(2,1263)	1:42:A:MET:HE1	1:39:A:LEU:HD23	8	0.8
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	8	0.8
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD13	10	0.8
(2,703)	1:18:A:ALA:HB2	1:15:A:PHE:HD2	7	0.8
(2,581)	1:180:A:VAL:HG22	1:183:A:LYS:H	10	0.8
(2,436)	1:39:A:LEU:HD11	1:61:A:PHE:HD2	15	0.8
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD13	3	0.8
(2,275)	1:121:A:ALA:HA	1:53:A:ILE:HG13	3	0.8
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	9	0.8
(2,5)	1:95:A:THR:HG21	1:94:A:VAL:HB	14	0.8
(2,4815)	1:165:A:GLU:HG3	1:167:A:LYS:H	9	0.79
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD22	12	0.79
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG11	10	0.79
(2,4539)	1:95:A:THR:HG21	1:91:A:HIS:HB2	8	0.79
(2,4475)	1:17:A:MET:HE3	1:17:A:MET:HB2	1	0.79
(2,4475)	1:17:A:MET:HE3	1:17:A:MET:HB2	4	0.79
(2,4475)	1:17:A:MET:HE1	1:17:A:MET:HB2	5	0.79
(2,4475)	1:17:A:MET:HE1	1:17:A:MET:HB2	14	0.79
(2,4475)	1:17:A:MET:HE1	1:17:A:MET:HB2	15	0.79
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	10	0.79
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	1	0.79
(2,4285)	1:97:A:ALA:HB1	1:172:A:ASP:HB3	9	0.79
(2,4258)	1:95:A:THR:HG21	1:75:A:PHE:HD2	2	0.79
(2,4195)	1:18:A:ALA:HB1	1:21:A:LEU:H	3	0.79
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	8	0.79
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	13	0.79
(2,4171)	1:134:A:LEU:HD21	1:129:A:GLN:H	8	0.79
(2,4171)	1:134:A:LEU:HD21	1:129:A:GLN:H	15	0.79
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	15	0.79
(2,4083)	1:163:A:CYS:HB2	1:162:A:CYS:H	5	0.79
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	13	0.79
(2,3554)	1:152:A:TYR:HD2	1:155:A:LEU:HD11	12	0.79
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG22	9	0.79
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG22	10	0.79
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD12	7	0.79
(2,3199)	1:5:A:SER:H	1:4:A:GLY:HA3	14	0.79
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	9	0.79
(2,2939)	1:178:A:LEU:HD12	1:177:A:MET:H	12	0.79
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	2	0.79
(2,2435)	1:73:A:ASN:HB2	1:73:A:ASN:H	2	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	6	0.79
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	4	0.79
(2,1866)	1:146:A:VAL:HG12	1:143:A:ILE:H	3	0.79
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG22	12	0.79
(2,1525)	1:143:A:ILE:HG21	1:144:A:LYS:HE3	9	0.79
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE2	4	0.79
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG21	12	0.79
(2,1190)	1:19:A:GLU:HA	1:22:A:GLN:HG2	3	0.79
(2,712)	1:157:A:LYS:HG2	1:157:A:LYS:HE2	2	0.79
(2,712)	1:157:A:LYS:HG2	1:157:A:LYS:HE2	11	0.79
(2,705)	1:18:A:ALA:HB3	1:21:A:LEU:HG	3	0.79
(2,687)	1:184:A:ALA:HB2	1:181:A:PRO:HD3	7	0.79
(2,586)	1:180:A:VAL:HG22	1:183:A:LYS:HG2	8	0.79
(2,581)	1:180:A:VAL:HG21	1:183:A:LYS:H	13	0.79
(2,461)	1:134:A:LEU:HD21	1:33:A:GLU:HG2	1	0.79
(2,381)	1:68:A:TYR:HE1	1:31:A:LEU:HD21	14	0.79
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD12	1	0.79
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD11	5	0.79
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	13	0.78
(2,4475)	1:17:A:MET:HE2	1:17:A:MET:HB2	8	0.78
(2,4475)	1:17:A:MET:HE3	1:17:A:MET:HB2	9	0.78
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	7	0.78
(2,4322)	1:20:A:LEU:HD11	1:152:A:TYR:H	3	0.78
(2,4322)	1:20:A:LEU:HD12	1:152:A:TYR:H	4	0.78
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	15	0.78
(2,4264)	1:16:A:ILE:HD12	1:19:A:GLU:HB3	14	0.78
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	6	0.78
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD11	3	0.78
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD12	6	0.78
(2,4058)	1:16:A:ILE:HD13	1:15:A:PHE:H	5	0.78
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD2	7	0.78
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	15	0.78
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD12	2	0.78
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD11	4	0.78
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	11	0.78
(2,2928)	1:173:A:GLY:H	1:172:A:ASP:HB3	3	0.78
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	14	0.78
(2,2435)	1:73:A:ASN:HB2	1:73:A:ASN:H	1	0.78
(2,2435)	1:73:A:ASN:HB2	1:73:A:ASN:H	3	0.78
(2,1990)	1:116:A:LEU:H	1:117:A:ILE:HG13	1	0.78
(2,1988)	1:49:A:ILE:HG22	1:55:A:ASN:H	9	0.78
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	14	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG23	1	0.78
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE1	3	0.78
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	7	0.78
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD23	3	0.78
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG22	4	0.78
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG12	4	0.78
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	6	0.78
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	13	0.78
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	11	0.78
(2,828)	1:128:A:ILE:HD12	1:47:A:GLU:HG2	5	0.78
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	4	0.78
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	9	0.78
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	14	0.78
(2,454)	1:53:A:ILE:HG22	1:60:A:ILE:HG21	10	0.78
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD12	2	0.78
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD13	11	0.78
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD12	12	0.78
(2,141)	1:36:A:GLU:HG3	1:35:A:LEU:HD23	15	0.78
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	6	0.78
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD12	3	0.77
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	13	0.77
(2,4594)	1:148:A:ARG:H	1:144:A:LYS:HD2	13	0.77
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	2	0.77
(2,4516)	1:138:A:ILE:HD13	1:39:A:LEU:H	9	0.77
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	3	0.77
(2,4475)	1:17:A:MET:HE1	1:17:A:MET:HB2	7	0.77
(2,4457)	1:164:A:GLU:HG3	1:164:A:GLU:HA	1	0.77
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	6	0.77
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD22	5	0.77
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD12	9	0.77
(2,3930)	1:184:A:ALA:HB2	1:107:A:CYS:H	5	0.77
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	1	0.77
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG23	7	0.77
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG22	2	0.77
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG21	3	0.77
(2,3199)	1:5:A:SER:H	1:4:A:GLY:HA3	1	0.77
(2,2780)	1:136:A:ASN:HB2	1:136:A:ASN:H	10	0.77
(2,2278)	1:153:A:GLN:HE21	1:149:A:VAL:HG22	13	0.77
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	3	0.77
(2,1988)	1:49:A:ILE:HG23	1:55:A:ASN:H	6	0.77
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	15	0.77
(2,1558)	1:20:A:LEU:HD21	1:89:A:VAL:HA	14	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	1	0.77
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE3	14	0.77
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	3	0.77
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG22	1	0.77
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG22	2	0.77
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG12	5	0.77
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	7	0.77
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD12	15	0.77
(2,828)	1:128:A:ILE:HD11	1:47:A:GLU:HG2	13	0.77
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	7	0.77
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	8	0.77
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE1	15	0.77
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD23	6	0.77
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD23	8	0.77
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG22	6	0.77
(2,436)	1:39:A:LEU:HD11	1:61:A:PHE:HD2	10	0.77
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	3	0.77
(2,316)	1:20:A:LEU:HD13	1:152:A:TYR:HB3	11	0.77
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD13	14	0.77
(2,31)	1:35:A:LEU:HD13	1:69:A:ASP:HB2	10	0.77
(2,31)	1:35:A:LEU:HD11	1:69:A:ASP:HB2	11	0.77
(2,4530)	1:60:A:ILE:HG22	1:57:A:GLU:HG2	2	0.76
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD11	6	0.76
(2,4295)	1:181:A:PRO:HG2	1:149:A:VAL:HG11	12	0.76
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	2	0.76
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	15	0.76
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	13	0.76
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	4	0.76
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD1	1	0.76
(2,3931)	1:156:A:LEU:HD21	1:177:A:MET:H	4	0.76
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	11	0.76
(2,3770)	1:117:A:ILE:HD13	1:118:A:LEU:H	13	0.76
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG21	13	0.76
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG22	8	0.76
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD13	6	0.76
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG23	14	0.76
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG22	7	0.76
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG23	8	0.76
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG21	10	0.76
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	7	0.76
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	11	0.76
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	10	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	8	0.76
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	10	0.76
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	5	0.76
(2,1517)	1:39:A:LEU:HD13	1:61:A:PHE:HB2	4	0.76
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD13	8	0.76
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG22	6	0.76
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	1	0.76
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG23	10	0.76
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG23	14	0.76
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG11	10	0.76
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	11	0.76
(2,687)	1:184:A:ALA:HB2	1:181:A:PRO:HD3	4	0.76
(2,593)	1:64:A:ILE:HD11	1:67:A:ILE:HD12	2	0.76
(2,581)	1:180:A:VAL:HG22	1:183:A:LYS:H	1	0.76
(2,528)	1:46:A:VAL:HG23	1:41:A:GLU:HB3	9	0.76
(2,461)	1:134:A:LEU:HD22	1:33:A:GLU:HG2	4	0.76
(2,454)	1:53:A:ILE:HG23	1:60:A:ILE:HG21	11	0.76
(2,378)	1:142:A:LEU:HD22	1:60:A:ILE:HG23	1	0.76
(2,378)	1:142:A:LEU:HD22	1:60:A:ILE:HG22	9	0.76
(2,318)	1:20:A:LEU:HD21	1:152:A:TYR:HD1	10	0.76
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	6	0.76
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD3	5	0.75
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD11	5	0.75
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD11	5	0.75
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	1	0.75
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	15	0.75
(2,4554)	1:146:A:VAL:HG21	1:110:A:LYS:HD3	12	0.75
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD2	5	0.75
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	3	0.75
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	12	0.75
(2,4475)	1:17:A:MET:HE1	1:17:A:MET:HB2	2	0.75
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG23	4	0.75
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG23	8	0.75
(2,4331)	1:95:A:THR:HG23	1:92:A:CYS:HG	7	0.75
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	5	0.75
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	1	0.75
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	5	0.75
(2,4287)	1:13:A:LYS:HD3	1:15:A:PHE:HD1	7	0.75
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	9	0.75
(2,4171)	1:134:A:LEU:HD23	1:129:A:GLN:H	10	0.75
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	8	0.75
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	10	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD12	12	0.75
(2,4058)	1:16:A:ILE:HD12	1:15:A:PHE:H	12	0.75
(2,3770)	1:117:A:ILE:HD12	1:118:A:LEU:H	3	0.75
(2,3770)	1:117:A:ILE:HD11	1:118:A:LEU:H	14	0.75
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD12	4	0.75
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG23	5	0.75
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG23	12	0.75
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG21	15	0.75
(2,3282)	1:102:A:MET:H	1:101:A:GLN:HB3	2	0.75
(2,2878)	1:157:A:LYS:HG2	1:157:A:LYS:H	2	0.75
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	9	0.75
(2,2116)	1:97:A:ALA:HB3	1:100:A:PHE:H	5	0.75
(2,1932)	1:10:A:GLY:H	1:11:A:ARG:HB3	15	0.75
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	5	0.75
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	5	0.75
(2,1517)	1:39:A:LEU:HD13	1:61:A:PHE:HB2	6	0.75
(2,1442)	1:74:A:ILE:HD12	1:99:A:LYS:HE2	10	0.75
(2,1442)	1:74:A:ILE:HD11	1:99:A:LYS:HE2	15	0.75
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE2	6	0.75
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE2	15	0.75
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	8	0.75
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	10	0.75
(2,1263)	1:42:A:MET:HE2	1:39:A:LEU:HD21	2	0.75
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG11	11	0.75
(2,1153)	1:101:A:GLN:HA	1:180:A:VAL:HG11	2	0.75
(2,933)	1:15:A:PHE:HB3	1:18:A:ALA:HB2	11	0.75
(2,824)	1:134:A:LEU:HD23	1:33:A:GLU:HG3	11	0.75
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG21	4	0.75
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE1	10	0.75
(2,703)	1:18:A:ALA:HB2	1:15:A:PHE:HD1	11	0.75
(2,581)	1:180:A:VAL:HG22	1:183:A:LYS:H	14	0.75
(2,528)	1:46:A:VAL:HG22	1:41:A:GLU:HB3	6	0.75
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG21	9	0.75
(2,405)	1:117:A:ILE:HD12	1:138:A:ILE:HD12	14	0.75
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG21	3	0.75
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG22	4	0.75
(2,378)	1:142:A:LEU:HD22	1:60:A:ILE:HG22	11	0.75
(2,378)	1:142:A:LEU:HD21	1:60:A:ILE:HG22	14	0.75
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD13	2	0.75
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD11	14	0.75
(2,316)	1:20:A:LEU:HD12	1:152:A:TYR:HB3	5	0.75
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD11	12	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:174:A:LEU:HD22	1:178:A:LEU:H	1	0.75
(2,60)	1:174:A:LEU:HD22	1:178:A:LEU:H	9	0.75
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	4	0.75
(2,31)	1:35:A:LEU:HD11	1:69:A:ASP:HB2	12	0.75
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	2	0.75
(2,5)	1:95:A:THR:HG22	1:94:A:VAL:HB	1	0.75
(2,5)	1:95:A:THR:HG22	1:94:A:VAL:HB	8	0.75
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD22	7	0.74
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD22	14	0.74
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	15	0.74
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG13	5	0.74
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD1	11	0.74
(2,4534)	1:76:A:LEU:HD12	1:73:A:ASN:H	7	0.74
(2,4530)	1:60:A:ILE:HG22	1:57:A:GLU:HG2	8	0.74
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	6	0.74
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD22	8	0.74
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	15	0.74
(2,4352)	1:28:A:VAL:HG22	1:25:A:LYS:HG2	3	0.74
(2,4322)	1:20:A:LEU:HD13	1:152:A:TYR:H	11	0.74
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	2	0.74
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	6	0.74
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	1	0.74
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	9	0.74
(2,4285)	1:97:A:ALA:HB3	1:172:A:ASP:HB3	11	0.74
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD11	4	0.74
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	8	0.74
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD11	5	0.74
(2,3770)	1:117:A:ILE:HD12	1:118:A:LEU:H	11	0.74
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	7	0.74
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG23	12	0.74
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD11	1	0.74
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD12	3	0.74
(2,3063)	1:29:A:ARG:HD3	1:30:A:ASP:H	12	0.74
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	12	0.74
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	9	0.74
(2,2166)	1:151:A:LYS:H	1:151:A:LYS:HB3	10	0.74
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	15	0.74
(2,1852)	1:130:A:GLN:HG2	1:130:A:GLN:H	1	0.74
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	10	0.74
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG21	3	0.74
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	8	0.74
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG11	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1368)	1:79:A:LEU:HD23	1:17:A:MET:HE2	2	0.74
(2,1368)	1:79:A:LEU:HD23	1:17:A:MET:HE2	9	0.74
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	5	0.74
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG21	13	0.74
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	1	0.74
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	7	0.74
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG12	8	0.74
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	12	0.74
(2,1127)	1:182:A:LYS:HA	1:185:A:ASN:HB2	3	0.74
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD11	5	0.74
(2,876)	1:97:A:ALA:HB1	1:98:A:ASP:HB2	2	0.74
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	1	0.74
(2,776)	1:121:A:ALA:HB3	1:138:A:ILE:HD12	6	0.74
(2,454)	1:53:A:ILE:HG22	1:60:A:ILE:HG23	3	0.74
(2,405)	1:117:A:ILE:HD12	1:138:A:ILE:HD12	6	0.74
(2,378)	1:142:A:LEU:HD21	1:60:A:ILE:HG21	8	0.74
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD12	8	0.74
(2,340)	1:102:A:MET:HE2	1:99:A:LYS:HE3	2	0.74
(2,287)	1:187:A:ALA:HA	1:183:A:LYS:HE2	6	0.74
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	9	0.74
(2,197)	1:81:A:LYS:HE3	1:78:A:GLU:H	2	0.74
(2,168)	1:33:A:GLU:HG3	1:37:A:THR:H	8	0.74
(2,55)	1:142:A:LEU:HD12	1:106:A:TYR:HH	13	0.74
(2,31)	1:35:A:LEU:HD13	1:69:A:ASP:HB2	5	0.74
(2,31)	1:35:A:LEU:HD11	1:69:A:ASP:HB2	8	0.74
(2,4766)	1:8:A:PHE:HD2	1:7:A:GLU:HB3	15	0.73
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	1	0.73
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	7	0.73
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG21	8	0.73
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG13	4	0.73
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	6	0.73
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG13	8	0.73
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD13	6	0.73
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG2	14	0.73
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	7	0.73
(2,4490)	1:79:A:LEU:HD21	1:93:A:PHE:HZ	13	0.73
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG11	3	0.73
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	11	0.73
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	13	0.73
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	15	0.73
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	1	0.73
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	7	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4265)	1:142:A:LEU:HD12	1:110:A:LYS:HB2	10	0.73
(2,4263)	1:178:A:LEU:HD22	1:175:A:GLU:HG2	4	0.73
(2,4120)	1:7:A:GLU:HG3	1:7:A:GLU:H	12	0.73
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	1	0.73
(2,3931)	1:156:A:LEU:HD21	1:177:A:MET:H	2	0.73
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD23	11	0.73
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG22	9	0.73
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	7	0.73
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	15	0.73
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	7	0.73
(2,2166)	1:151:A:LYS:H	1:151:A:LYS:HB3	9	0.73
(2,1988)	1:49:A:ILE:HG23	1:55:A:ASN:H	7	0.73
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	11	0.73
(2,1988)	1:49:A:ILE:HG23	1:55:A:ASN:H	13	0.73
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	12	0.73
(2,1852)	1:130:A:GLN:HG2	1:130:A:GLN:H	6	0.73
(2,1852)	1:130:A:GLN:HG2	1:130:A:GLN:H	12	0.73
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG23	7	0.73
(2,1439)	1:102:A:MET:HE1	1:106:A:TYR:HD2	11	0.73
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	5	0.73
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD21	4	0.73
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD23	5	0.73
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG21	8	0.73
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG12	2	0.73
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD11	4	0.73
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD12	13	0.73
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD13	14	0.73
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	1	0.73
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	3	0.73
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	10	0.73
(2,581)	1:180:A:VAL:HG22	1:183:A:LYS:H	15	0.73
(2,509)	1:174:A:LEU:HD23	1:156:A:LEU:HD21	14	0.73
(2,436)	1:39:A:LEU:HD13	1:61:A:PHE:HD2	12	0.73
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG21	2	0.73
(2,378)	1:142:A:LEU:HD22	1:60:A:ILE:HG22	5	0.73
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD13	3	0.73
(2,124)	1:187:A:ALA:HB2	1:183:A:LYS:HE2	7	0.73
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	9	0.73
(2,5)	1:95:A:THR:HG23	1:94:A:VAL:HB	4	0.73
(2,5)	1:95:A:THR:HG23	1:94:A:VAL:HB	11	0.73
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	15	0.72
(2,4669)	1:158:A:GLU:H	1:155:A:LEU:HD12	7	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG13	11	0.72
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG12	13	0.72
(2,4584)	1:170:A:LEU:HD22	1:90:A:GLY:H	8	0.72
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	11	0.72
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	5	0.72
(2,4516)	1:138:A:ILE:HD13	1:39:A:LEU:H	10	0.72
(2,4502)	1:14:A:GLU:HB3	1:15:A:PHE:HE2	12	0.72
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD11	8	0.72
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD13	11	0.72
(2,4358)	1:177:A:MET:HE1	1:173:A:GLY:HA3	11	0.72
(2,4328)	1:156:A:LEU:HD22	1:155:A:LEU:H	2	0.72
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	9	0.72
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	8	0.72
(2,3931)	1:156:A:LEU:HD22	1:177:A:MET:H	3	0.72
(2,3896)	1:134:A:LEU:HD22	1:132:A:HIS:H	6	0.72
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	3	0.72
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	6	0.72
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	8	0.72
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	14	0.72
(2,2878)	1:157:A:LYS:HG2	1:157:A:LYS:H	11	0.72
(2,2853)	1:150:A:THR:H	1:153:A:GLN:HE21	13	0.72
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	14	0.72
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	4	0.72
(2,1828)	1:131:A:ARG:HE	1:47:A:GLU:HG3	5	0.72
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG11	2	0.72
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	7	0.72
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD23	7	0.72
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	3	0.72
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG13	14	0.72
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG23	5	0.72
(2,705)	1:18:A:ALA:HB3	1:21:A:LEU:HG	7	0.72
(2,612)	1:28:A:VAL:HG13	1:68:A:TYR:HE1	1	0.72
(2,378)	1:142:A:LEU:HD23	1:60:A:ILE:HG21	7	0.72
(2,378)	1:142:A:LEU:HD21	1:60:A:ILE:HG22	12	0.72
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD12	5	0.72
(2,318)	1:20:A:LEU:HD23	1:152:A:TYR:HD1	3	0.72
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	4	0.72
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD11	6	0.72
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	11	0.72
(2,41)	1:31:A:LEU:HD12	1:67:A:ILE:HD12	14	0.72
(2,31)	1:35:A:LEU:HD13	1:69:A:ASP:HB2	14	0.72
(2,5)	1:95:A:THR:HG22	1:94:A:VAL:HB	10	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4772)	1:32:A:HIS:HE1	1:69:A:ASP:HA	13	0.71
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	7	0.71
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD11	1	0.71
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	5	0.71
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	2	0.71
(2,4554)	1:146:A:VAL:HG23	1:110:A:LYS:HD3	6	0.71
(2,4539)	1:95:A:THR:HG22	1:91:A:HIS:HB2	6	0.71
(2,4534)	1:76:A:LEU:HD13	1:24:A:GLU:H	14	0.71
(2,4530)	1:60:A:ILE:HG22	1:57:A:GLU:HG2	3	0.71
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG3	11	0.71
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	12	0.71
(2,4457)	1:164:A:GLU:HG3	1:164:A:GLU:HA	15	0.71
(2,4423)	1:174:A:LEU:HD12	1:157:A:LYS:HE2	7	0.71
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG23	10	0.71
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD12	14	0.71
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	1	0.71
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	9	0.71
(2,4358)	1:177:A:MET:HE3	1:173:A:GLY:HA3	6	0.71
(2,4331)	1:95:A:THR:HG23	1:92:A:CYS:HG	5	0.71
(2,4331)	1:95:A:THR:HG22	1:92:A:CYS:HG	12	0.71
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	11	0.71
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	4	0.71
(2,4195)	1:18:A:ALA:HB2	1:21:A:LEU:H	5	0.71
(2,4195)	1:18:A:ALA:HB1	1:21:A:LEU:H	7	0.71
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD13	11	0.71
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	10	0.71
(2,3928)	1:162:A:CYS:H	1:162:A:CYS:HB3	2	0.71
(2,3770)	1:117:A:ILE:HD11	1:118:A:LEU:H	2	0.71
(2,3770)	1:117:A:ILE:HD12	1:118:A:LEU:H	7	0.71
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD2	5	0.71
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	11	0.71
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD11	11	0.71
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG22	4	0.71
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG23	7	0.71
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	13	0.71
(2,1988)	1:49:A:ILE:HG22	1:55:A:ASN:H	8	0.71
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	2	0.71
(2,1866)	1:146:A:VAL:HG11	1:143:A:ILE:H	11	0.71
(2,1807)	1:104:A:VAL:H	1:105:A:THR:HG21	8	0.71
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	14	0.71
(2,1644)	1:174:A:LEU:H	1:175:A:GLU:HG3	2	0.71
(2,1593)	1:135:A:ALA:HB3	1:129:A:GLN:HE21	10	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1517)	1:39:A:LEU:HD13	1:61:A:PHE:HB2	11	0.71
(2,1267)	1:94:A:VAL:HG22	1:97:A:ALA:H	6	0.71
(2,1263)	1:42:A:MET:HE3	1:39:A:LEU:HD23	12	0.71
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG21	15	0.71
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD13	1	0.71
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	9	0.71
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD13	8	0.71
(2,687)	1:184:A:ALA:HB2	1:181:A:PRO:HD3	2	0.71
(2,581)	1:180:A:VAL:HG21	1:183:A:LYS:H	6	0.71
(2,461)	1:134:A:LEU:HD21	1:33:A:GLU:HG2	6	0.71
(2,378)	1:142:A:LEU:HD22	1:60:A:ILE:HG22	10	0.71
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD13	6	0.71
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD12	7	0.71
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE1	10	0.71
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	3	0.71
(2,31)	1:35:A:LEU:HD11	1:69:A:ASP:HB2	13	0.71
(2,29)	1:35:A:LEU:HD11	1:33:A:GLU:H	3	0.71
(2,5)	1:95:A:THR:HG23	1:94:A:VAL:HB	12	0.71
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	10	0.7
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG13	3	0.7
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	3	0.7
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	10	0.7
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD12	8	0.7
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	12	0.7
(2,4423)	1:174:A:LEU:HD11	1:157:A:LYS:HE2	11	0.7
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD13	3	0.7
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	9	0.7
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	7	0.7
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG22	1	0.7
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	12	0.7
(2,4322)	1:20:A:LEU:HD11	1:152:A:TYR:H	8	0.7
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	3	0.7
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	8	0.7
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	12	0.7
(2,4263)	1:178:A:LEU:HD23	1:175:A:GLU:HG2	10	0.7
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	14	0.7
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	9	0.7
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD13	2	0.7
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD11	9	0.7
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD13	10	0.7
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	4	0.7
(2,3770)	1:117:A:ILE:HD13	1:118:A:LEU:H	5	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3770)	1:117:A:ILE:HD13	1:118:A:LEU:H	12	0.7
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD23	8	0.7
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD12	1	0.7
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD11	10	0.7
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD13	12	0.7
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG22	1	0.7
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG21	14	0.7
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD23	1	0.7
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	4	0.7
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	15	0.7
(2,2902)	1:166:A:GLY:HA3	1:167:A:LYS:H	5	0.7
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	8	0.7
(2,2166)	1:151:A:LYS:H	1:151:A:LYS:HB3	3	0.7
(2,1988)	1:49:A:ILE:HG23	1:55:A:ASN:H	12	0.7
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	9	0.7
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	6	0.7
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG11	8	0.7
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG12	4	0.7
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE1	8	0.7
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE2	12	0.7
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	6	0.7
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG12	3	0.7
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG21	9	0.7
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG21	1	0.7
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD12	6	0.7
(2,866)	1:22:A:GLN:HG3	1:21:A:LEU:H	3	0.7
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	6	0.7
(2,608)	1:28:A:VAL:HG12	1:75:A:PHE:H	14	0.7
(2,581)	1:180:A:VAL:HG21	1:183:A:LYS:H	5	0.7
(2,497)	1:142:A:LEU:HD13	1:138:A:ILE:HA	4	0.7
(2,444)	1:31:A:LEU:HD13	1:30:A:ASP:HB2	5	0.7
(2,378)	1:142:A:LEU:HD21	1:60:A:ILE:HG22	15	0.7
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD11	9	0.7
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	2	0.7
(2,168)	1:33:A:GLU:HG3	1:37:A:THR:H	3	0.7
(2,5)	1:95:A:THR:HG21	1:94:A:VAL:HB	15	0.7
(2,4823)	1:13:A:LYS:H	1:13:A:LYS:HE3	11	0.69
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG3	10	0.69
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	3	0.69
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD22	10	0.69
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	11	0.69
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD22	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4587)	1:94:A:VAL:H	1:176:A:VAL:HB	6	0.69
(2,4551)	1:21:A:LEU:HD23	1:75:A:PHE:HD2	12	0.69
(2,4539)	1:95:A:THR:HG22	1:91:A:HIS:HB2	2	0.69
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	5	0.69
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	3	0.69
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG22	5	0.69
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG22	9	0.69
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	12	0.69
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD13	4	0.69
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	12	0.69
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD22	6	0.69
(2,4339)	1:134:A:LEU:HD22	1:129:A:GLN:HG3	15	0.69
(2,4328)	1:156:A:LEU:HD23	1:155:A:LEU:H	1	0.69
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	10	0.69
(2,4322)	1:20:A:LEU:HD12	1:152:A:TYR:H	7	0.69
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	10	0.69
(2,4305)	1:56:A:LYS:HE2	1:55:A:ASN:HD21	6	0.69
(2,4263)	1:178:A:LEU:HD23	1:175:A:GLU:HG2	6	0.69
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	11	0.69
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	9	0.69
(2,4083)	1:163:A:CYS:HB2	1:162:A:CYS:H	6	0.69
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	3	0.69
(2,3930)	1:184:A:ALA:HB2	1:107:A:CYS:H	2	0.69
(2,3770)	1:117:A:ILE:HD13	1:118:A:LEU:H	4	0.69
(2,3770)	1:117:A:ILE:HD13	1:118:A:LEU:H	8	0.69
(2,3770)	1:117:A:ILE:HD11	1:118:A:LEU:H	9	0.69
(2,3705)	1:74:A:ILE:HG21	1:74:A:ILE:H	3	0.69
(2,3705)	1:74:A:ILE:HG22	1:74:A:ILE:H	5	0.69
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG21	1	0.69
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	4	0.69
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD2	12	0.69
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD13	2	0.69
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD11	8	0.69
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG21	9	0.69
(2,3260)	1:161:A:THR:HG22	1:158:A:GLU:H	8	0.69
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD21	10	0.69
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG12	10	0.69
(2,2908)	1:169:A:GLU:H	1:168:A:GLY:HA2	6	0.69
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	10	0.69
(2,2613)	1:172:A:ASP:H	1:172:A:ASP:HB3	3	0.69
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	5	0.69
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	1	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG23	4	0.69
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG23	11	0.69
(2,1592)	1:135:A:ALA:HB2	1:129:A:GLN:HE22	14	0.69
(2,1516)	1:39:A:LEU:HD13	1:61:A:PHE:HB3	4	0.69
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG11	6	0.69
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG11	4	0.69
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	9	0.69
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	10	0.69
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	12	0.69
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	13	0.69
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD12	6	0.69
(2,705)	1:18:A:ALA:HB2	1:21:A:LEU:HG	10	0.69
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	12	0.69
(2,608)	1:28:A:VAL:HG11	1:75:A:PHE:H	11	0.69
(2,509)	1:174:A:LEU:HD23	1:156:A:LEU:HD21	11	0.69
(2,461)	1:134:A:LEU:HD23	1:33:A:GLU:HG2	7	0.69
(2,454)	1:53:A:ILE:HG23	1:60:A:ILE:HG21	4	0.69
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD12	15	0.69
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	3	0.69
(2,60)	1:174:A:LEU:HD23	1:178:A:LEU:H	6	0.69
(2,55)	1:142:A:LEU:HD11	1:106:A:TYR:HH	4	0.69
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	1	0.69
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	7	0.69
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	15	0.69
(2,5)	1:95:A:THR:HG22	1:94:A:VAL:HB	3	0.69
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD11	12	0.68
(2,4589)	1:97:A:ALA:H	1:94:A:VAL:HG11	9	0.68
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	11	0.68
(2,4584)	1:170:A:LEU:HD22	1:90:A:GLY:H	13	0.68
(2,4547)	1:102:A:MET:HE3	1:64:A:ILE:HA	12	0.68
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG3	5	0.68
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG3	10	0.68
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	7	0.68
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	1	0.68
(2,4352)	1:28:A:VAL:HG22	1:25:A:LYS:HG2	10	0.68
(2,4320)	1:188:A:MET:HA	1:108:A:LYS:HE3	5	0.68
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	7	0.68
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	15	0.68
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	2	0.68
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	11	0.68
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	12	0.68
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	6	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	14	0.68
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD11	7	0.68
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	5	0.68
(2,3931)	1:156:A:LEU:HD21	1:177:A:MET:H	11	0.68
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	12	0.68
(2,3907)	1:138:A:ILE:HD13	1:142:A:LEU:H	4	0.68
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	12	0.68
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	14	0.68
(2,3770)	1:117:A:ILE:HD13	1:118:A:LEU:H	10	0.68
(2,3705)	1:74:A:ILE:HG23	1:74:A:ILE:H	2	0.68
(2,3705)	1:74:A:ILE:HG22	1:74:A:ILE:H	6	0.68
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD22	9	0.68
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG23	12	0.68
(2,3559)	1:141:A:TYR:HD2	1:138:A:ILE:HD12	4	0.68
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG12	5	0.68
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	1	0.68
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	8	0.68
(2,1988)	1:49:A:ILE:HG21	1:55:A:ASN:H	15	0.68
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD11	13	0.68
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	7	0.68
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG23	1	0.68
(2,1593)	1:135:A:ALA:HB2	1:129:A:GLN:HE21	12	0.68
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	5	0.68
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	1	0.68
(2,1442)	1:74:A:ILE:HD11	1:99:A:LYS:HE2	14	0.68
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB2	5	0.68
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	7	0.68
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG23	9	0.68
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	15	0.68
(2,687)	1:184:A:ALA:HB3	1:181:A:PRO:HD3	15	0.68
(2,497)	1:142:A:LEU:HD13	1:138:A:ILE:HA	2	0.68
(2,497)	1:142:A:LEU:HD12	1:138:A:ILE:HA	8	0.68
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG23	13	0.68
(2,444)	1:31:A:LEU:HD13	1:30:A:ASP:HB2	4	0.68
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG21	1	0.68
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG22	14	0.68
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD13	4	0.68
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD13	5	0.68
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD11	9	0.68
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD13	12	0.68
(2,302)	1:136:A:ASN:HA	1:129:A:GLN:HE22	13	0.68
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	8	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,168)	1:33:A:GLU:HG3	1:37:A:THR:H	5	0.68
(2,55)	1:142:A:LEU:HD11	1:106:A:TYR:HH	3	0.68
(2,5)	1:95:A:THR:HG21	1:94:A:VAL:HB	13	0.68
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	1	0.67
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	9	0.67
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	2	0.67
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	9	0.67
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	4	0.67
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD12	15	0.67
(2,4551)	1:21:A:LEU:HD22	1:75:A:PHE:HD1	13	0.67
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	10	0.67
(2,4530)	1:60:A:ILE:HG21	1:57:A:GLU:HG3	6	0.67
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG3	12	0.67
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD11	10	0.67
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG21	7	0.67
(2,4358)	1:177:A:MET:HE2	1:173:A:GLY:HA3	5	0.67
(2,4358)	1:177:A:MET:HE2	1:173:A:GLY:HA3	13	0.67
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	4	0.67
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	5	0.67
(2,4331)	1:95:A:THR:HG21	1:92:A:CYS:HG	10	0.67
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	7	0.67
(2,4322)	1:20:A:LEU:HD11	1:152:A:TYR:H	15	0.67
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	13	0.67
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	14	0.67
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	1	0.67
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	3	0.67
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	14	0.67
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	13	0.67
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	6	0.67
(2,3931)	1:156:A:LEU:HD22	1:177:A:MET:H	15	0.67
(2,3907)	1:138:A:ILE:HD12	1:142:A:LEU:H	15	0.67
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	13	0.67
(2,3705)	1:74:A:ILE:HG21	1:74:A:ILE:H	1	0.67
(2,3705)	1:74:A:ILE:HG21	1:74:A:ILE:H	4	0.67
(2,3705)	1:74:A:ILE:HG23	1:74:A:ILE:H	7	0.67
(2,3705)	1:74:A:ILE:HG21	1:74:A:ILE:H	8	0.67
(2,3705)	1:74:A:ILE:HG22	1:74:A:ILE:H	9	0.67
(2,3705)	1:74:A:ILE:HG23	1:74:A:ILE:H	11	0.67
(2,3705)	1:74:A:ILE:HG23	1:74:A:ILE:H	13	0.67
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD11	15	0.67
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	4	0.67
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	9	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG12	11	0.67
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	6	0.67
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	5	0.67
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	6	0.67
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG21	5	0.67
(2,1522)	1:76:A:LEU:HD11	1:68:A:TYR:HE1	4	0.67
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	8	0.67
(2,1442)	1:74:A:ILE:HD11	1:99:A:LYS:HE2	1	0.67
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	10	0.67
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	11	0.67
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD13	11	0.67
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG21	10	0.67
(2,775)	1:121:A:ALA:HB1	1:60:A:ILE:HG21	11	0.67
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG23	13	0.67
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	9	0.67
(2,705)	1:18:A:ALA:HB3	1:21:A:LEU:HG	11	0.67
(2,705)	1:18:A:ALA:HB2	1:21:A:LEU:HG	12	0.67
(2,612)	1:28:A:VAL:HG11	1:68:A:TYR:HE1	5	0.67
(2,612)	1:28:A:VAL:HG12	1:68:A:TYR:HE1	7	0.67
(2,612)	1:28:A:VAL:HG13	1:68:A:TYR:HE1	15	0.67
(2,581)	1:180:A:VAL:HG22	1:183:A:LYS:H	8	0.67
(2,581)	1:180:A:VAL:HG21	1:183:A:LYS:H	11	0.67
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	1	0.67
(2,528)	1:46:A:VAL:HG23	1:41:A:GLU:HB3	12	0.67
(2,509)	1:174:A:LEU:HD21	1:156:A:LEU:HD21	2	0.67
(2,497)	1:142:A:LEU:HD13	1:138:A:ILE:HA	3	0.67
(2,461)	1:134:A:LEU:HD23	1:33:A:GLU:HG2	9	0.67
(2,444)	1:31:A:LEU:HD12	1:30:A:ASP:HB2	1	0.67
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG22	7	0.67
(2,337)	1:102:A:MET:HE3	1:66:A:GLU:HA	14	0.67
(2,316)	1:20:A:LEU:HD13	1:152:A:TYR:HB3	8	0.67
(2,284)	1:57:A:GLU:HA	1:60:A:ILE:HD11	10	0.67
(2,120)	1:161:A:THR:HG21	1:158:A:GLU:HG2	14	0.67
(2,60)	1:174:A:LEU:HD21	1:178:A:LEU:H	3	0.67
(2,60)	1:174:A:LEU:HD21	1:178:A:LEU:H	14	0.67
(2,55)	1:142:A:LEU:HD11	1:106:A:TYR:HH	12	0.67
(2,29)	1:35:A:LEU:HD12	1:33:A:GLU:H	5	0.67
(2,5)	1:95:A:THR:HG21	1:94:A:VAL:HB	7	0.67
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	6	0.66
(2,4609)	1:141:A:TYR:HE1	1:33:A:GLU:H	12	0.66
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD1	1	0.66
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	4	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4420)	1:103:A:TYR:HB3	1:104:A:VAL:HG23	1	0.66
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	2	0.66
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	3	0.66
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD21	14	0.66
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	14	0.66
(2,4348)	1:60:A:ILE:HD12	1:113:A:SER:H	1	0.66
(2,4348)	1:60:A:ILE:HD13	1:113:A:SER:H	3	0.66
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	4	0.66
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	5	0.66
(2,4272)	1:174:A:LEU:HD23	1:175:A:GLU:HB2	2	0.66
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD13	15	0.66
(2,4195)	1:18:A:ALA:HB1	1:21:A:LEU:H	4	0.66
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	11	0.66
(2,4123)	1:28:A:VAL:HG23	1:72:A:ASN:H	3	0.66
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	8	0.66
(2,4123)	1:28:A:VAL:HG23	1:72:A:ASN:H	11	0.66
(2,3907)	1:138:A:ILE:HD13	1:142:A:LEU:H	1	0.66
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	2	0.66
(2,3907)	1:138:A:ILE:HD12	1:142:A:LEU:H	5	0.66
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	8	0.66
(2,3810)	1:150:A:THR:HG23	1:150:A:THR:H	9	0.66
(2,3705)	1:74:A:ILE:HG22	1:74:A:ILE:H	14	0.66
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD13	12	0.66
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG21	11	0.66
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD21	15	0.66
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	4	0.66
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	3	0.66
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD22	7	0.66
(2,2296)	1:29:A:ARG:HD3	1:29:A:ARG:H	10	0.66
(2,2296)	1:29:A:ARG:HD3	1:29:A:ARG:H	13	0.66
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	11	0.66
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	10	0.66
(2,1900)	1:169:A:GLU:H	1:172:A:ASP:HB3	3	0.66
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	6	0.66
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD13	2	0.66
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG22	13	0.66
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG21	14	0.66
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG11	7	0.66
(2,1558)	1:20:A:LEU:HD22	1:89:A:VAL:HA	3	0.66
(2,1483)	1:36:A:GLU:HG2	1:33:A:GLU:H	11	0.66
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	3	0.66
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	10	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1267)	1:94:A:VAL:HG23	1:97:A:ALA:H	13	0.66
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	15	0.66
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB2	1	0.66
(2,1188)	1:179:A:SER:HA	1:180:A:VAL:HG12	15	0.66
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	11	0.66
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	15	0.66
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD13	12	0.66
(2,894)	1:99:A:LYS:HE3	1:75:A:PHE:H	9	0.66
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	5	0.66
(2,824)	1:134:A:LEU:HD23	1:33:A:GLU:HG3	14	0.66
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	15	0.66
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	3	0.66
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	7	0.66
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	12	0.66
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	14	0.66
(2,729)	1:97:A:ALA:HB2	1:100:A:PHE:HE1	2	0.66
(2,687)	1:184:A:ALA:HB2	1:181:A:PRO:HD3	5	0.66
(2,612)	1:28:A:VAL:HG11	1:68:A:TYR:HE1	11	0.66
(2,608)	1:28:A:VAL:HG12	1:75:A:PHE:H	9	0.66
(2,608)	1:28:A:VAL:HG12	1:75:A:PHE:H	13	0.66
(2,585)	1:180:A:VAL:HG22	1:181:A:PRO:HG3	3	0.66
(2,585)	1:180:A:VAL:HG21	1:181:A:PRO:HG3	14	0.66
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	4	0.66
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE1	6	0.66
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE3	14	0.66
(2,454)	1:53:A:ILE:HG23	1:60:A:ILE:HG21	14	0.66
(2,444)	1:31:A:LEU:HD11	1:30:A:ASP:HB2	2	0.66
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD13	15	0.66
(2,393)	1:39:A:LEU:HD21	1:57:A:GLU:HB3	6	0.66
(2,378)	1:142:A:LEU:HD21	1:60:A:ILE:HG21	13	0.66
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD13	12	0.66
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD11	11	0.66
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD13	13	0.66
(2,351)	1:188:A:MET:HE2	1:108:A:LYS:HA	10	0.66
(2,340)	1:102:A:MET:HE2	1:99:A:LYS:HE3	1	0.66
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	8	0.66
(2,318)	1:20:A:LEU:HD22	1:152:A:TYR:HD1	14	0.66
(2,291)	1:172:A:ASP:HA	1:171:A:LYS:HG2	11	0.66
(2,291)	1:172:A:ASP:HA	1:171:A:LYS:HG2	13	0.66
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD12	7	0.66
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD12	4	0.66
(2,120)	1:161:A:THR:HG21	1:158:A:GLU:HG2	15	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,94)	1:180:A:VAL:HG23	1:103:A:TYR:HA	10	0.66
(2,55)	1:142:A:LEU:HD12	1:106:A:TYR:HH	9	0.66
(2,5)	1:95:A:THR:HG23	1:94:A:VAL:HB	2	0.66
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD3	10	0.65
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD2	13	0.65
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG2	5	0.65
(2,4772)	1:32:A:HIS:HE1	1:69:A:ASP:HA	8	0.65
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD23	8	0.65
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	11	0.65
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	8	0.65
(2,4635)	1:23:A:THR:HG22	1:22:A:GLN:H	2	0.65
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HB3	4	0.65
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	15	0.65
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD12	14	0.65
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD1	10	0.65
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD11	1	0.65
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	7	0.65
(2,4448)	1:179:A:SER:HB2	1:180:A:VAL:HG11	4	0.65
(2,4417)	1:153:A:GLN:HG2	1:149:A:VAL:HG11	3	0.65
(2,4358)	1:177:A:MET:HE2	1:173:A:GLY:HA3	8	0.65
(2,4352)	1:28:A:VAL:HG23	1:25:A:LYS:HG2	13	0.65
(2,4265)	1:142:A:LEU:HD11	1:110:A:LYS:HB2	4	0.65
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	5	0.65
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	6	0.65
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	4	0.65
(2,4123)	1:28:A:VAL:HG21	1:72:A:ASN:H	13	0.65
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD11	5	0.65
(2,3928)	1:162:A:CYS:H	1:162:A:CYS:HB3	14	0.65
(2,3896)	1:134:A:LEU:HD22	1:132:A:HIS:H	9	0.65
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	6	0.65
(2,3810)	1:150:A:THR:HG23	1:150:A:THR:H	5	0.65
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	12	0.65
(2,3770)	1:117:A:ILE:HD11	1:118:A:LEU:H	6	0.65
(2,3705)	1:74:A:ILE:HG23	1:74:A:ILE:H	12	0.65
(2,3705)	1:74:A:ILE:HG21	1:74:A:ILE:H	15	0.65
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG21	8	0.65
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD12	5	0.65
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD22	2	0.65
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	14	0.65
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	3	0.65
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	6	0.65
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD11	12	0.65
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	14	0.65
(2,1442)	1:74:A:ILE:HD12	1:99:A:LYS:HE2	8	0.65
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD11	14	0.65
(2,1267)	1:94:A:VAL:HG23	1:97:A:ALA:H	12	0.65
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	7	0.65
(2,865)	1:22:A:GLN:HG3	1:22:A:GLN:H	3	0.65
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG22	6	0.65
(2,775)	1:121:A:ALA:HB1	1:60:A:ILE:HG21	15	0.65
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	2	0.65
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	6	0.65
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	15	0.65
(2,705)	1:18:A:ALA:HB2	1:21:A:LEU:HG	1	0.65
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	5	0.65
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	8	0.65
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	13	0.65
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	14	0.65
(2,638)	1:150:A:THR:HG21	1:153:A:GLN:HE21	11	0.65
(2,593)	1:64:A:ILE:HD13	1:67:A:ILE:HD12	6	0.65
(2,585)	1:180:A:VAL:HG21	1:181:A:PRO:HG3	15	0.65
(2,528)	1:46:A:VAL:HG21	1:41:A:GLU:HB3	3	0.65
(2,497)	1:142:A:LEU:HD11	1:138:A:ILE:HA	13	0.65
(2,497)	1:142:A:LEU:HD11	1:138:A:ILE:HA	14	0.65
(2,454)	1:53:A:ILE:HG22	1:60:A:ILE:HG22	1	0.65
(2,454)	1:53:A:ILE:HG22	1:60:A:ILE:HG21	15	0.65
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD11	7	0.65
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD11	8	0.65
(2,316)	1:20:A:LEU:HD13	1:152:A:TYR:HB3	2	0.65
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD13	14	0.65
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD22	10	0.65
(2,120)	1:161:A:THR:HG21	1:158:A:GLU:HG2	1	0.65
(2,120)	1:161:A:THR:HG23	1:158:A:GLU:HG2	6	0.65
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD13	1	0.65
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD12	6	0.65
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD12	15	0.65
(2,77)	1:76:A:LEU:HD11	1:80:A:GLU:HG3	10	0.65
(2,76)	1:116:A:LEU:HD23	1:56:A:LYS:H	11	0.65
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	12	0.65
(2,31)	1:35:A:LEU:HD12	1:69:A:ASP:HB2	2	0.65
(2,30)	1:32:A:HIS:HD2	1:35:A:LEU:HD12	10	0.65
(2,5)	1:95:A:THR:HG23	1:94:A:VAL:HB	6	0.65
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	15	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD23	4	0.64
(2,4635)	1:23:A:THR:HG23	1:22:A:GLN:H	8	0.64
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	5	0.64
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD11	1	0.64
(2,4551)	1:21:A:LEU:HD22	1:75:A:PHE:HD1	14	0.64
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD1	15	0.64
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	8	0.64
(2,4530)	1:60:A:ILE:HG22	1:57:A:GLU:HG3	13	0.64
(2,4457)	1:164:A:GLU:HG3	1:164:A:GLU:HA	8	0.64
(2,4328)	1:156:A:LEU:HD23	1:155:A:LEU:H	3	0.64
(2,4322)	1:20:A:LEU:HD12	1:152:A:TYR:H	14	0.64
(2,4312)	1:52:A:GLY:HA2	1:51:A:PRO:HG3	14	0.64
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	4	0.64
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	9	0.64
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	14	0.64
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	15	0.64
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	11	0.64
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	7	0.64
(2,3931)	1:156:A:LEU:HD21	1:177:A:MET:H	14	0.64
(2,3907)	1:138:A:ILE:HD12	1:142:A:LEU:H	7	0.64
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	9	0.64
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD13	6	0.64
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	9	0.64
(2,3705)	1:74:A:ILE:HG23	1:74:A:ILE:H	10	0.64
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG22	1	0.64
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	6	0.64
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD13	9	0.64
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	4	0.64
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	7	0.64
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	13	0.64
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	6	0.64
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	7	0.64
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	6	0.64
(2,2575)	1:36:A:GLU:HG2	1:35:A:LEU:H	11	0.64
(2,2116)	1:97:A:ALA:HB2	1:100:A:PHE:H	15	0.64
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	5	0.64
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG21	13	0.64
(2,1838)	1:16:A:ILE:HD13	1:158:A:GLU:H	6	0.64
(2,1838)	1:16:A:ILE:HD12	1:158:A:GLU:H	13	0.64
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD12	14	0.64
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	8	0.64
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG21	6	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG22	15	0.64
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD11	11	0.64
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	14	0.64
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD11	5	0.64
(2,1186)	1:179:A:SER:HA	1:182:A:LYS:HD3	8	0.64
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG23	8	0.64
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG22	15	0.64
(2,908)	1:73:A:ASN:HB3	1:74:A:ILE:HD12	9	0.64
(2,876)	1:97:A:ALA:HB3	1:98:A:ASP:HB2	15	0.64
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	5	0.64
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	14	0.64
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	6	0.64
(2,705)	1:18:A:ALA:HB1	1:21:A:LEU:HG	9	0.64
(2,658)	1:104:A:VAL:HG13	1:184:A:ALA:HA	2	0.64
(2,610)	1:28:A:VAL:HG11	1:74:A:ILE:H	11	0.64
(2,608)	1:28:A:VAL:HG13	1:75:A:PHE:H	4	0.64
(2,586)	1:180:A:VAL:HG23	1:183:A:LYS:HG2	9	0.64
(2,585)	1:180:A:VAL:HG23	1:181:A:PRO:HG3	11	0.64
(2,585)	1:180:A:VAL:HG22	1:181:A:PRO:HG3	12	0.64
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	9	0.64
(2,528)	1:46:A:VAL:HG21	1:41:A:GLU:HB3	10	0.64
(2,497)	1:142:A:LEU:HD13	1:138:A:ILE:HA	6	0.64
(2,497)	1:142:A:LEU:HD11	1:138:A:ILE:HA	10	0.64
(2,461)	1:134:A:LEU:HD23	1:33:A:GLU:HG2	8	0.64
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG21	12	0.64
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG22	6	0.64
(2,411)	1:138:A:ILE:HG21	1:117:A:ILE:HG22	11	0.64
(2,411)	1:138:A:ILE:HG21	1:117:A:ILE:HG22	12	0.64
(2,372)	1:95:A:THR:HG23	1:92:A:CYS:H	7	0.64
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	6	0.64
(2,168)	1:33:A:GLU:HG3	1:37:A:THR:H	15	0.64
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	12	0.64
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	13	0.64
(2,120)	1:161:A:THR:HG21	1:158:A:GLU:HG2	11	0.64
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	4	0.64
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	7	0.64
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	8	0.64
(2,76)	1:116:A:LEU:HD21	1:56:A:LYS:H	15	0.64
(2,62)	1:155:A:LEU:HD23	1:93:A:PHE:HZ	13	0.64
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	9	0.64
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB2	7	0.63
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD21	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	7	0.63
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	10	0.63
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	14	0.63
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	1	0.63
(2,4570)	1:128:A:ILE:HG22	1:38:A:TYR:H	2	0.63
(2,4570)	1:128:A:ILE:HG23	1:38:A:TYR:H	7	0.63
(2,4570)	1:128:A:ILE:HG23	1:38:A:TYR:H	8	0.63
(2,4554)	1:146:A:VAL:HG23	1:110:A:LYS:HD3	8	0.63
(2,4511)	1:46:A:VAL:HG22	1:46:A:VAL:HB	5	0.63
(2,4511)	1:46:A:VAL:HG11	1:46:A:VAL:HB	8	0.63
(2,4511)	1:46:A:VAL:HG23	1:46:A:VAL:HB	10	0.63
(2,4511)	1:46:A:VAL:HG22	1:46:A:VAL:HB	11	0.63
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD11	9	0.63
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	13	0.63
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	14	0.63
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD11	15	0.63
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	6	0.63
(2,4331)	1:95:A:THR:HG21	1:92:A:CYS:HG	3	0.63
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	3	0.63
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	4	0.63
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	13	0.63
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	15	0.63
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	2	0.63
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	1	0.63
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	5	0.63
(2,3896)	1:134:A:LEU:HD23	1:132:A:HIS:H	1	0.63
(2,3896)	1:134:A:LEU:HD21	1:132:A:HIS:H	5	0.63
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	4	0.63
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	7	0.63
(2,3810)	1:150:A:THR:HG23	1:150:A:THR:H	8	0.63
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG22	9	0.63
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	13	0.63
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG22	6	0.63
(2,3456)	1:71:A:HIS:HE1	1:67:A:ILE:HG22	6	0.63
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	14	0.63
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	8	0.63
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	10	0.63
(2,2296)	1:29:A:ARG:HD3	1:29:A:ARG:H	12	0.63
(2,2166)	1:151:A:LYS:H	1:151:A:LYS:HB3	13	0.63
(2,1988)	1:49:A:ILE:HG22	1:55:A:ASN:H	2	0.63
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	2	0.63
(2,1933)	1:186:A:ASP:H	1:104:A:VAL:HG12	8	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD12	3	0.63
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD13	13	0.63
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD13	10	0.63
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD12	11	0.63
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG22	13	0.63
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	15	0.63
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG23	9	0.63
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG21	10	0.63
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG13	11	0.63
(2,1498)	1:49:A:ILE:HG22	1:43:A:THR:H	3	0.63
(2,1442)	1:74:A:ILE:HD13	1:99:A:LYS:HE2	4	0.63
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	3	0.63
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	6	0.63
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	9	0.63
(2,1368)	1:79:A:LEU:HD21	1:17:A:MET:HE2	11	0.63
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	2	0.63
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	15	0.63
(2,1267)	1:94:A:VAL:HG23	1:97:A:ALA:H	3	0.63
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	1	0.63
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	2	0.63
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD13	4	0.63
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD11	13	0.63
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	15	0.63
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG21	2	0.63
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG22	6	0.63
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG23	2	0.63
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD23	12	0.63
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	6	0.63
(2,775)	1:121:A:ALA:HB1	1:60:A:ILE:HG23	7	0.63
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	1	0.63
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	10	0.63
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	11	0.63
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	12	0.63
(2,687)	1:184:A:ALA:HB2	1:181:A:PRO:HD3	13	0.63
(2,638)	1:150:A:THR:HG22	1:153:A:GLN:HE21	5	0.63
(2,612)	1:28:A:VAL:HG13	1:68:A:TYR:HE1	4	0.63
(2,581)	1:180:A:VAL:HG23	1:183:A:LYS:H	3	0.63
(2,581)	1:180:A:VAL:HG23	1:183:A:LYS:H	12	0.63
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE1	11	0.63
(2,528)	1:46:A:VAL:HG21	1:41:A:GLU:HB3	8	0.63
(2,497)	1:142:A:LEU:HD12	1:138:A:ILE:HA	7	0.63
(2,461)	1:134:A:LEU:HD21	1:33:A:GLU:HG2	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,461)	1:134:A:LEU:HD23	1:33:A:GLU:HG2	15	0.63
(2,444)	1:31:A:LEU:HD13	1:30:A:ASP:HB2	7	0.63
(2,436)	1:39:A:LEU:HD11	1:61:A:PHE:HD2	2	0.63
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG23	8	0.63
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG23	10	0.63
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG22	15	0.63
(2,372)	1:95:A:THR:HG22	1:92:A:CYS:H	2	0.63
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	15	0.63
(2,316)	1:20:A:LEU:HD13	1:152:A:TYR:HB3	10	0.63
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD13	5	0.63
(2,94)	1:180:A:VAL:HG22	1:103:A:TYR:HA	2	0.63
(2,94)	1:180:A:VAL:HG22	1:103:A:TYR:HA	11	0.63
(2,77)	1:76:A:LEU:HD13	1:80:A:GLU:HG3	8	0.63
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	12	0.63
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	2	0.63
(2,4814)	1:31:A:LEU:HD22	1:69:A:ASP:H	13	0.62
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD12	4	0.62
(2,4584)	1:170:A:LEU:HD23	1:90:A:GLY:H	7	0.62
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HB3	14	0.62
(2,4551)	1:21:A:LEU:HD23	1:75:A:PHE:HD2	9	0.62
(2,4511)	1:46:A:VAL:HG23	1:46:A:VAL:HB	1	0.62
(2,4511)	1:46:A:VAL:HG12	1:46:A:VAL:HB	6	0.62
(2,4511)	1:46:A:VAL:HG21	1:46:A:VAL:HB	7	0.62
(2,4511)	1:46:A:VAL:HG23	1:46:A:VAL:HB	12	0.62
(2,4457)	1:164:A:GLU:HG2	1:164:A:GLU:HA	11	0.62
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	14	0.62
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD12	13	0.62
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG2	10	0.62
(2,4322)	1:20:A:LEU:HD13	1:152:A:TYR:H	2	0.62
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	13	0.62
(2,4258)	1:95:A:THR:HG22	1:75:A:PHE:HD1	5	0.62
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	14	0.62
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD22	9	0.62
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	3	0.62
(2,4218)	1:85:A:LEU:HD12	1:84:A:GLN:H	11	0.62
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	14	0.62
(2,4195)	1:18:A:ALA:HB3	1:21:A:LEU:H	2	0.62
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	10	0.62
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	14	0.62
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	10	0.62
(2,4123)	1:28:A:VAL:HG21	1:72:A:ASN:H	15	0.62
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	10	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	8	0.62
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	13	0.62
(2,3861)	1:143:A:ILE:HG23	1:147:A:GLN:HE22	14	0.62
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	11	0.62
(2,3810)	1:150:A:THR:HG22	1:150:A:THR:H	11	0.62
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG22	5	0.62
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG23	10	0.62
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG23	2	0.62
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	2	0.62
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG21	15	0.62
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	2	0.62
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD21	3	0.62
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	2	0.62
(2,3063)	1:29:A:ARG:HD3	1:30:A:ASP:H	10	0.62
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	1	0.62
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD22	6	0.62
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	9	0.62
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	1	0.62
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	4	0.62
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD12	5	0.62
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD11	6	0.62
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD12	8	0.62
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD12	9	0.62
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	2	0.62
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	3	0.62
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	9	0.62
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG13	3	0.62
(2,1558)	1:20:A:LEU:HD22	1:89:A:VAL:HA	1	0.62
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	1	0.62
(2,1516)	1:39:A:LEU:HD13	1:61:A:PHE:HB3	6	0.62
(2,1516)	1:39:A:LEU:HD13	1:61:A:PHE:HB3	11	0.62
(2,1498)	1:49:A:ILE:HG23	1:43:A:THR:H	2	0.62
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	15	0.62
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG21	14	0.62
(2,1385)	1:33:A:GLU:HG3	1:29:A:ARG:HD3	15	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD12	4	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD12	5	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD12	7	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD11	8	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD11	10	0.62
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	15	0.62
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	14	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD11	6	0.62
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	9	0.62
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD13	11	0.62
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	14	0.62
(2,1216)	1:112:A:ASP:HA	1:59:A:ILE:HG23	7	0.62
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG22	7	0.62
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG23	13	0.62
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	6	0.62
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG21	8	0.62
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG21	10	0.62
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD22	9	0.62
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG23	2	0.62
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG21	9	0.62
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	4	0.62
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	13	0.62
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	14	0.62
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	4	0.62
(2,612)	1:28:A:VAL:HG13	1:68:A:TYR:HE1	2	0.62
(2,612)	1:28:A:VAL:HG12	1:68:A:TYR:HE1	3	0.62
(2,610)	1:28:A:VAL:HG13	1:74:A:ILE:H	10	0.62
(2,585)	1:180:A:VAL:HG22	1:181:A:PRO:HG3	9	0.62
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	5	0.62
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE3	8	0.62
(2,528)	1:46:A:VAL:HG22	1:41:A:GLU:HB3	2	0.62
(2,497)	1:142:A:LEU:HD13	1:138:A:ILE:HA	5	0.62
(2,497)	1:142:A:LEU:HD11	1:138:A:ILE:HA	9	0.62
(2,411)	1:138:A:ILE:HG23	1:117:A:ILE:HG21	14	0.62
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG21	11	0.62
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD11	11	0.62
(2,351)	1:188:A:MET:HE3	1:108:A:LYS:HA	2	0.62
(2,291)	1:172:A:ASP:HA	1:171:A:LYS:HG2	5	0.62
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD12	12	0.62
(2,120)	1:161:A:THR:HG23	1:158:A:GLU:HG2	12	0.62
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD13	3	0.62
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD13	11	0.62
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD12	14	0.62
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	1	0.62
(2,76)	1:116:A:LEU:HD21	1:56:A:LYS:H	6	0.62
(2,76)	1:116:A:LEU:HD23	1:56:A:LYS:H	14	0.62
(2,55)	1:142:A:LEU:HD11	1:106:A:TYR:HH	5	0.62
(2,55)	1:142:A:LEU:HD13	1:106:A:TYR:HH	7	0.62
(2,55)	1:142:A:LEU:HD12	1:106:A:TYR:HH	14	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:95:A:THR:HG21	1:94:A:VAL:HB	5	0.62
(2,4818)	1:7:A:GLU:H	1:5:A:SER:HB2	14	0.61
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	1	0.61
(2,4814)	1:31:A:LEU:HD23	1:69:A:ASP:H	7	0.61
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG3	14	0.61
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG3	4	0.61
(2,4674)	1:156:A:LEU:H	1:155:A:LEU:HD22	2	0.61
(2,4609)	1:141:A:TYR:HE1	1:33:A:GLU:H	13	0.61
(2,4570)	1:128:A:ILE:HG22	1:38:A:TYR:H	4	0.61
(2,4570)	1:128:A:ILE:HG22	1:38:A:TYR:H	5	0.61
(2,4570)	1:128:A:ILE:HG22	1:38:A:TYR:H	10	0.61
(2,4570)	1:128:A:ILE:HG23	1:38:A:TYR:H	15	0.61
(2,4561)	1:23:A:THR:HG23	1:16:A:ILE:HA	4	0.61
(2,4551)	1:21:A:LEU:HD22	1:75:A:PHE:HD1	3	0.61
(2,4551)	1:21:A:LEU:HD22	1:75:A:PHE:HD1	4	0.61
(2,4511)	1:46:A:VAL:HG21	1:46:A:VAL:HB	3	0.61
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD12	3	0.61
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG23	5	0.61
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG22	6	0.61
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	12	0.61
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	9	0.61
(2,4328)	1:156:A:LEU:HD22	1:155:A:LEU:H	11	0.61
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	6	0.61
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	10	0.61
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD13	10	0.61
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	4	0.61
(2,4218)	1:85:A:LEU:HD11	1:84:A:GLN:H	2	0.61
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD23	13	0.61
(2,4185)	1:178:A:LEU:HD12	1:179:A:SER:H	5	0.61
(2,4123)	1:28:A:VAL:HG23	1:72:A:ASN:H	10	0.61
(2,4069)	1:23:A:THR:HG22	1:24:A:GLU:H	2	0.61
(2,4022)	1:143:A:ILE:HD13	1:147:A:GLN:HE22	6	0.61
(2,4022)	1:143:A:ILE:HD13	1:147:A:GLN:HE22	10	0.61
(2,3896)	1:134:A:LEU:HD22	1:132:A:HIS:H	7	0.61
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD12	4	0.61
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	10	0.61
(2,3810)	1:150:A:THR:HG22	1:150:A:THR:H	15	0.61
(2,3689)	1:60:A:ILE:HD13	1:61:A:PHE:H	9	0.61
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	4	0.61
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD1	8	0.61
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	11	0.61
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	12	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	1	0.61
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	3	0.61
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	6	0.61
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	7	0.61
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	8	0.61
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	9	0.61
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	15	0.61
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG12	1	0.61
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG11	3	0.61
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD21	10	0.61
(2,1988)	1:49:A:ILE:HG23	1:55:A:ASN:H	1	0.61
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	15	0.61
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG22	9	0.61
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD12	3	0.61
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD13	5	0.61
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	4	0.61
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	5	0.61
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	7	0.61
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	8	0.61
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	10	0.61
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG23	2	0.61
(2,1669)	1:55:A:ASN:HD22	1:55:A:ASN:HB3	4	0.61
(2,1572)	1:49:A:ILE:HG21	1:55:A:ASN:HB2	4	0.61
(2,1547)	1:95:A:THR:HG22	1:78:A:GLU:HB2	2	0.61
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	5	0.61
(2,1498)	1:49:A:ILE:HG23	1:43:A:THR:H	12	0.61
(2,1483)	1:36:A:GLU:HG2	1:33:A:GLU:H	6	0.61
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	6	0.61
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD21	7	0.61
(2,1267)	1:94:A:VAL:HG23	1:97:A:ALA:H	8	0.61
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD13	3	0.61
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD11	8	0.61
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	15	0.61
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	2	0.61
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB3	9	0.61
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG21	11	0.61
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG23	15	0.61
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD23	3	0.61
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD21	4	0.61
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG22	10	0.61
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG23	12	0.61
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	6	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	3	0.61
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG23	3	0.61
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	5	0.61
(2,700)	1:23:A:THR:HG23	1:21:A:LEU:H	8	0.61
(2,612)	1:28:A:VAL:HG13	1:68:A:TYR:HE1	10	0.61
(2,610)	1:28:A:VAL:HG13	1:74:A:ILE:H	4	0.61
(2,610)	1:28:A:VAL:HG12	1:74:A:ILE:H	7	0.61
(2,610)	1:28:A:VAL:HG12	1:74:A:ILE:H	14	0.61
(2,603)	1:28:A:VAL:HG22	1:72:A:ASN:HB3	5	0.61
(2,585)	1:180:A:VAL:HG23	1:181:A:PRO:HG3	6	0.61
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	12	0.61
(2,528)	1:46:A:VAL:HG23	1:41:A:GLU:HB3	4	0.61
(2,508)	1:155:A:LEU:HD21	1:155:A:LEU:HB2	4	0.61
(2,508)	1:155:A:LEU:HD22	1:155:A:LEU:HB2	13	0.61
(2,461)	1:134:A:LEU:HD23	1:33:A:GLU:HG2	14	0.61
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG21	9	0.61
(2,411)	1:138:A:ILE:HG23	1:117:A:ILE:HG23	15	0.61
(2,393)	1:39:A:LEU:HD21	1:57:A:GLU:HB3	13	0.61
(2,372)	1:95:A:THR:HG23	1:92:A:CYS:H	5	0.61
(2,340)	1:102:A:MET:HE2	1:99:A:LYS:HE3	11	0.61
(2,140)	1:36:A:GLU:HG3	1:37:A:THR:H	6	0.61
(2,120)	1:161:A:THR:HG23	1:158:A:GLU:HG2	10	0.61
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD11	4	0.61
(2,88)	1:60:A:ILE:HD12	1:117:A:ILE:HD11	5	0.61
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD11	8	0.61
(2,88)	1:60:A:ILE:HD12	1:117:A:ILE:HD11	10	0.61
(2,82)	1:76:A:LEU:HD13	1:77:A:LYS:HE2	12	0.61
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	1	0.61
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	3	0.61
(2,77)	1:76:A:LEU:HD11	1:80:A:GLU:HG3	9	0.61
(2,77)	1:76:A:LEU:HD13	1:80:A:GLU:HG3	15	0.61
(2,76)	1:116:A:LEU:HD23	1:56:A:LYS:H	5	0.61
(2,76)	1:116:A:LEU:HD22	1:56:A:LYS:H	13	0.61
(2,43)	1:128:A:ILE:HG22	1:38:A:TYR:H	13	0.61
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	14	0.61
(2,5)	1:95:A:THR:HG22	1:94:A:VAL:HB	9	0.61
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD12	6	0.6
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	9	0.6
(2,4635)	1:23:A:THR:HG23	1:22:A:GLN:H	4	0.6
(2,4635)	1:23:A:THR:HG23	1:22:A:GLN:H	7	0.6
(2,4635)	1:23:A:THR:HG23	1:22:A:GLN:H	9	0.6
(2,4635)	1:23:A:THR:HG22	1:22:A:GLN:H	15	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HB3	11	0.6
(2,4561)	1:23:A:THR:HG21	1:16:A:ILE:HA	5	0.6
(2,4554)	1:146:A:VAL:HG23	1:110:A:LYS:HD2	5	0.6
(2,4551)	1:21:A:LEU:HD22	1:75:A:PHE:HD1	6	0.6
(2,4539)	1:95:A:THR:HG21	1:91:A:HIS:HB2	9	0.6
(2,4530)	1:60:A:ILE:HG21	1:57:A:GLU:HG2	1	0.6
(2,4511)	1:46:A:VAL:HG23	1:46:A:VAL:HB	4	0.6
(2,4511)	1:46:A:VAL:HG22	1:46:A:VAL:HB	9	0.6
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	4	0.6
(2,4486)	1:104:A:VAL:HG11	1:183:A:LYS:HD3	7	0.6
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD11	5	0.6
(2,4429)	1:11:A:ARG:HB3	1:11:A:ARG:HD2	12	0.6
(2,4358)	1:177:A:MET:HE3	1:173:A:GLY:HA3	10	0.6
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	9	0.6
(2,4331)	1:95:A:THR:HG22	1:92:A:CYS:HG	2	0.6
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	8	0.6
(2,4288)	1:60:A:ILE:HG12	1:42:A:MET:HB3	9	0.6
(2,4264)	1:16:A:ILE:HD13	1:19:A:GLU:HB3	4	0.6
(2,4263)	1:178:A:LEU:HD21	1:175:A:GLU:HG2	5	0.6
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD21	5	0.6
(2,4218)	1:85:A:LEU:HD12	1:84:A:GLN:H	1	0.6
(2,4218)	1:85:A:LEU:HD12	1:84:A:GLN:H	7	0.6
(2,4218)	1:85:A:LEU:HD12	1:84:A:GLN:H	9	0.6
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	6	0.6
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	1	0.6
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	14	0.6
(2,3930)	1:184:A:ALA:HB2	1:107:A:CYS:H	4	0.6
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	6	0.6
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	10	0.6
(2,3810)	1:150:A:THR:HG23	1:150:A:THR:H	2	0.6
(2,3810)	1:150:A:THR:HG23	1:150:A:THR:H	14	0.6
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	10	0.6
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG22	14	0.6
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	11	0.6
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG21	5	0.6
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	10	0.6
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	2	0.6
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	4	0.6
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	5	0.6
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	11	0.6
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	12	0.6
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	13	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	14	0.6
(2,3014)	1:16:A:ILE:H	1:14:A:GLU:HB3	15	0.6
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	4	0.6
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	2	0.6
(2,2614)	1:99:A:LYS:H	1:99:A:LYS:HE2	13	0.6
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	1	0.6
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	12	0.6
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	8	0.6
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	9	0.6
(2,1854)	1:143:A:ILE:HD11	1:147:A:GLN:H	12	0.6
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD11	15	0.6
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	11	0.6
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	13	0.6
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG22	8	0.6
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	14	0.6
(2,1516)	1:39:A:LEU:HD13	1:61:A:PHE:HB3	10	0.6
(2,1498)	1:49:A:ILE:HG23	1:43:A:THR:H	13	0.6
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	2	0.6
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	15	0.6
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	2	0.6
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD11	12	0.6
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	13	0.6
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	2	0.6
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD23	4	0.6
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD21	9	0.6
(2,1267)	1:94:A:VAL:HG22	1:97:A:ALA:H	1	0.6
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD13	10	0.6
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	12	0.6
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB2	13	0.6
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG22	3	0.6
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG22	14	0.6
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	3	0.6
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD22	1	0.6
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD23	8	0.6
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG21	4	0.6
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG21	6	0.6
(2,894)	1:99:A:LYS:HE3	1:75:A:PHE:H	13	0.6
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	6	0.6
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	8	0.6
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	11	0.6
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG22	1	0.6
(2,748)	1:117:A:ILE:HG12	1:117:A:ILE:H	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,734)	1:36:A:GLU:HG3	1:35:A:LEU:H	6	0.6
(2,700)	1:23:A:THR:HG22	1:21:A:LEU:H	2	0.6
(2,610)	1:28:A:VAL:HG11	1:74:A:ILE:H	8	0.6
(2,610)	1:28:A:VAL:HG12	1:74:A:ILE:H	9	0.6
(2,608)	1:28:A:VAL:HG11	1:75:A:PHE:H	8	0.6
(2,585)	1:180:A:VAL:HG23	1:181:A:PRO:HG3	4	0.6
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	7	0.6
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE2	13	0.6
(2,528)	1:46:A:VAL:HG22	1:41:A:GLU:HB3	11	0.6
(2,467)	1:178:A:LEU:HD23	1:175:A:GLU:H	6	0.6
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD11	15	0.6
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG21	2	0.6
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG23	3	0.6
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG21	4	0.6
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG21	6	0.6
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG22	13	0.6
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD11	13	0.6
(2,356)	1:138:A:ILE:HD11	1:60:A:ILE:HD11	14	0.6
(2,351)	1:188:A:MET:HE2	1:108:A:LYS:HA	14	0.6
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	7	0.6
(2,316)	1:20:A:LEU:HD12	1:152:A:TYR:HB3	9	0.6
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD12	13	0.6
(2,140)	1:36:A:GLU:HG3	1:37:A:THR:H	11	0.6
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE1	15	0.6
(2,77)	1:76:A:LEU:HD11	1:80:A:GLU:HG3	7	0.6
(2,76)	1:116:A:LEU:HD21	1:56:A:LYS:H	9	0.6
(2,55)	1:142:A:LEU:HD13	1:106:A:TYR:HH	8	0.6
(2,43)	1:128:A:ILE:HG21	1:38:A:TYR:H	14	0.6
(2,34)	1:39:A:LEU:HD12	1:35:A:LEU:H	6	0.6
(2,4802)	1:167:A:LYS:HD3	1:167:A:LYS:H	14	0.59
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD3	6	0.59
(2,4800)	1:164:A:GLU:HG2	1:164:A:GLU:H	15	0.59
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD12	10	0.59
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD22	9	0.59
(2,4570)	1:128:A:ILE:HG21	1:38:A:TYR:H	1	0.59
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD12	8	0.59
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	8	0.59
(2,4511)	1:46:A:VAL:HG22	1:46:A:VAL:HB	2	0.59
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD12	1	0.59
(2,4352)	1:28:A:VAL:HG23	1:25:A:LYS:HG2	15	0.59
(2,4328)	1:156:A:LEU:HD22	1:155:A:LEU:H	14	0.59
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	12	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	4	0.59
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	7	0.59
(2,4218)	1:85:A:LEU:HD11	1:84:A:GLN:H	5	0.59
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD23	8	0.59
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	7	0.59
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	1	0.59
(2,4022)	1:143:A:ILE:HD12	1:147:A:GLN:HE22	12	0.59
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	9	0.59
(2,3930)	1:184:A:ALA:HB3	1:107:A:CYS:H	15	0.59
(2,3913)	1:176:A:VAL:HG23	1:100:A:PHE:H	14	0.59
(2,3907)	1:138:A:ILE:HD11	1:142:A:LEU:H	11	0.59
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	3	0.59
(2,3861)	1:143:A:ILE:HG21	1:147:A:GLN:HE22	5	0.59
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	5	0.59
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	1	0.59
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	3	0.59
(2,3689)	1:60:A:ILE:HD12	1:61:A:PHE:H	4	0.59
(2,3689)	1:60:A:ILE:HD12	1:61:A:PHE:H	6	0.59
(2,3689)	1:60:A:ILE:HD12	1:61:A:PHE:H	13	0.59
(2,3689)	1:60:A:ILE:HD13	1:61:A:PHE:H	14	0.59
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD22	1	0.59
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG22	9	0.59
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG23	11	0.59
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD11	2	0.59
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	8	0.59
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	14	0.59
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	4	0.59
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD12	9	0.59
(2,3138)	1:52:A:GLY:HA3	1:52:A:GLY:H	10	0.59
(2,3063)	1:29:A:ARG:HD3	1:30:A:ASP:H	13	0.59
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	7	0.59
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD22	3	0.59
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD21	5	0.59
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	15	0.59
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	12	0.59
(2,2614)	1:99:A:LYS:H	1:99:A:LYS:HE2	9	0.59
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	3	0.59
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	5	0.59
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	1	0.59
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	12	0.59
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD11	1	0.59
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD12	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	1	0.59
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	4	0.59
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG12	5	0.59
(2,1522)	1:76:A:LEU:HD12	1:68:A:TYR:HE1	14	0.59
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	5	0.59
(2,1498)	1:49:A:ILE:HG23	1:43:A:THR:H	8	0.59
(2,1377)	1:74:A:ILE:HA	1:74:A:ILE:HD13	1	0.59
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	11	0.59
(2,1244)	1:20:A:LEU:HD12	1:21:A:LEU:H	8	0.59
(2,1243)	1:21:A:LEU:HD23	1:21:A:LEU:HB2	9	0.59
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD21	2	0.59
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD21	6	0.59
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD22	10	0.59
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG23	3	0.59
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG23	9	0.59
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG22	14	0.59
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	15	0.59
(2,658)	1:104:A:VAL:HG11	1:184:A:ALA:HA	14	0.59
(2,612)	1:28:A:VAL:HG12	1:68:A:TYR:HE1	9	0.59
(2,612)	1:28:A:VAL:HG12	1:68:A:TYR:HE1	14	0.59
(2,610)	1:28:A:VAL:HG13	1:74:A:ILE:H	2	0.59
(2,585)	1:180:A:VAL:HG21	1:181:A:PRO:HG3	8	0.59
(2,535)	1:76:A:LEU:HD21	1:71:A:HIS:HB3	7	0.59
(2,509)	1:174:A:LEU:HD22	1:156:A:LEU:HD22	3	0.59
(2,497)	1:142:A:LEU:HD12	1:138:A:ILE:HA	15	0.59
(2,467)	1:178:A:LEU:HD22	1:175:A:GLU:H	11	0.59
(2,441)	1:31:A:LEU:HD12	1:61:A:PHE:HE1	2	0.59
(2,441)	1:31:A:LEU:HD11	1:61:A:PHE:HE1	5	0.59
(2,441)	1:31:A:LEU:HD13	1:61:A:PHE:HE1	8	0.59
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG23	1	0.59
(2,356)	1:138:A:ILE:HD13	1:60:A:ILE:HD13	1	0.59
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	10	0.59
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD12	15	0.59
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD22	10	0.59
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD12	6	0.59
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD11	10	0.59
(2,120)	1:161:A:THR:HG22	1:158:A:GLU:HG2	4	0.59
(2,76)	1:116:A:LEU:HD21	1:56:A:LYS:H	4	0.59
(2,76)	1:116:A:LEU:HD21	1:56:A:LYS:H	10	0.59
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	7	0.59
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	13	0.59
(2,34)	1:39:A:LEU:HD12	1:35:A:LEU:H	2	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	12	0.59
(2,4814)	1:31:A:LEU:HD23	1:69:A:ASP:H	2	0.58
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	1	0.58
(2,4794)	1:115:A:GLN:HG2	1:115:A:GLN:H	2	0.58
(2,4635)	1:23:A:THR:HG21	1:22:A:GLN:H	5	0.58
(2,4635)	1:23:A:THR:HG21	1:22:A:GLN:H	6	0.58
(2,4635)	1:23:A:THR:HG21	1:22:A:GLN:H	12	0.58
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	10	0.58
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	13	0.58
(2,4570)	1:128:A:ILE:HG21	1:38:A:TYR:H	11	0.58
(2,4539)	1:95:A:THR:HG22	1:91:A:HIS:HB2	4	0.58
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	2	0.58
(2,4511)	1:46:A:VAL:HG22	1:46:A:VAL:HB	14	0.58
(2,4511)	1:46:A:VAL:HG21	1:46:A:VAL:HB	15	0.58
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD3	6	0.58
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	9	0.58
(2,4328)	1:156:A:LEU:HD21	1:155:A:LEU:H	6	0.58
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	6	0.58
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	4	0.58
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	15	0.58
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	7	0.58
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	5	0.58
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	13	0.58
(2,4022)	1:143:A:ILE:HD11	1:147:A:GLN:HE22	9	0.58
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	10	0.58
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	14	0.58
(2,3913)	1:176:A:VAL:HG21	1:100:A:PHE:H	13	0.58
(2,3904)	1:31:A:LEU:HD23	1:72:A:ASN:H	5	0.58
(2,3896)	1:134:A:LEU:HD23	1:132:A:HIS:H	2	0.58
(2,3896)	1:134:A:LEU:HD21	1:132:A:HIS:H	3	0.58
(2,3896)	1:134:A:LEU:HD22	1:132:A:HIS:H	11	0.58
(2,3810)	1:150:A:THR:HG21	1:150:A:THR:H	6	0.58
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD13	12	0.58
(2,3789)	1:128:A:ILE:HG22	1:128:A:ILE:H	7	0.58
(2,3719)	1:81:A:LYS:HE2	1:81:A:LYS:H	2	0.58
(2,3689)	1:60:A:ILE:HD13	1:61:A:PHE:H	3	0.58
(2,3689)	1:60:A:ILE:HD13	1:61:A:PHE:H	8	0.58
(2,3689)	1:60:A:ILE:HD11	1:61:A:PHE:H	10	0.58
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	12	0.58
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD22	14	0.58
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD23	14	0.58
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG22	14	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG23	7	0.58
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	12	0.58
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	5	0.58
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	13	0.58
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB2	13	0.58
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	15	0.58
(2,2910)	1:169:A:GLU:H	1:169:A:GLU:HG2	1	0.58
(2,2896)	1:164:A:GLU:H	1:163:A:CYS:H	3	0.58
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD22	4	0.58
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	8	0.58
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD21	11	0.58
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	5	0.58
(2,2575)	1:36:A:GLU:HG2	1:35:A:LEU:H	6	0.58
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	1	0.58
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG22	9	0.58
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	14	0.58
(2,2274)	1:189:A:HIS:H	1:188:A:MET:HB3	9	0.58
(2,2116)	1:97:A:ALA:HB2	1:100:A:PHE:H	4	0.58
(2,2116)	1:97:A:ALA:HB3	1:100:A:PHE:H	8	0.58
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	13	0.58
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	6	0.58
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD11	10	0.58
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD11	4	0.58
(2,1833)	1:13:A:LYS:H	1:13:A:LYS:HB2	12	0.58
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG22	12	0.58
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	15	0.58
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	7	0.58
(2,1517)	1:39:A:LEU:HD11	1:61:A:PHE:HB2	13	0.58
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	1	0.58
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG22	13	0.58
(2,1470)	1:53:A:ILE:HG21	1:54:A:LEU:HA	11	0.58
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	12	0.58
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	14	0.58
(2,1392)	1:31:A:LEU:HD21	1:27:A:TYR:H	7	0.58
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	12	0.58
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD23	5	0.58
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	15	0.58
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD23	5	0.58
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD21	11	0.58
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD21	13	0.58
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG23	3	0.58
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD11	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	12	0.58
(2,775)	1:121:A:ALA:HB1	1:60:A:ILE:HG21	12	0.58
(2,700)	1:23:A:THR:HG21	1:21:A:LEU:H	6	0.58
(2,700)	1:23:A:THR:HG23	1:21:A:LEU:H	9	0.58
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	1	0.58
(2,585)	1:180:A:VAL:HG23	1:181:A:PRO:HG3	13	0.58
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE1	2	0.58
(2,528)	1:46:A:VAL:HG21	1:41:A:GLU:HB3	1	0.58
(2,528)	1:46:A:VAL:HG21	1:41:A:GLU:HB3	7	0.58
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	11	0.58
(2,497)	1:142:A:LEU:HD13	1:138:A:ILE:HA	12	0.58
(2,467)	1:178:A:LEU:HD21	1:175:A:GLU:H	5	0.58
(2,467)	1:178:A:LEU:HD22	1:175:A:GLU:H	7	0.58
(2,415)	1:37:A:THR:HG21	1:36:A:GLU:HG3	2	0.58
(2,411)	1:138:A:ILE:HG23	1:117:A:ILE:HG22	3	0.58
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG22	7	0.58
(2,393)	1:39:A:LEU:HD23	1:57:A:GLU:HB3	5	0.58
(2,372)	1:95:A:THR:HG21	1:92:A:CYS:H	10	0.58
(2,372)	1:95:A:THR:HG22	1:92:A:CYS:H	11	0.58
(2,372)	1:95:A:THR:HG23	1:92:A:CYS:H	15	0.58
(2,351)	1:188:A:MET:HE1	1:108:A:LYS:HA	5	0.58
(2,309)	1:79:A:LEU:HD22	1:79:A:LEU:H	2	0.58
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	11	0.58
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD12	1	0.58
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	12	0.58
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	13	0.58
(2,156)	1:7:A:GLU:HG2	1:8:A:PHE:H	12	0.58
(2,112)	1:177:A:MET:HE3	1:100:A:PHE:HE2	11	0.58
(2,88)	1:60:A:ILE:HD12	1:117:A:ILE:HD12	2	0.58
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD12	9	0.58
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD11	12	0.58
(2,88)	1:60:A:ILE:HD13	1:117:A:ILE:HD11	13	0.58
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	4	0.58
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	1	0.58
(2,30)	1:32:A:HIS:HD2	1:35:A:LEU:HD13	8	0.58
(2,4818)	1:7:A:GLU:H	1:5:A:SER:HB2	4	0.57
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	8	0.57
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	5	0.57
(2,4794)	1:115:A:GLN:HG2	1:115:A:GLN:H	12	0.57
(2,4778)	1:11:A:ARG:HD2	1:12:A:LYS:H	15	0.57
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG3	9	0.57
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	13	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4654)	1:83:A:GLU:HG2	1:84:A:GLN:HE21	6	0.57
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD11	5	0.57
(2,4635)	1:23:A:THR:HG21	1:22:A:GLN:H	1	0.57
(2,4635)	1:23:A:THR:HG22	1:22:A:GLN:H	13	0.57
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	6	0.57
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	9	0.57
(2,4584)	1:170:A:LEU:HD23	1:90:A:GLY:H	12	0.57
(2,4570)	1:128:A:ILE:HG23	1:38:A:TYR:H	9	0.57
(2,4570)	1:128:A:ILE:HG21	1:38:A:TYR:H	12	0.57
(2,4511)	1:46:A:VAL:HG23	1:46:A:VAL:HB	13	0.57
(2,4502)	1:14:A:GLU:HB2	1:15:A:PHE:HE2	14	0.57
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD11	6	0.57
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	11	0.57
(2,4417)	1:153:A:GLN:HG2	1:149:A:VAL:HG11	7	0.57
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD11	13	0.57
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD11	8	0.57
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD23	13	0.57
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	8	0.57
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	12	0.57
(2,4272)	1:174:A:LEU:HD21	1:175:A:GLU:HB2	6	0.57
(2,4264)	1:16:A:ILE:HD11	1:19:A:GLU:HB3	8	0.57
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD12	6	0.57
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD11	11	0.57
(2,4218)	1:85:A:LEU:HD11	1:84:A:GLN:H	8	0.57
(2,4218)	1:85:A:LEU:HD12	1:84:A:GLN:H	10	0.57
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	11	0.57
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	1	0.57
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	1	0.57
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	5	0.57
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	13	0.57
(2,4123)	1:28:A:VAL:HG21	1:72:A:ASN:H	2	0.57
(2,4088)	1:33:A:GLU:H	1:31:A:LEU:HD12	2	0.57
(2,4069)	1:23:A:THR:HG21	1:24:A:GLU:H	3	0.57
(2,4069)	1:23:A:THR:HG23	1:24:A:GLU:H	8	0.57
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	1	0.57
(2,3913)	1:176:A:VAL:HG22	1:100:A:PHE:H	8	0.57
(2,3907)	1:138:A:ILE:HD12	1:142:A:LEU:H	3	0.57
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD11	1	0.57
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD11	4	0.57
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	13	0.57
(2,3789)	1:128:A:ILE:HG21	1:128:A:ILE:H	2	0.57
(2,3689)	1:60:A:ILE:HD13	1:61:A:PHE:H	11	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3689)	1:60:A:ILE:HD12	1:61:A:PHE:H	15	0.57
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	12	0.57
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG23	10	0.57
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	4	0.57
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	14	0.57
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD21	14	0.57
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB2	5	0.57
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD22	2	0.57
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	14	0.57
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	3	0.57
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG23	6	0.57
(2,2116)	1:97:A:ALA:HB3	1:100:A:PHE:H	3	0.57
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	9	0.57
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	4	0.57
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD12	11	0.57
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	11	0.57
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	14	0.57
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	2	0.57
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	6	0.57
(2,1630)	1:178:A:LEU:HD22	1:153:A:GLN:H	12	0.57
(2,1517)	1:39:A:LEU:HD13	1:61:A:PHE:HB2	2	0.57
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	4	0.57
(2,1498)	1:49:A:ILE:HG23	1:43:A:THR:H	7	0.57
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	11	0.57
(2,1470)	1:53:A:ILE:HG23	1:54:A:LEU:HA	1	0.57
(2,1470)	1:53:A:ILE:HG23	1:54:A:LEU:HA	3	0.57
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	6	0.57
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	7	0.57
(2,1463)	1:16:A:ILE:HG22	1:158:A:GLU:HG3	9	0.57
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG12	12	0.57
(2,1244)	1:20:A:LEU:HD11	1:21:A:LEU:H	11	0.57
(2,1243)	1:21:A:LEU:HD22	1:21:A:LEU:HB2	4	0.57
(2,1243)	1:21:A:LEU:HD21	1:21:A:LEU:HB2	10	0.57
(2,1243)	1:21:A:LEU:HD21	1:21:A:LEU:HB2	11	0.57
(2,1226)	1:53:A:ILE:HA	1:53:A:ILE:HD12	7	0.57
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB2	2	0.57
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	6	0.57
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB3	8	0.57
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	14	0.57
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG22	5	0.57
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD13	14	0.57
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD22	15	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG22	1	0.57
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG22	8	0.57
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG21	11	0.57
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG21	13	0.57
(2,933)	1:15:A:PHE:HB3	1:18:A:ALA:HB3	5	0.57
(2,933)	1:15:A:PHE:HB3	1:18:A:ALA:HB1	12	0.57
(2,921)	1:54:A:LEU:HD13	1:55:A:ASN:HB2	4	0.57
(2,836)	1:64:A:ILE:HG21	1:65:A:GLN:HG3	13	0.57
(2,824)	1:134:A:LEU:HD21	1:33:A:GLU:HG3	2	0.57
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	1	0.57
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	13	0.57
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE3	14	0.57
(2,705)	1:18:A:ALA:HB2	1:21:A:LEU:HG	2	0.57
(2,705)	1:18:A:ALA:HB3	1:21:A:LEU:HG	4	0.57
(2,700)	1:23:A:THR:HG21	1:21:A:LEU:H	3	0.57
(2,658)	1:104:A:VAL:HG13	1:184:A:ALA:HA	15	0.57
(2,610)	1:28:A:VAL:HG12	1:74:A:ILE:H	6	0.57
(2,610)	1:28:A:VAL:HG13	1:74:A:ILE:H	12	0.57
(2,610)	1:28:A:VAL:HG12	1:74:A:ILE:H	13	0.57
(2,608)	1:28:A:VAL:HG12	1:75:A:PHE:H	3	0.57
(2,608)	1:28:A:VAL:HG11	1:75:A:PHE:H	5	0.57
(2,608)	1:28:A:VAL:HG12	1:75:A:PHE:H	7	0.57
(2,585)	1:180:A:VAL:HG23	1:181:A:PRO:HG3	5	0.57
(2,581)	1:180:A:VAL:HG23	1:183:A:LYS:H	9	0.57
(2,505)	1:174:A:LEU:HD21	1:157:A:LYS:HE3	2	0.57
(2,505)	1:174:A:LEU:HD23	1:157:A:LYS:HE3	11	0.57
(2,467)	1:178:A:LEU:HD23	1:175:A:GLU:H	1	0.57
(2,461)	1:134:A:LEU:HD21	1:33:A:GLU:HG2	10	0.57
(2,444)	1:31:A:LEU:HD11	1:30:A:ASP:HB2	6	0.57
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG22	4	0.57
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD12	11	0.57
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG21	12	0.57
(2,372)	1:95:A:THR:HG21	1:92:A:CYS:H	8	0.57
(2,372)	1:95:A:THR:HG21	1:92:A:CYS:H	9	0.57
(2,372)	1:95:A:THR:HG23	1:92:A:CYS:H	13	0.57
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD12	10	0.57
(2,340)	1:102:A:MET:HE1	1:99:A:LYS:HE3	14	0.57
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD22	10	0.57
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD11	2	0.57
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD13	3	0.57
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD13	11	0.57
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	1	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,88)	1:60:A:ILE:HD11	1:117:A:ILE:HD13	7	0.57
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD11	10	0.57
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	6	0.57
(2,60)	1:174:A:LEU:HD23	1:178:A:LEU:H	12	0.57
(2,55)	1:142:A:LEU:HD12	1:106:A:TYR:HH	10	0.57
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	5	0.57
(2,34)	1:39:A:LEU:HD13	1:35:A:LEU:H	13	0.57
(2,30)	1:32:A:HIS:HD2	1:35:A:LEU:HD13	13	0.57
(2,11)	1:79:A:LEU:HD11	1:79:A:LEU:H	6	0.57
(2,4814)	1:31:A:LEU:HD23	1:69:A:ASP:H	12	0.56
(2,4814)	1:31:A:LEU:HD23	1:69:A:ASP:H	14	0.56
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	15	0.56
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG2	15	0.56
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB2	11	0.56
(2,4654)	1:83:A:GLU:HG2	1:84:A:GLN:HE21	4	0.56
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD11	4	0.56
(2,4635)	1:23:A:THR:HG22	1:22:A:GLN:H	14	0.56
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	8	0.56
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	4	0.56
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	1	0.56
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HB3	5	0.56
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG12	7	0.56
(2,4423)	1:174:A:LEU:HD12	1:157:A:LYS:HE2	8	0.56
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD11	5	0.56
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG23	3	0.56
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG2	6	0.56
(2,4358)	1:177:A:MET:HE1	1:173:A:GLY:HA3	9	0.56
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	7	0.56
(2,4352)	1:28:A:VAL:HG21	1:25:A:LYS:HG2	8	0.56
(2,4322)	1:20:A:LEU:HD12	1:152:A:TYR:H	9	0.56
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	3	0.56
(2,4287)	1:13:A:LYS:HD3	1:15:A:PHE:HD1	5	0.56
(2,4272)	1:174:A:LEU:HD22	1:175:A:GLU:HB2	14	0.56
(2,4271)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	7	0.56
(2,4268)	1:99:A:LYS:HG2	1:101:A:GLN:H	6	0.56
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD11	9	0.56
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	1	0.56
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD22	6	0.56
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	13	0.56
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	3	0.56
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	4	0.56
(2,4069)	1:23:A:THR:HG23	1:24:A:GLU:H	9	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4069)	1:23:A:THR:HG22	1:24:A:GLU:H	15	0.56
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD1	12	0.56
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	2	0.56
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	14	0.56
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	8	0.56
(2,3930)	1:184:A:ALA:HB2	1:107:A:CYS:H	13	0.56
(2,3913)	1:176:A:VAL:HG21	1:100:A:PHE:H	10	0.56
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	1	0.56
(2,3896)	1:134:A:LEU:HD21	1:132:A:HIS:H	8	0.56
(2,3896)	1:134:A:LEU:HD21	1:132:A:HIS:H	15	0.56
(2,3862)	1:101:A:GLN:HE21	1:104:A:VAL:HG13	1	0.56
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	7	0.56
(2,3816)	1:156:A:LEU:HD22	1:156:A:LEU:H	13	0.56
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD13	5	0.56
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD13	11	0.56
(2,3789)	1:128:A:ILE:HG23	1:128:A:ILE:H	6	0.56
(2,3789)	1:128:A:ILE:HG21	1:128:A:ILE:H	15	0.56
(2,3770)	1:117:A:ILE:HD11	1:118:A:LEU:H	15	0.56
(2,3689)	1:60:A:ILE:HD12	1:61:A:PHE:H	1	0.56
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	10	0.56
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG23	11	0.56
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	7	0.56
(2,3309)	1:28:A:VAL:HG21	1:31:A:LEU:H	10	0.56
(2,3260)	1:161:A:THR:HG21	1:158:A:GLU:H	4	0.56
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD21	9	0.56
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	11	0.56
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	11	0.56
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG22	13	0.56
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	8	0.56
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	2	0.56
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	11	0.56
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	4	0.56
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	10	0.56
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD22	6	0.56
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	15	0.56
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD13	6	0.56
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	2	0.56
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	14	0.56
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG11	15	0.56
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	3	0.56
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	7	0.56
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	15	0.56
(2,1392)	1:31:A:LEU:HD21	1:27:A:TYR:H	12	0.56
(2,1267)	1:94:A:VAL:HG21	1:97:A:ALA:H	4	0.56
(2,1244)	1:20:A:LEU:HD13	1:21:A:LEU:H	5	0.56
(2,1243)	1:21:A:LEU:HD22	1:21:A:LEU:HB2	3	0.56
(2,1243)	1:21:A:LEU:HD22	1:21:A:LEU:HB2	6	0.56
(2,1243)	1:21:A:LEU:HD23	1:21:A:LEU:HB2	8	0.56
(2,1243)	1:21:A:LEU:HD22	1:21:A:LEU:HB2	13	0.56
(2,1243)	1:21:A:LEU:HD22	1:21:A:LEU:HB2	14	0.56
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	3	0.56
(2,1210)	1:134:A:LEU:HD12	1:134:A:LEU:HA	6	0.56
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG21	4	0.56
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG22	2	0.56
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG22	7	0.56
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD23	7	0.56
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	2	0.56
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	13	0.56
(2,712)	1:157:A:LYS:HG2	1:157:A:LYS:HE2	15	0.56
(2,608)	1:28:A:VAL:HG13	1:75:A:PHE:H	2	0.56
(2,585)	1:180:A:VAL:HG21	1:181:A:PRO:HG3	10	0.56
(2,569)	1:49:A:ILE:HG13	1:42:A:MET:HE1	3	0.56
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	5	0.56
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	6	0.56
(2,508)	1:155:A:LEU:HD22	1:155:A:LEU:HB2	8	0.56
(2,505)	1:174:A:LEU:HD22	1:157:A:LYS:HE3	8	0.56
(2,467)	1:178:A:LEU:HD21	1:175:A:GLU:H	9	0.56
(2,467)	1:178:A:LEU:HD22	1:175:A:GLU:H	14	0.56
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG23	8	0.56
(2,441)	1:31:A:LEU:HD11	1:61:A:PHE:HE1	4	0.56
(2,441)	1:31:A:LEU:HD11	1:61:A:PHE:HE1	7	0.56
(2,411)	1:138:A:ILE:HG23	1:117:A:ILE:HG22	2	0.56
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG22	10	0.56
(2,393)	1:39:A:LEU:HD23	1:57:A:GLU:HB3	12	0.56
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG22	5	0.56
(2,373)	1:96:A:TRP:HH2	1:95:A:THR:HG23	9	0.56
(2,372)	1:95:A:THR:HG21	1:92:A:CYS:H	3	0.56
(2,372)	1:95:A:THR:HG22	1:92:A:CYS:H	12	0.56
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	12	0.56
(2,309)	1:79:A:LEU:HD21	1:79:A:LEU:H	14	0.56
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	15	0.56
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	11	0.56
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD13	13	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD12	8	0.56
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD22	8	0.56
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	1	0.56
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE3	14	0.56
(2,94)	1:180:A:VAL:HG22	1:103:A:TYR:HA	4	0.56
(2,77)	1:76:A:LEU:HD13	1:80:A:GLU:HG3	13	0.56
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	10	0.56
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	7	0.56
(2,11)	1:79:A:LEU:HD11	1:79:A:LEU:H	14	0.56
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD2	7	0.55
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	3	0.55
(2,4814)	1:31:A:LEU:HD22	1:69:A:ASP:H	6	0.55
(2,4802)	1:167:A:LYS:HD3	1:167:A:LYS:H	11	0.55
(2,4794)	1:115:A:GLN:HG2	1:115:A:GLN:H	4	0.55
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	6	0.55
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	8	0.55
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	9	0.55
(2,4778)	1:11:A:ARG:HD3	1:12:A:LYS:H	4	0.55
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB2	12	0.55
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD21	15	0.55
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD13	9	0.55
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD11	12	0.55
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	7	0.55
(2,4551)	1:21:A:LEU:HD23	1:75:A:PHE:HD1	8	0.55
(2,4530)	1:60:A:ILE:HG23	1:57:A:GLU:HG2	15	0.55
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG12	14	0.55
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD13	10	0.55
(2,4358)	1:177:A:MET:HE1	1:173:A:GLY:HA3	15	0.55
(2,4331)	1:95:A:THR:HG23	1:92:A:CYS:HG	15	0.55
(2,4328)	1:156:A:LEU:HD23	1:155:A:LEU:H	15	0.55
(2,4322)	1:20:A:LEU:HD13	1:152:A:TYR:H	12	0.55
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD2	11	0.55
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD12	2	0.55
(2,4272)	1:174:A:LEU:HD23	1:175:A:GLU:HB2	9	0.55
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD22	4	0.55
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD21	11	0.55
(2,4208)	1:64:A:ILE:HG21	1:66:A:GLU:H	3	0.55
(2,4185)	1:178:A:LEU:HD11	1:179:A:SER:H	14	0.55
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	5	0.55
(2,4123)	1:28:A:VAL:HG22	1:72:A:ASN:H	12	0.55
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	1	0.55
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	2	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4069)	1:23:A:THR:HG21	1:24:A:GLU:H	6	0.55
(2,4069)	1:23:A:THR:HG22	1:24:A:GLU:H	13	0.55
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD12	15	0.55
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	15	0.55
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	12	0.55
(2,3930)	1:184:A:ALA:HB2	1:107:A:CYS:H	7	0.55
(2,3913)	1:176:A:VAL:HG21	1:100:A:PHE:H	1	0.55
(2,3913)	1:176:A:VAL:HG22	1:100:A:PHE:H	5	0.55
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	6	0.55
(2,3789)	1:128:A:ILE:HG21	1:128:A:ILE:H	3	0.55
(2,3789)	1:128:A:ILE:HG21	1:128:A:ILE:H	4	0.55
(2,3789)	1:128:A:ILE:HG23	1:128:A:ILE:H	5	0.55
(2,3789)	1:128:A:ILE:HG22	1:128:A:ILE:H	8	0.55
(2,3789)	1:128:A:ILE:HG21	1:128:A:ILE:H	10	0.55
(2,3789)	1:128:A:ILE:HG22	1:128:A:ILE:H	11	0.55
(2,3689)	1:60:A:ILE:HD13	1:61:A:PHE:H	7	0.55
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	13	0.55
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG23	4	0.55
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG22	6	0.55
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	8	0.55
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG23	1	0.55
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	3	0.55
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG22	7	0.55
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG21	9	0.55
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	1	0.55
(2,3309)	1:28:A:VAL:HG21	1:31:A:LEU:H	3	0.55
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	5	0.55
(2,3257)	1:170:A:LEU:HD22	1:160:A:LEU:H	9	0.55
(2,3131)	1:49:A:ILE:HG22	1:49:A:ILE:H	7	0.55
(2,3131)	1:49:A:ILE:HG22	1:49:A:ILE:H	8	0.55
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG13	15	0.55
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	10	0.55
(2,2998)	1:185:A:ASN:H	1:185:A:ASN:HD22	3	0.55
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	9	0.55
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	13	0.55
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG22	14	0.55
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	2	0.55
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	1	0.55
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	13	0.55
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	4	0.55
(2,1854)	1:143:A:ILE:HD11	1:147:A:GLN:H	15	0.55
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG13	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	1:135:A:ALA:HA	1:129:A:GLN:HE22	12	0.55
(2,1555)	1:18:A:ALA:HB3	1:22:A:GLN:HB3	1	0.55
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	13	0.55
(2,1517)	1:39:A:LEU:HD13	1:61:A:PHE:HB2	10	0.55
(2,1517)	1:39:A:LEU:HD12	1:61:A:PHE:HB2	12	0.55
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG21	1	0.55
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	5	0.55
(2,1470)	1:53:A:ILE:HG23	1:54:A:LEU:HA	10	0.55
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG13	2	0.55
(2,1454)	1:103:A:TYR:HD2	1:149:A:VAL:HG13	10	0.55
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	9	0.55
(2,1267)	1:94:A:VAL:HG22	1:97:A:ALA:H	2	0.55
(2,1244)	1:20:A:LEU:HD11	1:21:A:LEU:H	12	0.55
(2,1243)	1:21:A:LEU:HD21	1:21:A:LEU:HB2	1	0.55
(2,1243)	1:21:A:LEU:HD21	1:21:A:LEU:HB2	5	0.55
(2,1243)	1:21:A:LEU:HD23	1:21:A:LEU:HB2	12	0.55
(2,1243)	1:21:A:LEU:HD21	1:21:A:LEU:HB2	15	0.55
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG22	10	0.55
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG23	12	0.55
(2,1144)	1:164:A:GLU:HA	1:163:A:CYS:HB3	6	0.55
(2,1122)	1:7:A:GLU:HG2	1:7:A:GLU:HA	7	0.55
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG22	5	0.55
(2,978)	1:104:A:VAL:HA	1:180:A:VAL:HG21	5	0.55
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	15	0.55
(2,836)	1:64:A:ILE:HG23	1:65:A:GLN:HG3	4	0.55
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	7	0.55
(2,608)	1:28:A:VAL:HG12	1:75:A:PHE:H	6	0.55
(2,608)	1:28:A:VAL:HG13	1:75:A:PHE:H	10	0.55
(2,585)	1:180:A:VAL:HG21	1:181:A:PRO:HG3	7	0.55
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	3	0.55
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	9	0.55
(2,505)	1:174:A:LEU:HD21	1:157:A:LYS:HE3	7	0.55
(2,467)	1:178:A:LEU:HD22	1:175:A:GLU:H	3	0.55
(2,461)	1:134:A:LEU:HD22	1:33:A:GLU:HG2	3	0.55
(2,461)	1:134:A:LEU:HD23	1:33:A:GLU:HG2	11	0.55
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG21	5	0.55
(2,441)	1:31:A:LEU:HD12	1:61:A:PHE:HE1	9	0.55
(2,419)	1:53:A:ILE:HD11	1:49:A:ILE:HB	11	0.55
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD11	1	0.55
(2,393)	1:39:A:LEU:HD21	1:57:A:GLU:HB3	11	0.55
(2,372)	1:95:A:THR:HG22	1:92:A:CYS:H	4	0.55
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	7	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	12	0.55
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD11	3	0.55
(2,309)	1:79:A:LEU:HD22	1:79:A:LEU:H	9	0.55
(2,309)	1:79:A:LEU:HD22	1:79:A:LEU:H	11	0.55
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD11	9	0.55
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD22	8	0.55
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	14	0.55
(2,187)	1:148:A:ARG:HD2	1:155:A:LEU:HD21	15	0.55
(2,132)	1:23:A:THR:HG21	1:148:A:ARG:HD2	14	0.55
(2,94)	1:180:A:VAL:HG22	1:103:A:TYR:HA	6	0.55
(2,66)	1:118:A:LEU:HD23	1:114:A:ASN:HD21	5	0.55
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	9	0.55
(2,66)	1:118:A:LEU:HD23	1:114:A:ASN:HD21	11	0.55
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	15	0.55
(2,61)	1:155:A:LEU:HD22	1:21:A:LEU:H	13	0.55
(2,35)	1:39:A:LEU:HD12	1:65:A:GLN:HG3	2	0.55
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	3	0.55
(2,34)	1:39:A:LEU:HD12	1:35:A:LEU:H	4	0.55
(2,34)	1:39:A:LEU:HD11	1:35:A:LEU:H	8	0.55
(2,34)	1:39:A:LEU:HD12	1:35:A:LEU:H	11	0.55
(2,11)	1:79:A:LEU:HD11	1:79:A:LEU:H	3	0.55
(2,11)	1:79:A:LEU:HD11	1:79:A:LEU:H	11	0.55
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	7	0.54
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	14	0.54
(2,4699)	1:7:A:GLU:H	1:6:A:PRO:HD3	14	0.54
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD13	9	0.54
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	4	0.54
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HB3	6	0.54
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	13	0.54
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	15	0.54
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD13	14	0.54
(2,4459)	1:57:A:GLU:HA	1:59:A:ILE:HD13	2	0.54
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG12	13	0.54
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD13	10	0.54
(2,4331)	1:95:A:THR:HG22	1:92:A:CYS:HG	11	0.54
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD12	4	0.54
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	13	0.54
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD21	14	0.54
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	2	0.54
(2,4208)	1:64:A:ILE:HG21	1:66:A:GLU:H	9	0.54
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	15	0.54
(2,4185)	1:178:A:LEU:HD11	1:179:A:SER:H	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	9	0.54
(2,4172)	1:18:A:ALA:HB3	1:22:A:GLN:HE22	2	0.54
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD12	9	0.54
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	5	0.54
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	5	0.54
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	12	0.54
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	7	0.54
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	15	0.54
(2,4069)	1:23:A:THR:HG22	1:24:A:GLU:H	14	0.54
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	11	0.54
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD12	3	0.54
(2,3961)	1:155:A:LEU:HD12	1:155:A:LEU:H	13	0.54
(2,3943)	1:18:A:ALA:HB1	1:17:A:MET:H	10	0.54
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	10	0.54
(2,3861)	1:143:A:ILE:HG22	1:147:A:GLN:HE22	3	0.54
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD12	4	0.54
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD13	3	0.54
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD13	7	0.54
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD13	15	0.54
(2,3789)	1:128:A:ILE:HG23	1:128:A:ILE:H	12	0.54
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	7	0.54
(2,3737)	1:95:A:THR:HG23	1:95:A:THR:H	1	0.54
(2,3737)	1:95:A:THR:HG22	1:95:A:THR:H	5	0.54
(2,3737)	1:95:A:THR:HG22	1:95:A:THR:H	13	0.54
(2,3689)	1:60:A:ILE:HD12	1:61:A:PHE:H	12	0.54
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG21	13	0.54
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	12	0.54
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	14	0.54
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	3	0.54
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	8	0.54
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD13	15	0.54
(2,3131)	1:49:A:ILE:HG21	1:49:A:ILE:H	3	0.54
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG11	2	0.54
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG12	14	0.54
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG21	12	0.54
(2,3041)	1:22:A:GLN:HG2	1:23:A:THR:H	3	0.54
(2,2901)	1:166:A:GLY:HA2	1:167:A:LYS:H	4	0.54
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG23	8	0.54
(2,2311)	1:55:A:ASN:HB2	1:55:A:ASN:HD21	4	0.54
(2,2273)	1:189:A:HIS:H	1:189:A:HIS:HB2	6	0.54
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD21	9	0.54
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG23	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2116)	1:97:A:ALA:HB3	1:100:A:PHE:H	7	0.54
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	14	0.54
(2,1965)	1:39:A:LEU:HD11	1:39:A:LEU:H	10	0.54
(2,1965)	1:39:A:LEU:HD11	1:39:A:LEU:H	15	0.54
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	9	0.54
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	14	0.54
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	10	0.54
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	11	0.54
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	12	0.54
(2,1861)	1:141:A:TYR:HE2	1:136:A:ASN:H	11	0.54
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	1	0.54
(2,1838)	1:16:A:ILE:HD13	1:158:A:GLU:H	7	0.54
(2,1837)	1:121:A:ALA:H	1:60:A:ILE:HD11	1	0.54
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	3	0.54
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	7	0.54
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	11	0.54
(2,1768)	1:86:A:PRO:HB3	1:87:A:GLU:H	12	0.54
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	7	0.54
(2,1555)	1:18:A:ALA:HB3	1:22:A:GLN:HB3	12	0.54
(2,1498)	1:49:A:ILE:HG21	1:43:A:THR:H	10	0.54
(2,1470)	1:53:A:ILE:HG21	1:54:A:LEU:HA	4	0.54
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	8	0.54
(2,1470)	1:53:A:ILE:HG21	1:54:A:LEU:HA	14	0.54
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	3	0.54
(2,1392)	1:31:A:LEU:HD21	1:27:A:TYR:H	14	0.54
(2,1368)	1:79:A:LEU:HD22	1:17:A:MET:HE3	7	0.54
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	1	0.54
(2,1243)	1:21:A:LEU:HD23	1:21:A:LEU:HB2	2	0.54
(2,1243)	1:21:A:LEU:HD21	1:21:A:LEU:HB2	7	0.54
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	9	0.54
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	12	0.54
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	3	0.54
(2,831)	1:84:A:GLN:HG3	1:83:A:GLU:HA	1	0.54
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE1	15	0.54
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	6	0.54
(2,658)	1:104:A:VAL:HG13	1:184:A:ALA:HA	12	0.54
(2,638)	1:150:A:THR:HG22	1:153:A:GLN:HE21	14	0.54
(2,612)	1:28:A:VAL:HG13	1:68:A:TYR:HE1	12	0.54
(2,610)	1:28:A:VAL:HG13	1:74:A:ILE:H	15	0.54
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	1	0.54
(2,508)	1:155:A:LEU:HD21	1:155:A:LEU:HB2	2	0.54
(2,467)	1:178:A:LEU:HD21	1:175:A:GLU:H	8	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,441)	1:31:A:LEU:HD13	1:61:A:PHE:HE1	13	0.54
(2,411)	1:138:A:ILE:HG22	1:117:A:ILE:HG22	8	0.54
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD13	3	0.54
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD12	8	0.54
(2,372)	1:95:A:THR:HG21	1:92:A:CYS:H	1	0.54
(2,372)	1:95:A:THR:HG22	1:92:A:CYS:H	6	0.54
(2,351)	1:188:A:MET:HE1	1:108:A:LYS:HA	3	0.54
(2,351)	1:188:A:MET:HE1	1:108:A:LYS:HA	9	0.54
(2,270)	1:103:A:TYR:HA	1:67:A:ILE:HD12	3	0.54
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD12	5	0.54
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE1	6	0.54
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD21	7	0.54
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD13	2	0.54
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	3	0.54
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	12	0.54
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	3	0.54
(2,30)	1:32:A:HIS:HD2	1:35:A:LEU:HD13	12	0.54
(2,11)	1:79:A:LEU:HD13	1:79:A:LEU:H	2	0.54
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	15	0.53
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	9	0.53
(2,4794)	1:115:A:GLN:HG2	1:115:A:GLN:H	10	0.53
(2,4654)	1:83:A:GLU:HG2	1:84:A:GLN:HE21	11	0.53
(2,4609)	1:141:A:TYR:HE1	1:33:A:GLU:H	1	0.53
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	9	0.53
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	14	0.53
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG21	13	0.53
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	15	0.53
(2,4570)	1:128:A:ILE:HG21	1:38:A:TYR:H	6	0.53
(2,4492)	1:79:A:LEU:HD23	1:25:A:LYS:HG3	1	0.53
(2,4404)	1:115:A:GLN:HG3	1:118:A:LEU:HD22	11	0.53
(2,4348)	1:60:A:ILE:HD11	1:113:A:SER:H	5	0.53
(2,4339)	1:134:A:LEU:HD23	1:129:A:GLN:HG3	6	0.53
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD12	2	0.53
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	8	0.53
(2,4208)	1:64:A:ILE:HG23	1:66:A:GLU:H	4	0.53
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	11	0.53
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	3	0.53
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	6	0.53
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	11	0.53
(2,4069)	1:23:A:THR:HG23	1:24:A:GLU:H	7	0.53
(2,4069)	1:23:A:THR:HG21	1:24:A:GLU:H	11	0.53
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	14	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3896)	1:134:A:LEU:HD23	1:132:A:HIS:H	10	0.53
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD12	6	0.53
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	8	0.53
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	9	0.53
(2,3789)	1:128:A:ILE:HG21	1:128:A:ILE:H	9	0.53
(2,3737)	1:95:A:THR:HG23	1:95:A:THR:H	3	0.53
(2,3737)	1:95:A:THR:HG23	1:95:A:THR:H	8	0.53
(2,3689)	1:60:A:ILE:HD11	1:61:A:PHE:H	5	0.53
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	13	0.53
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD12	1	0.53
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	2	0.53
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	6	0.53
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	9	0.53
(2,3508)	1:27:A:TYR:HE2	1:75:A:PHE:HD2	9	0.53
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	6	0.53
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD12	11	0.53
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG11	7	0.53
(2,3131)	1:49:A:ILE:HG22	1:49:A:ILE:H	2	0.53
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	5	0.53
(2,3131)	1:49:A:ILE:HG21	1:49:A:ILE:H	9	0.53
(2,3131)	1:49:A:ILE:HG22	1:49:A:ILE:H	13	0.53
(2,3084)	1:82:A:TYR:H	1:89:A:VAL:HG11	12	0.53
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB3	11	0.53
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	2	0.53
(2,2901)	1:166:A:GLY:HA2	1:167:A:LYS:H	5	0.53
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	9	0.53
(2,2822)	1:143:A:ILE:H	1:142:A:LEU:HD23	12	0.53
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	13	0.53
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	12	0.53
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	13	0.53
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	14	0.53
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	15	0.53
(2,2288)	1:21:A:LEU:HD12	1:22:A:GLN:H	6	0.53
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD21	11	0.53
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG23	2	0.53
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	11	0.53
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	11	0.53
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	1	0.53
(2,1965)	1:39:A:LEU:HD11	1:39:A:LEU:H	2	0.53
(2,1965)	1:39:A:LEU:HD11	1:39:A:LEU:H	6	0.53
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	7	0.53
(2,1965)	1:39:A:LEU:HD12	1:39:A:LEU:H	13	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	15	0.53
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD11	8	0.53
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	2	0.53
(2,1854)	1:143:A:ILE:HD13	1:147:A:GLN:H	9	0.53
(2,1838)	1:16:A:ILE:HD13	1:158:A:GLU:H	4	0.53
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	9	0.53
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	2	0.53
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	3	0.53
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	9	0.53
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	8	0.53
(2,1547)	1:95:A:THR:HG23	1:78:A:GLU:HB2	5	0.53
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD22	11	0.53
(2,1522)	1:76:A:LEU:HD13	1:68:A:TYR:HE1	1	0.53
(2,1519)	1:39:A:LEU:HD13	1:65:A:GLN:H	2	0.53
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	3	0.53
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	5	0.53
(2,1470)	1:53:A:ILE:HG23	1:54:A:LEU:HA	15	0.53
(2,1439)	1:102:A:MET:HE2	1:106:A:TYR:HD2	14	0.53
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD12	5	0.53
(2,1392)	1:31:A:LEU:HD21	1:27:A:TYR:H	5	0.53
(2,1392)	1:31:A:LEU:HD23	1:27:A:TYR:H	13	0.53
(2,1386)	1:33:A:GLU:HG2	1:29:A:ARG:HD3	5	0.53
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG23	10	0.53
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD23	2	0.53
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	6	0.53
(2,1244)	1:20:A:LEU:HD11	1:21:A:LEU:H	2	0.53
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	13	0.53
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	4	0.53
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	1	0.53
(2,836)	1:64:A:ILE:HG21	1:65:A:GLN:HG3	9	0.53
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	11	0.53
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	7	0.53
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG21	5	0.53
(2,734)	1:36:A:GLU:HG3	1:35:A:LEU:H	11	0.53
(2,712)	1:157:A:LYS:HG2	1:157:A:LYS:HE2	10	0.53
(2,700)	1:23:A:THR:HG23	1:21:A:LEU:H	10	0.53
(2,700)	1:23:A:THR:HG21	1:21:A:LEU:H	11	0.53
(2,612)	1:28:A:VAL:HG12	1:68:A:TYR:HE1	6	0.53
(2,608)	1:28:A:VAL:HG13	1:75:A:PHE:H	1	0.53
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE3	15	0.53
(2,508)	1:155:A:LEU:HD21	1:155:A:LEU:HB2	10	0.53
(2,508)	1:155:A:LEU:HD21	1:155:A:LEU:HB2	14	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,508)	1:155:A:LEU:HD23	1:155:A:LEU:HB2	15	0.53
(2,505)	1:174:A:LEU:HD22	1:157:A:LYS:HE3	12	0.53
(2,467)	1:178:A:LEU:HD21	1:175:A:GLU:H	2	0.53
(2,454)	1:53:A:ILE:HG21	1:60:A:ILE:HG23	2	0.53
(2,441)	1:31:A:LEU:HD12	1:61:A:PHE:HE1	6	0.53
(2,441)	1:31:A:LEU:HD12	1:61:A:PHE:HE1	12	0.53
(2,411)	1:138:A:ILE:HG21	1:117:A:ILE:HG23	5	0.53
(2,393)	1:39:A:LEU:HD21	1:57:A:GLU:HB3	4	0.53
(2,318)	1:20:A:LEU:HD23	1:152:A:TYR:HD2	15	0.53
(2,313)	1:20:A:LEU:HD13	1:22:A:GLN:H	5	0.53
(2,313)	1:20:A:LEU:HD12	1:22:A:GLN:H	8	0.53
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	3	0.53
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	7	0.53
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	13	0.53
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	11	0.53
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	1	0.53
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD21	2	0.53
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	14	0.53
(2,87)	1:67:A:ILE:HG22	1:31:A:LEU:HD12	5	0.53
(2,34)	1:39:A:LEU:HD12	1:35:A:LEU:H	10	0.53
(2,11)	1:79:A:LEU:HD13	1:79:A:LEU:H	7	0.53
(2,11)	1:79:A:LEU:HD13	1:79:A:LEU:H	8	0.53
(2,11)	1:79:A:LEU:HD12	1:79:A:LEU:H	10	0.53
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	2	0.52
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG3	7	0.52
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	3	0.52
(2,4778)	1:11:A:ARG:HD2	1:12:A:LYS:H	8	0.52
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	9	0.52
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB3	5	0.52
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	14	0.52
(2,4558)	1:99:A:LYS:HD2	1:98:A:ASP:HB2	11	0.52
(2,4358)	1:177:A:MET:HE2	1:173:A:GLY:HA3	3	0.52
(2,4358)	1:177:A:MET:HE1	1:173:A:GLY:HA3	4	0.52
(2,4304)	1:186:A:ASP:HB3	1:183:A:LYS:HG3	1	0.52
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	12	0.52
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	9	0.52
(2,4208)	1:64:A:ILE:HG21	1:66:A:GLU:H	13	0.52
(2,4185)	1:178:A:LEU:HD12	1:179:A:SER:H	3	0.52
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	8	0.52
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	10	0.52
(2,4160)	1:53:A:ILE:HG22	1:122:A:GLY:H	15	0.52
(2,4069)	1:23:A:THR:HG21	1:24:A:GLU:H	1	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	6	0.52
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	13	0.52
(2,3931)	1:156:A:LEU:HD23	1:177:A:MET:H	10	0.52
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	6	0.52
(2,3904)	1:31:A:LEU:HD23	1:72:A:ASN:H	11	0.52
(2,3896)	1:134:A:LEU:HD22	1:132:A:HIS:H	14	0.52
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD12	8	0.52
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	2	0.52
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	2	0.52
(2,3802)	1:138:A:ILE:H	1:138:A:ILE:HD12	14	0.52
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	1	0.52
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	9	0.52
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	12	0.52
(2,3737)	1:95:A:THR:HG21	1:95:A:THR:H	6	0.52
(2,3737)	1:95:A:THR:HG23	1:95:A:THR:H	9	0.52
(2,3737)	1:95:A:THR:HG23	1:95:A:THR:H	10	0.52
(2,3737)	1:95:A:THR:HG21	1:95:A:THR:H	12	0.52
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	8	0.52
(2,3689)	1:60:A:ILE:HD11	1:61:A:PHE:H	2	0.52
(2,3683)	1:59:A:ILE:HG21	1:59:A:ILE:H	3	0.52
(2,3683)	1:59:A:ILE:HG21	1:59:A:ILE:H	6	0.52
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG22	6	0.52
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG21	8	0.52
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD11	15	0.52
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG23	5	0.52
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG22	15	0.52
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG23	2	0.52
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG21	11	0.52
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	8	0.52
(2,3372)	1:141:A:TYR:HE1	1:141:A:TYR:H	9	0.52
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG23	10	0.52
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	6	0.52
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG21	14	0.52
(2,3264)	1:94:A:VAL:HG21	1:172:A:ASP:H	13	0.52
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	6	0.52
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD13	7	0.52
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD13	13	0.52
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	14	0.52
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	4	0.52
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	14	0.52
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	15	0.52
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB2	2	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	14	0.52
(2,2971)	1:180:A:VAL:H	1:182:A:LYS:HB2	13	0.52
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG22	7	0.52
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	5	0.52
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG23	11	0.52
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	9	0.52
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	4	0.52
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG23	12	0.52
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG23	13	0.52
(2,2165)	1:151:A:LYS:H	1:151:A:LYS:HB2	13	0.52
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	8	0.52
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	3	0.52
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	5	0.52
(2,1965)	1:39:A:LEU:HD11	1:39:A:LEU:H	11	0.52
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	1	0.52
(2,1854)	1:143:A:ILE:HD13	1:147:A:GLN:H	4	0.52
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	5	0.52
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	8	0.52
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	10	0.52
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	15	0.52
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	5	0.52
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	8	0.52
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG12	13	0.52
(2,1593)	1:135:A:ALA:HB1	1:129:A:GLN:HE21	4	0.52
(2,1592)	1:135:A:ALA:HB2	1:129:A:GLN:HE22	1	0.52
(2,1543)	1:128:A:ILE:HD12	1:132:A:HIS:HD2	13	0.52
(2,1543)	1:128:A:ILE:HD13	1:132:A:HIS:HD2	14	0.52
(2,1498)	1:49:A:ILE:HG22	1:43:A:THR:H	9	0.52
(2,1470)	1:53:A:ILE:HG22	1:54:A:LEU:HA	9	0.52
(2,1392)	1:31:A:LEU:HD21	1:27:A:TYR:H	2	0.52
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	4	0.52
(2,1370)	1:176:A:VAL:HG21	1:100:A:PHE:HE2	2	0.52
(2,1317)	1:43:A:THR:HG21	1:57:A:GLU:HB3	14	0.52
(2,1254)	1:17:A:MET:HE1	1:82:A:TYR:H	2	0.52
(2,1254)	1:17:A:MET:HE1	1:82:A:TYR:H	15	0.52
(2,1244)	1:20:A:LEU:HD13	1:21:A:LEU:H	7	0.52
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	14	0.52
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD11	6	0.52
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	5	0.52
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	4	0.52
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	8	0.52
(2,775)	1:121:A:ALA:HB2	1:60:A:ILE:HG23	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,775)	1:121:A:ALA:HB3	1:60:A:ILE:HG21	14	0.52
(2,700)	1:23:A:THR:HG23	1:21:A:LEU:H	7	0.52
(2,610)	1:28:A:VAL:HG13	1:74:A:ILE:H	1	0.52
(2,610)	1:28:A:VAL:HG11	1:74:A:ILE:H	5	0.52
(2,585)	1:180:A:VAL:HG21	1:181:A:PRO:HG3	1	0.52
(2,467)	1:178:A:LEU:HD23	1:175:A:GLU:H	13	0.52
(2,444)	1:31:A:LEU:HD12	1:30:A:ASP:HB2	8	0.52
(2,441)	1:31:A:LEU:HD11	1:61:A:PHE:HE1	3	0.52
(2,441)	1:31:A:LEU:HD13	1:61:A:PHE:HE1	10	0.52
(2,441)	1:31:A:LEU:HD13	1:61:A:PHE:HE1	15	0.52
(2,411)	1:138:A:ILE:HG21	1:117:A:ILE:HG22	13	0.52
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD11	4	0.52
(2,405)	1:117:A:ILE:HD13	1:138:A:ILE:HD13	7	0.52
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD23	4	0.52
(2,356)	1:138:A:ILE:HD13	1:60:A:ILE:HD13	4	0.52
(2,318)	1:20:A:LEU:HD21	1:152:A:TYR:HD1	6	0.52
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	6	0.52
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	4	0.52
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD11	10	0.52
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD13	1	0.52
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD12	7	0.52
(2,156)	1:7:A:GLU:HG2	1:8:A:PHE:H	1	0.52
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	4	0.52
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE1	11	0.52
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	13	0.52
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	5	0.52
(2,66)	1:118:A:LEU:HD23	1:114:A:ASN:HD21	2	0.52
(2,66)	1:118:A:LEU:HD23	1:114:A:ASN:HD21	8	0.52
(2,60)	1:174:A:LEU:HD21	1:178:A:LEU:H	11	0.52
(2,55)	1:142:A:LEU:HD13	1:106:A:TYR:HH	15	0.52
(2,34)	1:39:A:LEU:HD12	1:35:A:LEU:H	15	0.52
(2,16)	1:79:A:LEU:HD13	1:75:A:PHE:HA	15	0.52
(2,11)	1:79:A:LEU:HD13	1:79:A:LEU:H	12	0.52
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	4	0.51
(2,4814)	1:31:A:LEU:HD23	1:69:A:ASP:H	11	0.51
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	8	0.51
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG2	10	0.51
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	13	0.51
(2,4776)	1:11:A:ARG:HG3	1:11:A:ARG:H	4	0.51
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	8	0.51
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	15	0.51
(2,4715)	1:7:A:GLU:H	1:6:A:PRO:HD2	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4699)	1:7:A:GLU:H	1:5:A:SER:HB2	4	0.51
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD23	10	0.51
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	7	0.51
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	3	0.51
(2,4539)	1:95:A:THR:HG23	1:91:A:HIS:HB2	5	0.51
(2,4539)	1:95:A:THR:HG23	1:91:A:HIS:HB2	15	0.51
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	3	0.51
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	4	0.51
(2,4518)	1:128:A:ILE:HG23	1:124:A:PHE:HZ	15	0.51
(2,4492)	1:79:A:LEU:HD21	1:25:A:LYS:HG3	8	0.51
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	12	0.51
(2,4331)	1:95:A:THR:HG22	1:92:A:CYS:HG	6	0.51
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD2	9	0.51
(2,4272)	1:174:A:LEU:HD21	1:175:A:GLU:HB2	3	0.51
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	5	0.51
(2,4258)	1:95:A:THR:HG23	1:75:A:PHE:HD2	3	0.51
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD12	3	0.51
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	10	0.51
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	2	0.51
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	12	0.51
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	13	0.51
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD22	15	0.51
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	4	0.51
(2,4223)	1:159:A:LEU:HD13	1:156:A:LEU:H	5	0.51
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD22	15	0.51
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	10	0.51
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	15	0.51
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	2	0.51
(2,4150)	1:118:A:LEU:HD11	1:115:A:GLN:H	1	0.51
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	5	0.51
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	14	0.51
(2,4069)	1:23:A:THR:HG23	1:24:A:GLU:H	10	0.51
(2,3913)	1:176:A:VAL:HG21	1:100:A:PHE:H	4	0.51
(2,3904)	1:31:A:LEU:HD23	1:72:A:ASN:H	2	0.51
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	4	0.51
(2,3896)	1:134:A:LEU:HD23	1:132:A:HIS:H	4	0.51
(2,3896)	1:134:A:LEU:HD22	1:132:A:HIS:H	12	0.51
(2,3896)	1:134:A:LEU:HD23	1:132:A:HIS:H	13	0.51
(2,3889)	1:85:A:LEU:HD22	1:84:A:GLN:H	12	0.51
(2,3862)	1:101:A:GLN:HE21	1:104:A:VAL:HG13	3	0.51
(2,3862)	1:101:A:GLN:HE21	1:104:A:VAL:HG11	5	0.51
(2,3861)	1:143:A:ILE:HG21	1:147:A:GLN:HE22	15	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	15	0.51
(2,3832)	1:179:A:SER:HB2	1:179:A:SER:H	10	0.51
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD12	7	0.51
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD13	8	0.51
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD12	14	0.51
(2,3789)	1:128:A:ILE:HG22	1:128:A:ILE:H	1	0.51
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	4	0.51
(2,3737)	1:95:A:THR:HG22	1:95:A:THR:H	15	0.51
(2,3683)	1:59:A:ILE:HG23	1:59:A:ILE:H	2	0.51
(2,3683)	1:59:A:ILE:HG21	1:59:A:ILE:H	5	0.51
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	9	0.51
(2,3619)	1:93:A:PHE:HE1	1:79:A:LEU:HD21	15	0.51
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	7	0.51
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG21	4	0.51
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG22	13	0.51
(2,3477)	1:103:A:TYR:HE2	1:149:A:VAL:HG22	2	0.51
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	2	0.51
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	14	0.51
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG23	1	0.51
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG22	15	0.51
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	3	0.51
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	8	0.51
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	1	0.51
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	2	0.51
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD13	5	0.51
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD12	12	0.51
(2,3163)	1:42:A:MET:HE1	1:54:A:LEU:H	2	0.51
(2,3163)	1:42:A:MET:HE1	1:54:A:LEU:H	3	0.51
(2,3163)	1:42:A:MET:HE1	1:54:A:LEU:H	11	0.51
(2,3131)	1:49:A:ILE:HG22	1:49:A:ILE:H	12	0.51
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	9	0.51
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB3	12	0.51
(2,2902)	1:166:A:GLY:HA3	1:167:A:LYS:H	4	0.51
(2,2675)	1:117:A:ILE:HD13	1:113:A:SER:H	5	0.51
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG22	3	0.51
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	14	0.51
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	6	0.51
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	15	0.51
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	13	0.51
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	8	0.51
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD12	2	0.51
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1854)	1:143:A:ILE:HD11	1:147:A:GLN:H	3	0.51
(2,1854)	1:143:A:ILE:HD11	1:147:A:GLN:H	8	0.51
(2,1838)	1:16:A:ILE:HD12	1:158:A:GLU:H	10	0.51
(2,1838)	1:16:A:ILE:HD13	1:158:A:GLU:H	15	0.51
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	1	0.51
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	14	0.51
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG23	5	0.51
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG23	14	0.51
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	14	0.51
(2,1630)	1:178:A:LEU:HD23	1:153:A:GLN:H	11	0.51
(2,1512)	1:142:A:LEU:HD13	1:117:A:ILE:H	2	0.51
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	1	0.51
(2,1392)	1:31:A:LEU:HD21	1:27:A:TYR:H	11	0.51
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG23	2	0.51
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	13	0.51
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	3	0.51
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	4	0.51
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	6	0.51
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD12	10	0.51
(2,1088)	1:161:A:THR:HG22	1:158:A:GLU:HA	4	0.51
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG22	10	0.51
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD22	7	0.51
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	10	0.51
(2,712)	1:157:A:LYS:HG2	1:157:A:LYS:HE2	14	0.51
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	4	0.51
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE1	6	0.51
(2,700)	1:23:A:THR:HG22	1:21:A:LEU:H	14	0.51
(2,687)	1:184:A:ALA:HB1	1:181:A:PRO:HD3	9	0.51
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	11	0.51
(2,528)	1:46:A:VAL:HG22	1:41:A:GLU:HB3	5	0.51
(2,508)	1:155:A:LEU:HD21	1:155:A:LEU:HB2	12	0.51
(2,497)	1:142:A:LEU:HD11	1:138:A:ILE:HA	1	0.51
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	15	0.51
(2,419)	1:53:A:ILE:HD11	1:49:A:ILE:HB	3	0.51
(2,419)	1:53:A:ILE:HD12	1:49:A:ILE:HB	5	0.51
(2,393)	1:39:A:LEU:HD22	1:57:A:GLU:HB3	10	0.51
(2,316)	1:20:A:LEU:HD11	1:152:A:TYR:HB3	1	0.51
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG21	5	0.51
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	3	0.51
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD21	4	0.51
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD12	8	0.51
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE3	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	12	0.51
(2,94)	1:180:A:VAL:HG23	1:103:A:TYR:HA	7	0.51
(2,94)	1:180:A:VAL:HG21	1:103:A:TYR:HA	12	0.51
(2,82)	1:76:A:LEU:HD12	1:77:A:LYS:HE2	7	0.51
(2,77)	1:76:A:LEU:HD11	1:80:A:GLU:HG3	14	0.51
(2,60)	1:174:A:LEU:HD21	1:178:A:LEU:H	8	0.51
(2,55)	1:142:A:LEU:HD11	1:106:A:TYR:HH	6	0.51
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	1	0.51
(2,11)	1:79:A:LEU:HD12	1:79:A:LEU:H	13	0.51
(2,4802)	1:167:A:LYS:HD2	1:167:A:LYS:H	8	0.5
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD2	10	0.5
(2,4794)	1:115:A:GLN:HG3	1:115:A:GLN:H	11	0.5
(2,4778)	1:11:A:ARG:HD2	1:12:A:LYS:H	9	0.5
(2,4715)	1:7:A:GLU:H	1:6:A:PRO:HD2	4	0.5
(2,4654)	1:83:A:GLU:HG3	1:84:A:GLN:HE21	14	0.5
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD12	7	0.5
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD11	11	0.5
(2,4635)	1:23:A:THR:HG23	1:22:A:GLN:H	10	0.5
(2,4635)	1:23:A:THR:HG21	1:22:A:GLN:H	11	0.5
(2,4630)	1:126:A:ASP:H	1:127:A:GLU:HG3	6	0.5
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD23	13	0.5
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	11	0.5
(2,4596)	1:166:A:GLY:H	1:167:A:LYS:HD2	9	0.5
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	13	0.5
(2,4570)	1:128:A:ILE:HG23	1:38:A:TYR:H	3	0.5
(2,4551)	1:21:A:LEU:HD21	1:75:A:PHE:HD2	7	0.5
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD11	15	0.5
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG11	8	0.5
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	2	0.5
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG21	2	0.5
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	10	0.5
(2,4263)	1:178:A:LEU:HD23	1:175:A:GLU:HG2	15	0.5
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	8	0.5
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD12	14	0.5
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	3	0.5
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	11	0.5
(2,4197)	1:16:A:ILE:HG21	1:158:A:GLU:H	13	0.5
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD13	2	0.5
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	3	0.5
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	9	0.5
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	12	0.5
(2,4037)	1:21:A:LEU:HD23	1:22:A:GLN:H	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	8	0.5
(2,3931)	1:156:A:LEU:HD22	1:177:A:MET:H	1	0.5
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	3	0.5
(2,3913)	1:176:A:VAL:HG23	1:100:A:PHE:H	15	0.5
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD13	7	0.5
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD11	3	0.5
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD11	5	0.5
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD13	10	0.5
(2,3789)	1:128:A:ILE:HG22	1:128:A:ILE:H	14	0.5
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	15	0.5
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	7	0.5
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	9	0.5
(2,3737)	1:95:A:THR:HG21	1:95:A:THR:H	11	0.5
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	14	0.5
(2,3683)	1:59:A:ILE:HG23	1:59:A:ILE:H	11	0.5
(2,3652)	1:161:A:THR:HG23	1:162:A:CYS:H	11	0.5
(2,3613)	1:100:A:PHE:HE1	1:74:A:ILE:HG22	14	0.5
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG23	2	0.5
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	4	0.5
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	12	0.5
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	12	0.5
(2,3250)	1:153:A:GLN:H	1:154:A:LEU:HD11	10	0.5
(2,3169)	1:53:A:ILE:HG21	1:54:A:LEU:H	11	0.5
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	13	0.5
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	1	0.5
(2,3131)	1:49:A:ILE:HG22	1:49:A:ILE:H	6	0.5
(2,3131)	1:49:A:ILE:HG23	1:49:A:ILE:H	10	0.5
(2,3004)	1:3:A:LEU:H	1:3:A:LEU:HA	13	0.5
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB1	3	0.5
(2,2835)	1:146:A:VAL:HG12	1:148:A:ARG:H	9	0.5
(2,2614)	1:99:A:LYS:H	1:99:A:LYS:HE2	5	0.5
(2,2614)	1:99:A:LYS:H	1:99:A:LYS:HE2	12	0.5
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG22	5	0.5
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD22	7	0.5
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG21	10	0.5
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	6	0.5
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB2	7	0.5
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	9	0.5
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	8	0.5
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	8	0.5
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	7	0.5
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG21	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	6	0.5
(2,1555)	1:18:A:ALA:HB3	1:22:A:GLN:HB3	2	0.5
(2,1555)	1:18:A:ALA:HB3	1:22:A:GLN:HB3	10	0.5
(2,1522)	1:76:A:LEU:HD13	1:68:A:TYR:HE1	5	0.5
(2,1519)	1:39:A:LEU:HD13	1:65:A:GLN:H	10	0.5
(2,1517)	1:39:A:LEU:HD13	1:61:A:PHE:HB2	15	0.5
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	8	0.5
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	3	0.5
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	8	0.5
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG21	3	0.5
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG21	8	0.5
(2,1244)	1:20:A:LEU:HD13	1:21:A:LEU:H	9	0.5
(2,1244)	1:20:A:LEU:HD12	1:21:A:LEU:H	15	0.5
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	7	0.5
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	6	0.5
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	15	0.5
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG21	11	0.5
(2,933)	1:15:A:PHE:HB3	1:18:A:ALA:HB1	1	0.5
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD13	10	0.5
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE2	14	0.5
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	2	0.5
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	9	0.5
(2,804)	1:86:A:PRO:HB2	1:87:A:GLU:H	10	0.5
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG21	7	0.5
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	9	0.5
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	3	0.5
(2,658)	1:104:A:VAL:HG13	1:184:A:ALA:HA	8	0.5
(2,612)	1:28:A:VAL:HG12	1:68:A:TYR:HE1	13	0.5
(2,610)	1:28:A:VAL:HG12	1:74:A:ILE:H	3	0.5
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD22	12	0.5
(2,592)	1:64:A:ILE:HD13	1:31:A:LEU:HD23	15	0.5
(2,508)	1:155:A:LEU:HD21	1:155:A:LEU:HB2	7	0.5
(2,498)	1:142:A:LEU:HD12	1:60:A:ILE:HA	11	0.5
(2,467)	1:178:A:LEU:HD23	1:175:A:GLU:H	10	0.5
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	2	0.5
(2,415)	1:37:A:THR:HG21	1:36:A:GLU:HG3	12	0.5
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD11	10	0.5
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	8	0.5
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD23	11	0.5
(2,356)	1:138:A:ILE:HD13	1:60:A:ILE:HD13	15	0.5
(2,328)	1:42:A:MET:HE2	1:60:A:ILE:HB	2	0.5
(2,318)	1:20:A:LEU:HD22	1:152:A:TYR:HD1	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,313)	1:20:A:LEU:HD11	1:22:A:GLN:H	2	0.5
(2,309)	1:79:A:LEU:HD21	1:79:A:LEU:H	1	0.5
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD21	1	0.5
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD22	4	0.5
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	5	0.5
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	6	0.5
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD11	2	0.5
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE1	2	0.5
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	9	0.5
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD22	3	0.5
(2,66)	1:118:A:LEU:HD22	1:114:A:ASN:HD21	14	0.5
(2,60)	1:174:A:LEU:HD23	1:178:A:LEU:H	13	0.5
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	5	0.5
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	8	0.5
(2,11)	1:79:A:LEU:HD12	1:79:A:LEU:H	5	0.5
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	3	0.49
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG23	6	0.49
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	10	0.49
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	2	0.49
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD11	5	0.49
(2,4554)	1:146:A:VAL:HG22	1:110:A:LYS:HD2	7	0.49
(2,4547)	1:102:A:MET:HE2	1:64:A:ILE:HA	13	0.49
(2,4539)	1:95:A:THR:HG23	1:91:A:HIS:HB2	13	0.49
(2,4518)	1:128:A:ILE:HG21	1:124:A:PHE:HZ	6	0.49
(2,4492)	1:79:A:LEU:HD21	1:25:A:LYS:HG3	11	0.49
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	15	0.49
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	4	0.49
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG22	14	0.49
(2,4348)	1:60:A:ILE:HD13	1:113:A:SER:H	11	0.49
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD13	9	0.49
(2,4292)	1:48:A:GLU:HB3	1:49:A:ILE:HG23	10	0.49
(2,4272)	1:174:A:LEU:HD23	1:175:A:GLU:HB2	1	0.49
(2,4265)	1:142:A:LEU:HD13	1:110:A:LYS:HB2	15	0.49
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD13	8	0.49
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	2	0.49
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD13	5	0.49
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD11	15	0.49
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	15	0.49
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD23	7	0.49
(2,4238)	1:60:A:ILE:H	1:116:A:LEU:HD22	10	0.49
(2,4223)	1:159:A:LEU:HD13	1:156:A:LEU:H	8	0.49
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD21	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD21	4	0.49
(2,4185)	1:178:A:LEU:HD13	1:179:A:SER:H	4	0.49
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	14	0.49
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD11	4	0.49
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD11	5	0.49
(2,4160)	1:53:A:ILE:HG23	1:122:A:GLY:H	4	0.49
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	4	0.49
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	5	0.49
(2,4150)	1:118:A:LEU:HD13	1:115:A:GLN:H	12	0.49
(2,4150)	1:118:A:LEU:HD11	1:115:A:GLN:H	13	0.49
(2,4119)	1:7:A:GLU:HG2	1:7:A:GLU:H	12	0.49
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	10	0.49
(2,4069)	1:23:A:THR:HG21	1:24:A:GLU:H	12	0.49
(2,4037)	1:21:A:LEU:HD23	1:22:A:GLN:H	12	0.49
(2,4021)	1:18:A:ALA:HB1	1:20:A:LEU:H	12	0.49
(2,3933)	1:94:A:VAL:HG21	1:95:A:THR:H	2	0.49
(2,3913)	1:176:A:VAL:HG22	1:100:A:PHE:H	11	0.49
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD13	1	0.49
(2,3832)	1:179:A:SER:HB2	1:179:A:SER:H	15	0.49
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD13	12	0.49
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD12	15	0.49
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	3	0.49
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	4	0.49
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	13	0.49
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	14	0.49
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	3	0.49
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	11	0.49
(2,3771)	1:118:A:LEU:HD11	1:119:A:GLU:H	13	0.49
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	15	0.49
(2,3768)	1:117:A:ILE:HD11	1:117:A:ILE:H	5	0.49
(2,3737)	1:95:A:THR:HG21	1:95:A:THR:H	2	0.49
(2,3683)	1:59:A:ILE:HG23	1:59:A:ILE:H	1	0.49
(2,3683)	1:59:A:ILE:HG21	1:59:A:ILE:H	7	0.49
(2,3683)	1:59:A:ILE:HG22	1:59:A:ILE:H	12	0.49
(2,3683)	1:59:A:ILE:HG22	1:59:A:ILE:H	15	0.49
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	7	0.49
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	15	0.49
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG22	3	0.49
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD12	8	0.49
(2,3526)	1:96:A:TRP:HZ2	1:95:A:THR:HG22	12	0.49
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG23	6	0.49
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD12	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3163)	1:42:A:MET:HE1	1:54:A:LEU:H	6	0.49
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	7	0.49
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	11	0.49
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	14	0.49
(2,2901)	1:166:A:GLY:HA2	1:167:A:LYS:H	2	0.49
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	12	0.49
(2,2675)	1:117:A:ILE:HD13	1:113:A:SER:H	4	0.49
(2,2614)	1:99:A:LYS:H	1:99:A:LYS:HE2	6	0.49
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	4	0.49
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	13	0.49
(2,2528)	1:87:A:GLU:HG2	1:87:A:GLU:H	12	0.49
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	11	0.49
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	15	0.49
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	5	0.49
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG21	11	0.49
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB2	11	0.49
(2,2116)	1:97:A:ALA:HB3	1:100:A:PHE:H	2	0.49
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	10	0.49
(2,1965)	1:39:A:LEU:HD13	1:39:A:LEU:H	12	0.49
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	7	0.49
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	9	0.49
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	13	0.49
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	14	0.49
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	12	0.49
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG22	3	0.49
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG21	5	0.49
(2,1854)	1:143:A:ILE:HD13	1:147:A:GLN:H	5	0.49
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	14	0.49
(2,1838)	1:16:A:ILE:HD12	1:158:A:GLU:H	11	0.49
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	6	0.49
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG22	12	0.49
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	13	0.49
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG12	10	0.49
(2,1592)	1:135:A:ALA:HB2	1:129:A:GLN:HE22	7	0.49
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	6	0.49
(2,1522)	1:76:A:LEU:HD12	1:68:A:TYR:HE1	9	0.49
(2,1522)	1:76:A:LEU:HD13	1:68:A:TYR:HE1	11	0.49
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	3	0.49
(2,1476)	1:134:A:LEU:HD22	1:34:A:CYS:HA	4	0.49
(2,1476)	1:134:A:LEU:HD21	1:34:A:CYS:HA	6	0.49
(2,1392)	1:31:A:LEU:HD23	1:27:A:TYR:H	6	0.49
(2,1392)	1:31:A:LEU:HD22	1:27:A:TYR:H	10	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	2	0.49
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG23	4	0.49
(2,1244)	1:20:A:LEU:HD13	1:21:A:LEU:H	4	0.49
(2,1244)	1:20:A:LEU:HD13	1:21:A:LEU:H	13	0.49
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD22	4	0.49
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	5	0.49
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	11	0.49
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	4	0.49
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	9	0.49
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD22	14	0.49
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG22	13	0.49
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD12	15	0.49
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	3	0.49
(2,729)	1:97:A:ALA:HB1	1:100:A:PHE:HE1	8	0.49
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	1	0.49
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	12	0.49
(2,700)	1:23:A:THR:HG21	1:21:A:LEU:H	1	0.49
(2,577)	1:89:A:VAL:HG11	1:93:A:PHE:HE2	11	0.49
(2,505)	1:174:A:LEU:HD21	1:157:A:LYS:HE3	5	0.49
(2,498)	1:142:A:LEU:HD11	1:60:A:ILE:HA	5	0.49
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	7	0.49
(2,419)	1:53:A:ILE:HD12	1:49:A:ILE:HB	8	0.49
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	12	0.49
(2,415)	1:37:A:THR:HG21	1:36:A:GLU:HG3	7	0.49
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD13	9	0.49
(2,380)	1:31:A:LEU:HD23	1:70:A:PHE:H	2	0.49
(2,318)	1:20:A:LEU:HD23	1:152:A:TYR:HD2	7	0.49
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	12	0.49
(2,313)	1:20:A:LEU:HD13	1:22:A:GLN:H	4	0.49
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	4	0.49
(2,309)	1:79:A:LEU:HD22	1:79:A:LEU:H	5	0.49
(2,309)	1:79:A:LEU:HD22	1:79:A:LEU:H	8	0.49
(2,309)	1:79:A:LEU:HD23	1:79:A:LEU:H	10	0.49
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	8	0.49
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	14	0.49
(2,170)	1:37:A:THR:HG21	1:33:A:GLU:HG3	15	0.49
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	7	0.49
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD12	4	0.49
(2,87)	1:67:A:ILE:HG22	1:31:A:LEU:HD11	11	0.49
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	2	0.49
(2,25)	1:37:A:THR:HG22	1:33:A:GLU:HG2	14	0.49
(2,16)	1:79:A:LEU:HD11	1:75:A:PHE:HA	14	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	1:79:A:LEU:HD11	1:79:A:LEU:H	15	0.49
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	1	0.48
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD2	3	0.48
(2,4755)	1:124:A:PHE:HE2	1:50:A:PRO:HG2	2	0.48
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD13	1	0.48
(2,4641)	1:57:A:GLU:H	1:54:A:LEU:HD13	14	0.48
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD22	7	0.48
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	11	0.48
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	8	0.48
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD13	11	0.48
(2,4539)	1:95:A:THR:HG21	1:91:A:HIS:HB2	3	0.48
(2,4539)	1:95:A:THR:HG21	1:91:A:HIS:HB2	10	0.48
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	1	0.48
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG11	5	0.48
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE2	5	0.48
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE2	8	0.48
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD12	12	0.48
(2,4303)	1:186:A:ASP:HB2	1:182:A:LYS:HD2	12	0.48
(2,4287)	1:13:A:LYS:HD2	1:15:A:PHE:HD1	11	0.48
(2,4272)	1:174:A:LEU:HD21	1:175:A:GLU:HB2	12	0.48
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	10	0.48
(2,4264)	1:16:A:ILE:HD13	1:19:A:GLU:HB3	6	0.48
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	10	0.48
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	14	0.48
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	5	0.48
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	12	0.48
(2,4185)	1:178:A:LEU:HD11	1:179:A:SER:H	7	0.48
(2,4172)	1:18:A:ALA:HB3	1:22:A:GLN:HE22	10	0.48
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	9	0.48
(2,4160)	1:53:A:ILE:HG23	1:122:A:GLY:H	14	0.48
(2,4150)	1:118:A:LEU:HD13	1:115:A:GLN:H	2	0.48
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	7	0.48
(2,4069)	1:23:A:THR:HG23	1:24:A:GLU:H	4	0.48
(2,4037)	1:21:A:LEU:HD23	1:22:A:GLN:H	8	0.48
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	2	0.48
(2,3913)	1:176:A:VAL:HG21	1:100:A:PHE:H	6	0.48
(2,3904)	1:31:A:LEU:HD22	1:72:A:ASN:H	6	0.48
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD11	11	0.48
(2,3861)	1:143:A:ILE:HG22	1:147:A:GLN:HE22	4	0.48
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD13	1	0.48
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD13	9	0.48
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD11	11	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	5	0.48
(2,3772)	1:118:A:LEU:HD22	1:119:A:GLU:H	2	0.48
(2,3772)	1:118:A:LEU:HD22	1:119:A:GLU:H	5	0.48
(2,3772)	1:118:A:LEU:HD22	1:119:A:GLU:H	8	0.48
(2,3772)	1:118:A:LEU:HD22	1:119:A:GLU:H	11	0.48
(2,3771)	1:118:A:LEU:HD11	1:119:A:GLU:H	1	0.48
(2,3771)	1:118:A:LEU:HD13	1:119:A:GLU:H	2	0.48
(2,3771)	1:118:A:LEU:HD13	1:119:A:GLU:H	6	0.48
(2,3771)	1:118:A:LEU:HD11	1:119:A:GLU:H	10	0.48
(2,3771)	1:118:A:LEU:HD13	1:119:A:GLU:H	14	0.48
(2,3768)	1:117:A:ILE:HD13	1:117:A:ILE:H	1	0.48
(2,3737)	1:95:A:THR:HG21	1:95:A:THR:H	4	0.48
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	1	0.48
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	2	0.48
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	5	0.48
(2,3683)	1:59:A:ILE:HG21	1:59:A:ILE:H	10	0.48
(2,3683)	1:59:A:ILE:HG21	1:59:A:ILE:H	14	0.48
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	2	0.48
(2,3652)	1:161:A:THR:HG23	1:162:A:CYS:H	7	0.48
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD21	3	0.48
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	13	0.48
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	15	0.48
(2,3309)	1:28:A:VAL:HG23	1:31:A:LEU:H	9	0.48
(2,3264)	1:94:A:VAL:HG23	1:172:A:ASP:H	1	0.48
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG11	6	0.48
(2,3169)	1:53:A:ILE:HG23	1:54:A:LEU:H	3	0.48
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	9	0.48
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	1	0.48
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG21	2	0.48
(2,3032)	1:20:A:LEU:HD22	1:20:A:LEU:H	2	0.48
(2,3032)	1:20:A:LEU:HD23	1:20:A:LEU:H	6	0.48
(2,2948)	1:178:A:LEU:H	1:177:A:MET:HB3	14	0.48
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG23	1	0.48
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG21	2	0.48
(2,2675)	1:117:A:ILE:HD12	1:113:A:SER:H	1	0.48
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG22	2	0.48
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	15	0.48
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD21	1	0.48
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD22	2	0.48
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD22	3	0.48
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD21	10	0.48
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG21	1	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	1	0.48
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	14	0.48
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	10	0.48
(2,1926)	1:185:A:ASN:H	1:185:A:ASN:HB2	3	0.48
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD13	4	0.48
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD13	15	0.48
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	10	0.48
(2,1854)	1:143:A:ILE:HD13	1:147:A:GLN:H	11	0.48
(2,1826)	1:131:A:ARG:HE	1:128:A:ILE:HG21	15	0.48
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	13	0.48
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG23	2	0.48
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	1	0.48
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG23	2	0.48
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	1	0.48
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	15	0.48
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD23	2	0.48
(2,1516)	1:39:A:LEU:HD13	1:61:A:PHE:HB3	15	0.48
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	12	0.48
(2,1395)	1:188:A:MET:HE1	1:188:A:MET:HG3	4	0.48
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG21	9	0.48
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	3	0.48
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	14	0.48
(2,1244)	1:20:A:LEU:HD12	1:21:A:LEU:H	3	0.48
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD22	3	0.48
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	1	0.48
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	9	0.48
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	14	0.48
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	13	0.48
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	6	0.48
(2,851)	1:134:A:LEU:HD23	1:129:A:GLN:HB3	6	0.48
(2,836)	1:64:A:ILE:HG21	1:65:A:GLN:HG3	7	0.48
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	12	0.48
(2,832)	1:85:A:LEU:HG	1:84:A:GLN:HG3	1	0.48
(2,729)	1:97:A:ALA:HB1	1:100:A:PHE:HE1	15	0.48
(2,700)	1:23:A:THR:HG22	1:21:A:LEU:H	15	0.48
(2,687)	1:184:A:ALA:HB2	1:181:A:PRO:HD3	11	0.48
(2,679)	1:157:A:LYS:HG3	1:157:A:LYS:HE2	9	0.48
(2,612)	1:28:A:VAL:HG11	1:68:A:TYR:HE1	8	0.48
(2,608)	1:28:A:VAL:HG13	1:75:A:PHE:H	15	0.48
(2,505)	1:174:A:LEU:HD23	1:157:A:LYS:HE3	4	0.48
(2,497)	1:142:A:LEU:HD11	1:138:A:ILE:HA	11	0.48
(2,473)	1:59:A:ILE:HG22	1:112:A:ASP:HB2	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD13	5	0.48
(2,380)	1:31:A:LEU:HD23	1:70:A:PHE:H	7	0.48
(2,370)	1:138:A:ILE:HG13	1:142:A:LEU:HD11	1	0.48
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	9	0.48
(2,346)	1:102:A:MET:HE1	1:67:A:ILE:HD11	11	0.48
(2,337)	1:102:A:MET:HE3	1:66:A:GLU:HA	5	0.48
(2,336)	1:102:A:MET:HE2	1:100:A:PHE:HA	4	0.48
(2,328)	1:42:A:MET:HE1	1:60:A:ILE:HB	5	0.48
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	7	0.48
(2,316)	1:20:A:LEU:HD12	1:152:A:TYR:HB3	4	0.48
(2,316)	1:20:A:LEU:HD11	1:152:A:TYR:HB3	6	0.48
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD22	3	0.48
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	13	0.48
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	6	0.48
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD21	5	0.48
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD22	7	0.48
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	3	0.48
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD21	4	0.48
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE2	5	0.48
(2,120)	1:161:A:THR:HG23	1:158:A:GLU:HG2	8	0.48
(2,94)	1:180:A:VAL:HG22	1:103:A:TYR:HA	13	0.48
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD11	1	0.48
(2,60)	1:174:A:LEU:HD22	1:178:A:LEU:H	2	0.48
(2,60)	1:174:A:LEU:HD22	1:178:A:LEU:H	10	0.48
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	14	0.48
(2,19)	1:79:A:LEU:HD13	1:92:A:CYS:HG	9	0.48
(2,11)	1:79:A:LEU:HD12	1:79:A:LEU:H	1	0.48
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	2	0.47
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	13	0.47
(2,4776)	1:11:A:ARG:HG3	1:11:A:ARG:H	12	0.47
(2,4749)	1:15:A:PHE:HD1	1:14:A:GLU:HG2	8	0.47
(2,4749)	1:15:A:PHE:HD2	1:14:A:GLU:HG3	14	0.47
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG23	2	0.47
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	12	0.47
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	4	0.47
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD12	15	0.47
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	3	0.47
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	6	0.47
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	12	0.47
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD13	10	0.47
(2,4518)	1:128:A:ILE:HG23	1:124:A:PHE:HZ	7	0.47
(2,4518)	1:128:A:ILE:HG23	1:124:A:PHE:HZ	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4373)	1:167:A:LYS:HD3	1:167:A:LYS:HE2	10	0.47
(2,4373)	1:182:A:LYS:HD3	1:182:A:LYS:HE2	11	0.47
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE3	13	0.47
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	4	0.47
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD2	8	0.47
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD12	14	0.47
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	6	0.47
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	11	0.47
(2,4223)	1:159:A:LEU:HD13	1:156:A:LEU:H	12	0.47
(2,4223)	1:159:A:LEU:HD11	1:156:A:LEU:H	13	0.47
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD22	6	0.47
(2,4208)	1:64:A:ILE:HG21	1:66:A:GLU:H	7	0.47
(2,4208)	1:64:A:ILE:HG23	1:66:A:GLU:H	14	0.47
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD12	11	0.47
(2,4160)	1:53:A:ILE:HG22	1:122:A:GLY:H	1	0.47
(2,4160)	1:53:A:ILE:HG22	1:122:A:GLY:H	10	0.47
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	13	0.47
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	9	0.47
(2,4150)	1:118:A:LEU:HD11	1:115:A:GLN:H	10	0.47
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	7	0.47
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	1	0.47
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	11	0.47
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	7	0.47
(2,4037)	1:21:A:LEU:HD22	1:22:A:GLN:H	3	0.47
(2,4037)	1:21:A:LEU:HD22	1:22:A:GLN:H	6	0.47
(2,4037)	1:21:A:LEU:HD21	1:22:A:GLN:H	10	0.47
(2,4037)	1:21:A:LEU:HD22	1:22:A:GLN:H	14	0.47
(2,4033)	1:15:A:PHE:HD1	1:13:A:LYS:H	12	0.47
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	5	0.47
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	5	0.47
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	10	0.47
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	12	0.47
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD11	2	0.47
(2,3789)	1:128:A:ILE:HG23	1:128:A:ILE:H	13	0.47
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	5	0.47
(2,3771)	1:118:A:LEU:HD12	1:119:A:GLU:H	8	0.47
(2,3771)	1:118:A:LEU:HD13	1:119:A:GLU:H	12	0.47
(2,3768)	1:117:A:ILE:HD11	1:117:A:ILE:H	13	0.47
(2,3737)	1:95:A:THR:HG22	1:95:A:THR:H	7	0.47
(2,3683)	1:59:A:ILE:HG23	1:59:A:ILE:H	4	0.47
(2,3683)	1:59:A:ILE:HG22	1:59:A:ILE:H	8	0.47
(2,3683)	1:59:A:ILE:HG22	1:59:A:ILE:H	13	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3670)	1:43:A:THR:HG22	1:44:A:SER:H	5	0.47
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD13	3	0.47
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD11	12	0.47
(2,3485)	1:106:A:TYR:HE2	1:31:A:LEU:HD12	14	0.47
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD11	1	0.47
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD12	5	0.47
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD13	8	0.47
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG21	6	0.47
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG23	7	0.47
(2,3309)	1:28:A:VAL:HG21	1:31:A:LEU:H	11	0.47
(2,3309)	1:28:A:VAL:HG22	1:31:A:LEU:H	13	0.47
(2,3309)	1:28:A:VAL:HG22	1:31:A:LEU:H	15	0.47
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	9	0.47
(2,3257)	1:170:A:LEU:HD21	1:160:A:LEU:H	11	0.47
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	5	0.47
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	2	0.47
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	5	0.47
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	6	0.47
(2,3169)	1:53:A:ILE:HG23	1:54:A:LEU:H	10	0.47
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	13	0.47
(2,3169)	1:53:A:ILE:HG23	1:54:A:LEU:H	15	0.47
(2,3163)	1:42:A:MET:HE3	1:54:A:LEU:H	8	0.47
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG23	14	0.47
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD13	7	0.47
(2,3032)	1:20:A:LEU:HD23	1:20:A:LEU:H	10	0.47
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	13	0.47
(2,2948)	1:178:A:LEU:H	1:177:A:MET:HB3	1	0.47
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD22	4	0.47
(2,2853)	1:150:A:THR:H	1:153:A:GLN:HE21	2	0.47
(2,2835)	1:146:A:VAL:HG11	1:148:A:ARG:H	8	0.47
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	10	0.47
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG23	13	0.47
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG23	9	0.47
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG23	2	0.47
(2,2303)	1:41:A:GLU:HG2	1:41:A:GLU:H	14	0.47
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	1	0.47
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD21	5	0.47
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	3	0.47
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	3	0.47
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB2	13	0.47
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	4	0.47
(2,1752)	1:76:A:LEU:HD23	1:78:A:GLU:H	7	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG23	1	0.47
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG21	8	0.47
(2,1710)	1:62:A:GLY:H	1:59:A:ILE:HG21	7	0.47
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	4	0.47
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	10	0.47
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	11	0.47
(2,1593)	1:135:A:ALA:HB2	1:129:A:GLN:HE21	6	0.47
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	12	0.47
(2,1480)	1:99:A:LYS:HD2	1:100:A:PHE:H	10	0.47
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	7	0.47
(2,1421)	1:116:A:LEU:HD22	1:116:A:LEU:H	15	0.47
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	13	0.47
(2,1369)	1:156:A:LEU:HD12	1:170:A:LEU:HB3	5	0.47
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	13	0.47
(2,1179)	1:116:A:LEU:HA	1:59:A:ILE:HG21	1	0.47
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	3	0.47
(2,586)	1:180:A:VAL:HG21	1:183:A:LYS:HG2	5	0.47
(2,498)	1:142:A:LEU:HD12	1:60:A:ILE:HA	1	0.47
(2,498)	1:142:A:LEU:HD11	1:60:A:ILE:HA	6	0.47
(2,498)	1:142:A:LEU:HD13	1:60:A:ILE:HA	8	0.47
(2,498)	1:142:A:LEU:HD12	1:60:A:ILE:HA	14	0.47
(2,427)	1:35:A:LEU:HD12	1:35:A:LEU:HA	12	0.47
(2,427)	1:35:A:LEU:HD12	1:35:A:LEU:HA	13	0.47
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	3	0.47
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	9	0.47
(2,419)	1:53:A:ILE:HD11	1:49:A:ILE:HB	4	0.47
(2,419)	1:53:A:ILE:HD12	1:49:A:ILE:HB	13	0.47
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	14	0.47
(2,415)	1:37:A:THR:HG21	1:36:A:GLU:HG3	10	0.47
(2,405)	1:117:A:ILE:HD12	1:138:A:ILE:HD12	2	0.47
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	3	0.47
(2,380)	1:31:A:LEU:HD23	1:70:A:PHE:H	12	0.47
(2,372)	1:95:A:THR:HG23	1:92:A:CYS:H	14	0.47
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	4	0.47
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	7	0.47
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	8	0.47
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD22	14	0.47
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD22	9	0.47
(2,239)	1:36:A:GLU:HA	1:35:A:LEU:HD23	15	0.47
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD13	9	0.47
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD22	9	0.47
(2,35)	1:39:A:LEU:HD12	1:65:A:GLN:HG3	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,19)	1:79:A:LEU:HD12	1:92:A:CYS:HG	5	0.47
(2,16)	1:79:A:LEU:HD13	1:75:A:PHE:HA	11	0.47
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	13	0.47
(1,117)	1:151:A:LYS:O	1:155:A:LEU:H	13	0.47
(2,4814)	1:31:A:LEU:HD23	1:69:A:ASP:H	5	0.46
(2,4814)	1:31:A:LEU:HD21	1:69:A:ASP:H	10	0.46
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	2	0.46
(2,4803)	1:167:A:LYS:H	1:167:A:LYS:HE3	6	0.46
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	6	0.46
(2,4785)	1:56:A:LYS:HE2	1:56:A:LYS:H	10	0.46
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	14	0.46
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	10	0.46
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	4	0.46
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG21	14	0.46
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	10	0.46
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	8	0.46
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	7	0.46
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD13	3	0.46
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	5	0.46
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	8	0.46
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	12	0.46
(2,4635)	1:23:A:THR:HG21	1:22:A:GLN:H	3	0.46
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD23	2	0.46
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD23	4	0.46
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	7	0.46
(2,4518)	1:128:A:ILE:HG23	1:124:A:PHE:HZ	3	0.46
(2,4518)	1:128:A:ILE:HG22	1:124:A:PHE:HZ	10	0.46
(2,4518)	1:128:A:ILE:HG21	1:124:A:PHE:HZ	12	0.46
(2,4489)	1:184:A:ALA:HB3	1:108:A:LYS:HE3	13	0.46
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD3	9	0.46
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG12	6	0.46
(2,4413)	1:42:A:MET:HG3	1:53:A:ILE:HD12	15	0.46
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG21	12	0.46
(2,4358)	1:177:A:MET:HE1	1:176:A:VAL:HA	2	0.46
(2,4358)	1:177:A:MET:HE1	1:173:A:GLY:HA3	12	0.46
(2,4348)	1:60:A:ILE:HD12	1:113:A:SER:H	6	0.46
(2,4348)	1:60:A:ILE:HD13	1:113:A:SER:H	14	0.46
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD2	6	0.46
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD12	11	0.46
(2,4287)	1:13:A:LYS:HD3	1:15:A:PHE:HD1	10	0.46
(2,4264)	1:16:A:ILE:HD12	1:19:A:GLU:HB3	13	0.46
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD22	12	0.46
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	1	0.46
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD12	1	0.46
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD13	6	0.46
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	6	0.46
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	8	0.46
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	11	0.46
(2,4150)	1:118:A:LEU:HD13	1:115:A:GLN:H	14	0.46
(2,4150)	1:118:A:LEU:HD12	1:115:A:GLN:H	15	0.46
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	15	0.46
(2,4108)	1:52:A:GLY:H	1:53:A:ILE:HG12	8	0.46
(2,4078)	1:28:A:VAL:HG21	1:30:A:ASP:H	3	0.46
(2,4037)	1:21:A:LEU:HD22	1:22:A:GLN:H	13	0.46
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD11	9	0.46
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD12	12	0.46
(2,3943)	1:18:A:ALA:HB2	1:17:A:MET:H	11	0.46
(2,3937)	1:184:A:ALA:HB1	1:182:A:LYS:H	2	0.46
(2,3930)	1:184:A:ALA:HB1	1:107:A:CYS:H	9	0.46
(2,3930)	1:184:A:ALA:HB2	1:107:A:CYS:H	11	0.46
(2,3913)	1:176:A:VAL:HG23	1:100:A:PHE:H	9	0.46
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	8	0.46
(2,3889)	1:85:A:LEU:HD22	1:84:A:GLN:H	7	0.46
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD11	14	0.46
(2,3861)	1:143:A:ILE:HG23	1:147:A:GLN:HE22	8	0.46
(2,3832)	1:179:A:SER:HB2	1:179:A:SER:H	11	0.46
(2,3772)	1:118:A:LEU:HD22	1:119:A:GLU:H	6	0.46
(2,3772)	1:118:A:LEU:HD21	1:119:A:GLU:H	10	0.46
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	14	0.46
(2,3683)	1:59:A:ILE:HG23	1:59:A:ILE:H	9	0.46
(2,3670)	1:43:A:THR:HG22	1:44:A:SER:H	11	0.46
(2,3670)	1:43:A:THR:HG21	1:44:A:SER:H	13	0.46
(2,3670)	1:43:A:THR:HG22	1:44:A:SER:H	15	0.46
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	11	0.46
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD13	5	0.46
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD12	10	0.46
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD12	1	0.46
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG21	8	0.46
(2,3289)	1:21:A:LEU:HD12	1:21:A:LEU:H	1	0.46
(2,3289)	1:21:A:LEU:HD12	1:21:A:LEU:H	3	0.46
(2,3289)	1:21:A:LEU:HD12	1:21:A:LEU:H	6	0.46
(2,3257)	1:170:A:LEU:HD22	1:160:A:LEU:H	2	0.46
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD21	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3169)	1:53:A:ILE:HG23	1:54:A:LEU:H	1	0.46
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	12	0.46
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG21	10	0.46
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	7	0.46
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB3	9	0.46
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG22	14	0.46
(2,2644)	1:108:A:LYS:H	1:109:A:ASN:HB2	9	0.46
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	6	0.46
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	7	0.46
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD13	14	0.46
(2,2326)	1:56:A:LYS:H	1:49:A:ILE:HG23	7	0.46
(2,2303)	1:41:A:GLU:HG2	1:41:A:GLU:H	13	0.46
(2,2288)	1:21:A:LEU:HD12	1:22:A:GLN:H	14	0.46
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG23	9	0.46
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG21	11	0.46
(2,2151)	1:105:A:THR:HG22	1:105:A:THR:H	2	0.46
(2,2151)	1:105:A:THR:HG23	1:105:A:THR:H	4	0.46
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB2	4	0.46
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	12	0.46
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB3	15	0.46
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	6	0.46
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG12	4	0.46
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	3	0.46
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG21	11	0.46
(2,1694)	1:142:A:LEU:H	1:142:A:LEU:HB3	12	0.46
(2,1562)	1:13:A:LYS:HB3	1:13:A:LYS:H	7	0.46
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	6	0.46
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD23	9	0.46
(2,1498)	1:49:A:ILE:HG23	1:43:A:THR:H	6	0.46
(2,1476)	1:134:A:LEU:HD23	1:34:A:CYS:HA	15	0.46
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	2	0.46
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	3	0.46
(2,1421)	1:116:A:LEU:HD21	1:116:A:LEU:H	11	0.46
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG23	5	0.46
(2,1280)	1:35:A:LEU:HD23	1:31:A:LEU:HA	4	0.46
(2,1280)	1:35:A:LEU:HD21	1:31:A:LEU:HA	10	0.46
(2,1244)	1:20:A:LEU:HD12	1:21:A:LEU:H	6	0.46
(2,1244)	1:20:A:LEU:HD11	1:21:A:LEU:H	10	0.46
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	2	0.46
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	8	0.46
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	8	0.46
(2,1210)	1:134:A:LEU:HD11	1:134:A:LEU:HA	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	7	0.46
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB1	7	0.46
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG21	4	0.46
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG23	11	0.46
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG22	14	0.46
(2,851)	1:134:A:LEU:HD23	1:129:A:GLN:HB3	13	0.46
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE1	11	0.46
(2,700)	1:23:A:THR:HG21	1:21:A:LEU:H	12	0.46
(2,624)	1:39:A:LEU:HD12	1:43:A:THR:HG22	12	0.46
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	6	0.46
(2,586)	1:180:A:VAL:HG23	1:183:A:LYS:HG2	3	0.46
(2,585)	1:180:A:VAL:HG23	1:181:A:PRO:HG3	2	0.46
(2,498)	1:142:A:LEU:HD11	1:60:A:ILE:HA	3	0.46
(2,498)	1:142:A:LEU:HD12	1:60:A:ILE:HA	10	0.46
(2,427)	1:35:A:LEU:HD11	1:35:A:LEU:HA	10	0.46
(2,427)	1:35:A:LEU:HD12	1:35:A:LEU:HA	11	0.46
(2,425)	1:35:A:LEU:HD12	1:35:A:LEU:H	5	0.46
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	9	0.46
(2,415)	1:37:A:THR:HG22	1:36:A:GLU:HG3	13	0.46
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	1	0.46
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD23	14	0.46
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	12	0.46
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD11	11	0.46
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD21	5	0.46
(2,134)	1:18:A:ALA:HB1	1:22:A:GLN:HB2	4	0.46
(2,127)	1:49:A:ILE:HG12	1:42:A:MET:HE1	3	0.46
(2,94)	1:180:A:VAL:HG23	1:103:A:TYR:HA	8	0.46
(2,87)	1:67:A:ILE:HG22	1:31:A:LEU:HD12	3	0.46
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD13	9	0.46
(2,60)	1:174:A:LEU:HD22	1:178:A:LEU:H	7	0.46
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	7	0.46
(2,35)	1:39:A:LEU:HD12	1:65:A:GLN:HG3	10	0.46
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	12	0.46
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	7	0.45
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	13	0.45
(2,4776)	1:11:A:ARG:HG3	1:11:A:ARG:H	15	0.45
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB2	3	0.45
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD11	10	0.45
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD13	13	0.45
(2,4609)	1:141:A:TYR:HE1	1:33:A:GLU:H	7	0.45
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	8	0.45
(2,4518)	1:128:A:ILE:HG23	1:124:A:PHE:HZ	9	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG12	9	0.45
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	13	0.45
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	8	0.45
(2,4373)	1:167:A:LYS:HD3	1:167:A:LYS:HE2	14	0.45
(2,4358)	1:177:A:MET:HE2	1:173:A:GLY:HA3	7	0.45
(2,4348)	1:60:A:ILE:HD11	1:113:A:SER:H	10	0.45
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	10	0.45
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD13	1	0.45
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD13	10	0.45
(2,4292)	1:48:A:GLU:HB3	1:49:A:ILE:HG21	9	0.45
(2,4284)	1:171:A:LYS:HG2	1:172:A:ASP:H	3	0.45
(2,4264)	1:16:A:ILE:HD12	1:19:A:GLU:HB3	11	0.45
(2,4223)	1:159:A:LEU:HD12	1:156:A:LEU:H	7	0.45
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD21	13	0.45
(2,4186)	1:178:A:LEU:HD22	1:179:A:SER:H	2	0.45
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD11	7	0.45
(2,4150)	1:118:A:LEU:HD13	1:115:A:GLN:H	6	0.45
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG13	6	0.45
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG13	11	0.45
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	6	0.45
(2,4085)	1:169:A:GLU:HG3	1:169:A:GLU:H	8	0.45
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD22	8	0.45
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD23	11	0.45
(2,4037)	1:21:A:LEU:HD22	1:22:A:GLN:H	4	0.45
(2,4037)	1:21:A:LEU:HD21	1:22:A:GLN:H	5	0.45
(2,4037)	1:21:A:LEU:HD21	1:22:A:GLN:H	7	0.45
(2,4037)	1:21:A:LEU:HD21	1:22:A:GLN:H	11	0.45
(2,4037)	1:21:A:LEU:HD21	1:22:A:GLN:H	15	0.45
(2,3933)	1:94:A:VAL:HG22	1:95:A:THR:H	12	0.45
(2,3889)	1:85:A:LEU:HD23	1:84:A:GLN:H	13	0.45
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	1	0.45
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	6	0.45
(2,3818)	1:157:A:LYS:H	1:156:A:LEU:HD12	13	0.45
(2,3816)	1:156:A:LEU:HD22	1:156:A:LEU:H	4	0.45
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	12	0.45
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD12	12	0.45
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	3	0.45
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	8	0.45
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	12	0.45
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD23	4	0.45
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG22	3	0.45
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG22	12	0.45
(2,3169)	1:53:A:ILE:HG21	1:54:A:LEU:H	4	0.45
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	8	0.45
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	12	0.45
(2,3169)	1:53:A:ILE:HG21	1:54:A:LEU:H	14	0.45
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG23	9	0.45
(2,3032)	1:20:A:LEU:HD22	1:20:A:LEU:H	4	0.45
(2,3032)	1:20:A:LEU:HD23	1:20:A:LEU:H	8	0.45
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	12	0.45
(2,3031)	1:20:A:LEU:HD11	1:20:A:LEU:H	12	0.45
(2,2908)	1:169:A:GLU:H	1:168:A:GLY:HA2	1	0.45
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG23	14	0.45
(2,2713)	1:117:A:ILE:HG13	1:117:A:ILE:H	1	0.45
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG23	8	0.45
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG23	2	0.45
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG22	10	0.45
(2,2171)	1:174:A:LEU:HD23	1:174:A:LEU:H	2	0.45
(2,2151)	1:105:A:THR:HG21	1:105:A:THR:H	11	0.45
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	12	0.45
(2,1965)	1:39:A:LEU:HD11	1:39:A:LEU:H	4	0.45
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	3	0.45
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	6	0.45
(2,1828)	1:131:A:ARG:HE	1:47:A:GLU:HG3	6	0.45
(2,1752)	1:76:A:LEU:HD21	1:78:A:GLU:H	12	0.45
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG22	3	0.45
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG21	13	0.45
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG22	15	0.45
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG22	3	0.45
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	15	0.45
(2,1558)	1:20:A:LEU:HD23	1:89:A:VAL:HA	10	0.45
(2,1547)	1:95:A:THR:HG23	1:78:A:GLU:HB2	7	0.45
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	8	0.45
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD22	14	0.45
(2,1421)	1:116:A:LEU:HD22	1:116:A:LEU:H	6	0.45
(2,1421)	1:116:A:LEU:HD22	1:116:A:LEU:H	10	0.45
(2,1369)	1:156:A:LEU:HD12	1:170:A:LEU:HB3	13	0.45
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	12	0.45
(2,1318)	1:177:A:MET:HE3	1:173:A:GLY:H	5	0.45
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	1	0.45
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	1	0.45
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	2	0.45
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	1	0.45
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	8	0.45
(2,1143)	1:43:A:THR:HB	1:39:A:LEU:HD23	7	0.45
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG23	8	0.45
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD11	4	0.45
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	13	0.45
(2,828)	1:128:A:ILE:HD13	1:47:A:GLU:HG2	3	0.45
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG23	14	0.45
(2,712)	1:157:A:LYS:HG2	1:157:A:LYS:HE2	6	0.45
(2,658)	1:104:A:VAL:HG11	1:184:A:ALA:HA	10	0.45
(2,638)	1:150:A:THR:HG23	1:153:A:GLN:HE21	1	0.45
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG22	6	0.45
(2,624)	1:39:A:LEU:HD12	1:43:A:THR:HG22	8	0.45
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD21	13	0.45
(2,586)	1:180:A:VAL:HG23	1:183:A:LYS:HG2	12	0.45
(2,557)	1:60:A:ILE:HD13	1:42:A:MET:HE1	10	0.45
(2,498)	1:142:A:LEU:HD11	1:60:A:ILE:HA	2	0.45
(2,498)	1:142:A:LEU:HD11	1:60:A:ILE:HA	4	0.45
(2,498)	1:142:A:LEU:HD13	1:60:A:ILE:HA	7	0.45
(2,498)	1:142:A:LEU:HD12	1:60:A:ILE:HA	9	0.45
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	1	0.45
(2,427)	1:35:A:LEU:HD12	1:35:A:LEU:HA	8	0.45
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	6	0.45
(2,415)	1:37:A:THR:HG23	1:36:A:GLU:HG3	1	0.45
(2,415)	1:37:A:THR:HG21	1:36:A:GLU:HG3	4	0.45
(2,415)	1:37:A:THR:HG23	1:36:A:GLU:HG3	5	0.45
(2,415)	1:37:A:THR:HG23	1:36:A:GLU:HG3	6	0.45
(2,406)	1:156:A:LEU:HD13	1:93:A:PHE:HZ	2	0.45
(2,387)	1:31:A:LEU:HD21	1:67:A:ILE:HD11	13	0.45
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	4	0.45
(2,380)	1:31:A:LEU:HD22	1:70:A:PHE:H	6	0.45
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD21	3	0.45
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	5	0.45
(2,356)	1:138:A:ILE:HD12	1:60:A:ILE:HD13	6	0.45
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	10	0.45
(2,170)	1:37:A:THR:HG21	1:33:A:GLU:HG3	8	0.45
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD12	12	0.45
(2,160)	1:177:A:MET:HB3	1:156:A:LEU:HD22	14	0.45
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD22	15	0.45
(2,94)	1:180:A:VAL:HG23	1:103:A:TYR:HA	14	0.45
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD13	6	0.45
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD12	7	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:174:A:LEU:HD21	1:178:A:LEU:H	4	0.45
(2,35)	1:39:A:LEU:HD12	1:65:A:GLN:HG3	4	0.45
(2,35)	1:39:A:LEU:HD12	1:65:A:GLN:HG3	11	0.45
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	8	0.45
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	12	0.45
(2,11)	1:79:A:LEU:HD12	1:79:A:LEU:H	4	0.45
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	1	0.44
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD13	6	0.44
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD12	12	0.44
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD13	14	0.44
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD21	5	0.44
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	9	0.44
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	14	0.44
(2,4584)	1:170:A:LEU:HD21	1:90:A:GLY:H	10	0.44
(2,4539)	1:95:A:THR:HG22	1:91:A:HIS:HB2	11	0.44
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG21	9	0.44
(2,4373)	1:167:A:LYS:HD3	1:167:A:LYS:HE2	4	0.44
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE3	9	0.44
(2,4348)	1:60:A:ILE:HD12	1:113:A:SER:H	12	0.44
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD11	8	0.44
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD12	13	0.44
(2,4263)	1:178:A:LEU:HD23	1:175:A:GLU:HG2	1	0.44
(2,4256)	1:80:A:GLU:H	1:79:A:LEU:HD12	1	0.44
(2,4223)	1:159:A:LEU:HD11	1:156:A:LEU:H	1	0.44
(2,4223)	1:159:A:LEU:HD11	1:156:A:LEU:H	3	0.44
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD22	3	0.44
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD23	7	0.44
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD21	12	0.44
(2,4186)	1:178:A:LEU:HD22	1:179:A:SER:H	12	0.44
(2,4177)	1:144:A:LYS:H	1:144:A:LYS:HD2	13	0.44
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	13	0.44
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD11	14	0.44
(2,4160)	1:53:A:ILE:HG22	1:122:A:GLY:H	3	0.44
(2,4160)	1:53:A:ILE:HG23	1:122:A:GLY:H	11	0.44
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	8	0.44
(2,4037)	1:21:A:LEU:HD21	1:22:A:GLN:H	1	0.44
(2,4021)	1:18:A:ALA:HB2	1:20:A:LEU:H	4	0.44
(2,3913)	1:176:A:VAL:HG23	1:100:A:PHE:H	7	0.44
(2,3886)	1:161:A:THR:H	1:162:A:CYS:HB2	10	0.44
(2,3861)	1:143:A:ILE:HG22	1:147:A:GLN:HE22	2	0.44
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	4	0.44
(2,3833)	1:178:A:LEU:HD12	1:178:A:LEU:H	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	11	0.44
(2,3833)	1:178:A:LEU:HD11	1:178:A:LEU:H	12	0.44
(2,3832)	1:179:A:SER:HB2	1:179:A:SER:H	12	0.44
(2,3816)	1:156:A:LEU:HD22	1:156:A:LEU:H	2	0.44
(2,3768)	1:117:A:ILE:HD11	1:117:A:ILE:H	4	0.44
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG21	6	0.44
(2,3737)	1:95:A:THR:HG22	1:95:A:THR:H	14	0.44
(2,3728)	1:87:A:GLU:HG3	1:87:A:GLU:H	6	0.44
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	3	0.44
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	13	0.44
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	2	0.44
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	6	0.44
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	10	0.44
(2,3670)	1:43:A:THR:HG21	1:44:A:SER:H	14	0.44
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	1	0.44
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD13	7	0.44
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG22	12	0.44
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD11	15	0.44
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG23	5	0.44
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	6	0.44
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	15	0.44
(2,3257)	1:170:A:LEU:HD22	1:160:A:LEU:H	4	0.44
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	12	0.44
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	4	0.44
(2,3032)	1:20:A:LEU:HD23	1:20:A:LEU:H	1	0.44
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	11	0.44
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB2	1	0.44
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	10	0.44
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD23	3	0.44
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	5	0.44
(2,2675)	1:117:A:ILE:HD12	1:113:A:SER:H	3	0.44
(2,2643)	1:108:A:LYS:H	1:107:A:CYS:HB2	1	0.44
(2,2643)	1:108:A:LYS:H	1:107:A:CYS:HB2	5	0.44
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	3	0.44
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD13	5	0.44
(2,2275)	1:190:A:VAL:H	1:189:A:HIS:HB3	11	0.44
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD23	14	0.44
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	7	0.44
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	13	0.44
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG23	4	0.44
(2,2151)	1:105:A:THR:HG21	1:105:A:THR:H	6	0.44
(2,2151)	1:105:A:THR:HG23	1:105:A:THR:H	14	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB1	10	0.44
(2,2116)	1:97:A:ALA:HB1	1:100:A:PHE:H	13	0.44
(2,2028)	1:8:A:PHE:H	1:8:A:PHE:HB3	15	0.44
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	7	0.44
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD13	7	0.44
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG23	1	0.44
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG22	10	0.44
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG23	12	0.44
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG23	13	0.44
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	14	0.44
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG11	4	0.44
(2,1555)	1:18:A:ALA:HB2	1:22:A:GLN:HB3	9	0.44
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	13	0.44
(2,1519)	1:39:A:LEU:HD13	1:65:A:GLN:H	4	0.44
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	8	0.44
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	12	0.44
(2,1512)	1:142:A:LEU:HD12	1:117:A:ILE:H	8	0.44
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	1	0.44
(2,1421)	1:116:A:LEU:HD21	1:116:A:LEU:H	5	0.44
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	8	0.44
(2,1421)	1:116:A:LEU:HD21	1:116:A:LEU:H	14	0.44
(2,1395)	1:188:A:MET:HE3	1:188:A:MET:HG3	12	0.44
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	1	0.44
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	2	0.44
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	7	0.44
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG22	12	0.44
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG21	15	0.44
(2,1280)	1:35:A:LEU:HD23	1:31:A:LEU:HA	5	0.44
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	6	0.44
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	11	0.44
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	15	0.44
(2,1254)	1:17:A:MET:HE2	1:82:A:TYR:H	8	0.44
(2,1244)	1:20:A:LEU:HD13	1:21:A:LEU:H	14	0.44
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	14	0.44
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD12	9	0.44
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD12	11	0.44
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG23	7	0.44
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG21	12	0.44
(2,913)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	5	0.44
(2,913)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	15	0.44
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD21	2	0.44
(2,851)	1:134:A:LEU:HD22	1:129:A:GLN:HB3	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,824)	1:134:A:LEU:HD21	1:33:A:GLU:HG3	9	0.44
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE1	2	0.44
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE1	3	0.44
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE3	8	0.44
(2,704)	1:18:A:ALA:HB3	1:21:A:LEU:HB3	1	0.44
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	7	0.44
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG21	4	0.44
(2,581)	1:180:A:VAL:HG21	1:183:A:LYS:H	2	0.44
(2,528)	1:46:A:VAL:HG21	1:41:A:GLU:HB3	15	0.44
(2,498)	1:142:A:LEU:HD12	1:60:A:ILE:HA	13	0.44
(2,498)	1:142:A:LEU:HD13	1:60:A:ILE:HA	15	0.44
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	4	0.44
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	2	0.44
(2,425)	1:35:A:LEU:HD13	1:35:A:LEU:H	11	0.44
(2,425)	1:35:A:LEU:HD12	1:35:A:LEU:H	14	0.44
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG21	10	0.44
(2,419)	1:53:A:ILE:HD11	1:49:A:ILE:HB	10	0.44
(2,415)	1:37:A:THR:HG23	1:36:A:GLU:HG3	3	0.44
(2,415)	1:37:A:THR:HG23	1:36:A:GLU:HG3	9	0.44
(2,415)	1:37:A:THR:HG22	1:36:A:GLU:HG3	15	0.44
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD12	10	0.44
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	15	0.44
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD11	13	0.44
(2,302)	1:136:A:ASN:HA	1:129:A:GLN:HE22	12	0.44
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD22	9	0.44
(2,170)	1:37:A:THR:HG22	1:33:A:GLU:HG3	3	0.44
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD13	15	0.44
(2,134)	1:18:A:ALA:HB2	1:22:A:GLN:HB2	5	0.44
(2,87)	1:67:A:ILE:HG22	1:31:A:LEU:HD11	15	0.44
(2,43)	1:128:A:ILE:HG22	1:38:A:TYR:H	2	0.44
(2,43)	1:128:A:ILE:HG23	1:38:A:TYR:H	7	0.44
(2,35)	1:39:A:LEU:HD13	1:65:A:GLN:HG3	13	0.44
(2,35)	1:39:A:LEU:HD12	1:65:A:GLN:HG3	15	0.44
(2,19)	1:79:A:LEU:HD12	1:92:A:CYS:HG	4	0.44
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	7	0.44
(2,16)	1:79:A:LEU:HD13	1:75:A:PHE:HA	9	0.44
(2,11)	1:79:A:LEU:HD13	1:79:A:LEU:H	9	0.44
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	15	0.43
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	14	0.43
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD2	14	0.43
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	9	0.43
(2,4778)	1:11:A:ARG:HD3	1:12:A:LYS:H	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	11	0.43
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	13	0.43
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG22	3	0.43
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG21	11	0.43
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD12	8	0.43
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	2	0.43
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	3	0.43
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	5	0.43
(2,4609)	1:33:A:GLU:H	1:37:A:THR:H	15	0.43
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG21	12	0.43
(2,4448)	1:179:A:SER:HB3	1:180:A:VAL:HG11	2	0.43
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD2	8	0.43
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD13	11	0.43
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE3	2	0.43
(2,4373)	1:182:A:LYS:HD3	1:182:A:LYS:HE2	3	0.43
(2,4348)	1:60:A:ILE:HD11	1:113:A:SER:H	2	0.43
(2,4329)	1:156:A:LEU:HD23	1:175:A:GLU:HG3	12	0.43
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD13	5	0.43
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	3	0.43
(2,4272)	1:174:A:LEU:HD22	1:175:A:GLU:HB2	11	0.43
(2,4271)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	8	0.43
(2,4271)	1:116:A:LEU:HD23	1:56:A:LYS:HE2	15	0.43
(2,4265)	1:142:A:LEU:HD11	1:110:A:LYS:HB2	2	0.43
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD23	5	0.43
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD22	9	0.43
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD21	10	0.43
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD21	11	0.43
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD23	14	0.43
(2,4186)	1:178:A:LEU:HD23	1:179:A:SER:H	3	0.43
(2,4186)	1:178:A:LEU:HD21	1:179:A:SER:H	10	0.43
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD11	12	0.43
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	8	0.43
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG13	2	0.43
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG13	13	0.43
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	4	0.43
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	9	0.43
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD12	13	0.43
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD13	14	0.43
(2,4064)	1:17:A:MET:HE1	1:20:A:LEU:H	13	0.43
(2,4037)	1:21:A:LEU:HD23	1:22:A:GLN:H	2	0.43
(2,4021)	1:18:A:ALA:HB2	1:20:A:LEU:H	11	0.43
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	13	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3943)	1:18:A:ALA:HB1	1:17:A:MET:H	12	0.43
(2,3942)	1:102:A:MET:HE2	1:102:A:MET:H	10	0.43
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	1	0.43
(2,3872)	1:60:A:ILE:HD12	1:62:A:GLY:H	4	0.43
(2,3872)	1:60:A:ILE:HD12	1:62:A:GLY:H	15	0.43
(2,3862)	1:101:A:GLN:HE21	1:104:A:VAL:HG12	8	0.43
(2,3832)	1:179:A:SER:HB2	1:179:A:SER:H	1	0.43
(2,3768)	1:117:A:ILE:HD12	1:117:A:ILE:H	2	0.43
(2,3768)	1:117:A:ILE:HD13	1:117:A:ILE:H	11	0.43
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	5	0.43
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD13	5	0.43
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD12	8	0.43
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	1	0.43
(2,3670)	1:43:A:THR:HG22	1:44:A:SER:H	4	0.43
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD13	12	0.43
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD12	15	0.43
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG23	4	0.43
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG22	13	0.43
(2,3309)	1:28:A:VAL:HG22	1:31:A:LEU:H	2	0.43
(2,3289)	1:21:A:LEU:HD11	1:21:A:LEU:H	12	0.43
(2,3264)	1:94:A:VAL:HG21	1:172:A:ASP:H	8	0.43
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	10	0.43
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	11	0.43
(2,3264)	1:94:A:VAL:HG21	1:172:A:ASP:H	12	0.43
(2,3169)	1:53:A:ILE:HG22	1:54:A:LEU:H	7	0.43
(2,3163)	1:42:A:MET:HE3	1:54:A:LEU:H	14	0.43
(2,3032)	1:20:A:LEU:HD22	1:20:A:LEU:H	3	0.43
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	14	0.43
(2,3032)	1:20:A:LEU:HD21	1:20:A:LEU:H	15	0.43
(2,2927)	1:156:A:LEU:HD21	1:173:A:GLY:H	11	0.43
(2,2895)	1:164:A:GLU:H	1:163:A:CYS:HB2	15	0.43
(2,2835)	1:146:A:VAL:HG11	1:148:A:ARG:H	3	0.43
(2,2763)	1:146:A:VAL:HG22	1:147:A:GLN:H	12	0.43
(2,2675)	1:117:A:ILE:HD13	1:113:A:SER:H	13	0.43
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	6	0.43
(2,2288)	1:21:A:LEU:HD12	1:22:A:GLN:H	1	0.43
(2,2274)	1:189:A:HIS:H	1:188:A:MET:HB3	5	0.43
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD23	13	0.43
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	6	0.43
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	14	0.43
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG12	8	0.43
(2,1838)	1:16:A:ILE:HD11	1:158:A:GLU:H	3	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG22	12	0.43
(2,1771)	1:88:A:ASP:H	1:86:A:PRO:HB3	12	0.43
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG21	9	0.43
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	6	0.43
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	10	0.43
(2,1630)	1:178:A:LEU:HD22	1:153:A:GLN:H	2	0.43
(2,1590)	1:18:A:ALA:HB3	1:20:A:LEU:HA	8	0.43
(2,1558)	1:20:A:LEU:HD22	1:89:A:VAL:HA	6	0.43
(2,1543)	1:128:A:ILE:HD11	1:132:A:HIS:HD2	1	0.43
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD22	10	0.43
(2,1496)	1:41:A:GLU:HG2	1:128:A:ILE:HG23	15	0.43
(2,1439)	1:102:A:MET:HE3	1:106:A:TYR:HD2	1	0.43
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	12	0.43
(2,1421)	1:116:A:LEU:HD22	1:116:A:LEU:H	4	0.43
(2,1421)	1:116:A:LEU:HD23	1:116:A:LEU:H	13	0.43
(2,1351)	1:94:A:VAL:HG13	1:96:A:TRP:H	8	0.43
(2,1318)	1:177:A:MET:HE1	1:173:A:GLY:H	6	0.43
(2,1318)	1:177:A:MET:HE2	1:173:A:GLY:H	11	0.43
(2,1317)	1:43:A:THR:HG21	1:57:A:GLU:HB3	7	0.43
(2,1317)	1:43:A:THR:HG22	1:57:A:GLU:HB3	15	0.43
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG22	11	0.43
(2,1282)	1:64:A:ILE:HG21	1:35:A:LEU:H	3	0.43
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	8	0.43
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD22	5	0.43
(2,1210)	1:134:A:LEU:HD13	1:134:A:LEU:HA	13	0.43
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	12	0.43
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD12	6	0.43
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD13	14	0.43
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	8	0.43
(2,824)	1:134:A:LEU:HD23	1:33:A:GLU:HG3	12	0.43
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	13	0.43
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	5	0.43
(2,700)	1:23:A:THR:HG22	1:21:A:LEU:H	13	0.43
(2,652)	1:177:A:MET:HE3	1:179:A:SER:H	3	0.43
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	15	0.43
(2,644)	1:105:A:THR:HG22	1:108:A:LYS:HD3	5	0.43
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG21	9	0.43
(2,586)	1:180:A:VAL:HG22	1:183:A:LYS:HG2	14	0.43
(2,528)	1:46:A:VAL:HG22	1:41:A:GLU:HB3	14	0.43
(2,498)	1:142:A:LEU:HD11	1:60:A:ILE:HA	12	0.43
(2,473)	1:59:A:ILE:HG22	1:112:A:ASP:HB2	3	0.43
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	9	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,427)	1:35:A:LEU:HD11	1:35:A:LEU:HA	14	0.43
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	4	0.43
(2,415)	1:37:A:THR:HG22	1:36:A:GLU:HG3	8	0.43
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD12	12	0.43
(2,405)	1:117:A:ILE:HD11	1:138:A:ILE:HD12	13	0.43
(2,380)	1:31:A:LEU:HD23	1:70:A:PHE:H	5	0.43
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	10	0.43
(2,380)	1:31:A:LEU:HD22	1:70:A:PHE:H	13	0.43
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD21	1	0.43
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	6	0.43
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	12	0.43
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD21	15	0.43
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD12	15	0.43
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	9	0.43
(2,318)	1:20:A:LEU:HD22	1:152:A:TYR:HD1	9	0.43
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD23	2	0.43
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB2	2	0.43
(2,170)	1:37:A:THR:HG22	1:33:A:GLU:HG3	5	0.43
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD21	2	0.43
(2,114)	1:177:A:MET:HE2	1:93:A:PHE:HE1	1	0.43
(2,87)	1:67:A:ILE:HG22	1:31:A:LEU:HD11	8	0.43
(2,87)	1:67:A:ILE:HG21	1:31:A:LEU:HD11	13	0.43
(2,60)	1:174:A:LEU:HD23	1:178:A:LEU:H	5	0.43
(2,43)	1:128:A:ILE:HG23	1:38:A:TYR:H	8	0.43
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	2	0.43
(2,16)	1:79:A:LEU:HD11	1:75:A:PHE:HA	1	0.43
(2,16)	1:79:A:LEU:HD11	1:75:A:PHE:HA	3	0.43
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	10	0.43
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	11	0.42
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	7	0.42
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	14	0.42
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD3	2	0.42
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	1	0.42
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	3	0.42
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	5	0.42
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	6	0.42
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	8	0.42
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	11	0.42
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	15	0.42
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	14	0.42
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD11	3	0.42
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4551)	1:21:A:LEU:HD23	1:75:A:PHE:HD1	2	0.42
(2,4495)	1:154:A:LEU:HD11	1:154:A:LEU:HG	1	0.42
(2,4495)	1:154:A:LEU:HD12	1:154:A:LEU:HG	2	0.42
(2,4495)	1:154:A:LEU:HD12	1:154:A:LEU:HG	3	0.42
(2,4495)	1:154:A:LEU:HD13	1:154:A:LEU:HG	5	0.42
(2,4495)	1:154:A:LEU:HD13	1:154:A:LEU:HG	7	0.42
(2,4495)	1:154:A:LEU:HD12	1:154:A:LEU:HG	8	0.42
(2,4495)	1:154:A:LEU:HD11	1:154:A:LEU:HG	10	0.42
(2,4495)	1:154:A:LEU:HG	1:154:A:LEU:HD23	11	0.42
(2,4495)	1:154:A:LEU:HD13	1:154:A:LEU:HG	13	0.42
(2,4495)	1:154:A:LEU:HD12	1:154:A:LEU:HG	14	0.42
(2,4495)	1:154:A:LEU:HD13	1:154:A:LEU:HG	15	0.42
(2,4373)	1:167:A:LYS:HD3	1:167:A:LYS:HE2	7	0.42
(2,4348)	1:60:A:ILE:HD12	1:113:A:SER:H	4	0.42
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	10	0.42
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD13	15	0.42
(2,4284)	1:171:A:LYS:HG2	1:172:A:ASP:H	12	0.42
(2,4265)	1:142:A:LEU:HD11	1:110:A:LYS:HB2	5	0.42
(2,4265)	1:142:A:LEU:HD11	1:110:A:LYS:HB2	12	0.42
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD11	14	0.42
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD22	7	0.42
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD22	14	0.42
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	2	0.42
(2,4186)	1:178:A:LEU:HD23	1:179:A:SER:H	4	0.42
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	12	0.42
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG13	9	0.42
(2,4022)	1:143:A:ILE:HD13	1:147:A:GLN:HE22	7	0.42
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	8	0.42
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	8	0.42
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD22	8	0.42
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD22	10	0.42
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	12	0.42
(2,3933)	1:94:A:VAL:HG22	1:95:A:THR:H	8	0.42
(2,3904)	1:31:A:LEU:HD23	1:72:A:ASN:H	7	0.42
(2,3889)	1:85:A:LEU:HD21	1:84:A:GLN:H	5	0.42
(2,3889)	1:85:A:LEU:HD22	1:84:A:GLN:H	14	0.42
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD12	8	0.42
(2,3872)	1:60:A:ILE:HD12	1:62:A:GLY:H	6	0.42
(2,3872)	1:60:A:ILE:HD11	1:62:A:GLY:H	10	0.42
(2,3872)	1:60:A:ILE:HD12	1:62:A:GLY:H	13	0.42
(2,3842)	1:182:A:LYS:HD2	1:183:A:LYS:H	12	0.42
(2,3833)	1:178:A:LEU:HD12	1:178:A:LEU:H	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	10	0.42
(2,3816)	1:156:A:LEU:HD23	1:156:A:LEU:H	1	0.42
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	6	0.42
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	10	0.42
(2,3670)	1:43:A:THR:HG22	1:44:A:SER:H	9	0.42
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	3	0.42
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	14	0.42
(2,3512)	1:91:A:HIS:HD2	1:95:A:THR:HG23	11	0.42
(2,3371)	1:136:A:ASN:HD22	1:136:A:ASN:H	10	0.42
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	7	0.42
(2,3257)	1:170:A:LEU:HD22	1:160:A:LEU:H	6	0.42
(2,3251)	1:158:A:GLU:H	1:159:A:LEU:HD22	8	0.42
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG11	3	0.42
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG11	4	0.42
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG11	9	0.42
(2,3182)	1:15:A:PHE:HB2	1:15:A:PHE:H	7	0.42
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG22	8	0.42
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG22	15	0.42
(2,3031)	1:20:A:LEU:HD11	1:20:A:LEU:H	8	0.42
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG23	6	0.42
(2,2835)	1:146:A:VAL:HG12	1:148:A:ARG:H	7	0.42
(2,2643)	1:108:A:LYS:H	1:107:A:CYS:HB2	12	0.42
(2,2638)	1:180:A:VAL:HG23	1:104:A:VAL:H	12	0.42
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	1	0.42
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG23	7	0.42
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	15	0.42
(2,2460)	1:74:A:ILE:H	1:75:A:PHE:HB2	8	0.42
(2,2455)	1:73:A:ASN:HB2	1:74:A:ILE:H	3	0.42
(2,2275)	1:190:A:VAL:H	1:189:A:HIS:HB3	5	0.42
(2,2273)	1:189:A:HIS:H	1:189:A:HIS:HB2	7	0.42
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	14	0.42
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG21	8	0.42
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG22	15	0.42
(2,2171)	1:174:A:LEU:HD23	1:174:A:LEU:H	9	0.42
(2,2165)	1:151:A:LYS:H	1:151:A:LYS:HB2	3	0.42
(2,2151)	1:105:A:THR:HG22	1:105:A:THR:H	10	0.42
(2,2151)	1:105:A:THR:HG21	1:105:A:THR:H	13	0.42
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	6	0.42
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	13	0.42
(2,1919)	1:183:A:LYS:H	1:183:A:LYS:HG3	1	0.42
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	7	0.42
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD11	9	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG23	6	0.42
(2,1854)	1:143:A:ILE:HD12	1:147:A:GLN:H	13	0.42
(2,1838)	1:16:A:ILE:HD11	1:158:A:GLU:H	9	0.42
(2,1826)	1:131:A:ARG:HE	1:128:A:ILE:HG21	8	0.42
(2,1752)	1:76:A:LEU:HD23	1:78:A:GLU:H	8	0.42
(2,1713)	1:172:A:ASP:H	1:175:A:GLU:HG3	2	0.42
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG23	4	0.42
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	7	0.42
(2,1630)	1:178:A:LEU:HD21	1:153:A:GLN:H	10	0.42
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD13	4	0.42
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	4	0.42
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD13	12	0.42
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD13	15	0.42
(2,1395)	1:188:A:MET:HE2	1:188:A:MET:HG3	7	0.42
(2,1395)	1:188:A:MET:HE2	1:188:A:MET:HG3	11	0.42
(2,1351)	1:94:A:VAL:HG11	1:96:A:TRP:H	9	0.42
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	15	0.42
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	12	0.42
(2,1282)	1:64:A:ILE:HG21	1:35:A:LEU:H	7	0.42
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	15	0.42
(2,1280)	1:35:A:LEU:HD21	1:31:A:LEU:HA	8	0.42
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE1	4	0.42
(2,1244)	1:20:A:LEU:HD12	1:21:A:LEU:H	1	0.42
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	4	0.42
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	5	0.42
(2,1210)	1:134:A:LEU:HD13	1:134:A:LEU:HA	3	0.42
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	10	0.42
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD11	5	0.42
(2,1037)	1:143:A:ILE:HG22	1:140:A:SER:HB2	11	0.42
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG22	2	0.42
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	10	0.42
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG21	9	0.42
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG21	11	0.42
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG23	13	0.42
(2,533)	1:49:A:ILE:HD12	1:42:A:MET:HE1	15	0.42
(2,437)	1:39:A:LEU:HD12	1:42:A:MET:HG3	13	0.42
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	2	0.42
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	6	0.42
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	15	0.42
(2,415)	1:37:A:THR:HG23	1:36:A:GLU:HG3	14	0.42
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	8	0.42
(2,380)	1:31:A:LEU:HD23	1:70:A:PHE:H	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,380)	1:31:A:LEU:HD23	1:70:A:PHE:H	14	0.42
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD23	2	0.42
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	10	0.42
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	12	0.42
(2,316)	1:20:A:LEU:HD11	1:152:A:TYR:HB3	3	0.42
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	11	0.42
(2,313)	1:20:A:LEU:HD12	1:22:A:GLN:H	3	0.42
(2,313)	1:20:A:LEU:HD13	1:22:A:GLN:H	9	0.42
(2,313)	1:20:A:LEU:HD11	1:22:A:GLN:H	11	0.42
(2,294)	1:86:A:PRO:HA	1:159:A:LEU:HD22	15	0.42
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	6	0.42
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD13	4	0.42
(2,171)	1:74:A:ILE:HG23	1:78:A:GLU:HG3	11	0.42
(2,120)	1:161:A:THR:HG23	1:158:A:GLU:HG2	9	0.42
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD22	1	0.42
(2,94)	1:180:A:VAL:HG21	1:103:A:TYR:HA	9	0.42
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	3	0.42
(2,4801)	1:168:A:GLY:H	1:167:A:LYS:HD2	11	0.41
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	12	0.41
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB3	9	0.41
(2,4687)	1:11:A:ARG:HG2	1:12:A:LYS:H	4	0.41
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	4	0.41
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD13	7	0.41
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	7	0.41
(2,4495)	1:154:A:LEU:HG	1:154:A:LEU:HD23	12	0.41
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG21	13	0.41
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE3	12	0.41
(2,4338)	1:39:A:LEU:HD13	1:39:A:LEU:HG	4	0.41
(2,4338)	1:39:A:LEU:HD13	1:39:A:LEU:HG	11	0.41
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	12	0.41
(2,4338)	1:39:A:LEU:HD11	1:39:A:LEU:HG	13	0.41
(2,4338)	1:39:A:LEU:HD13	1:39:A:LEU:HG	15	0.41
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD11	3	0.41
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	1	0.41
(2,4272)	1:174:A:LEU:HD21	1:175:A:GLU:HB2	13	0.41
(2,4265)	1:142:A:LEU:HD12	1:110:A:LYS:HB2	11	0.41
(2,4223)	1:159:A:LEU:HD11	1:156:A:LEU:H	2	0.41
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	1	0.41
(2,4186)	1:178:A:LEU:HD21	1:179:A:SER:H	1	0.41
(2,4186)	1:178:A:LEU:HD22	1:179:A:SER:H	8	0.41
(2,4186)	1:178:A:LEU:HD23	1:179:A:SER:H	11	0.41
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	15	0.41
(2,4064)	1:17:A:MET:HE2	1:20:A:LEU:H	1	0.41
(2,4064)	1:17:A:MET:HE3	1:20:A:LEU:H	7	0.41
(2,4021)	1:18:A:ALA:HB2	1:20:A:LEU:H	3	0.41
(2,4021)	1:18:A:ALA:HB1	1:20:A:LEU:H	10	0.41
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	14	0.41
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG21	3	0.41
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD12	1	0.41
(2,3943)	1:18:A:ALA:HB1	1:17:A:MET:H	2	0.41
(2,3933)	1:94:A:VAL:HG21	1:95:A:THR:H	1	0.41
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	4	0.41
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD23	12	0.41
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD21	13	0.41
(2,3889)	1:85:A:LEU:HD21	1:84:A:GLN:H	2	0.41
(2,3889)	1:85:A:LEU:HD21	1:84:A:GLN:H	8	0.41
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	15	0.41
(2,3861)	1:143:A:ILE:HG21	1:147:A:GLN:HE22	11	0.41
(2,3833)	1:178:A:LEU:HD11	1:178:A:LEU:H	7	0.41
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	9	0.41
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	13	0.41
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	7	0.41
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	10	0.41
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	10	0.41
(2,3622)	1:4:A:GLY:HA2	1:5:A:SER:H	1	0.41
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	5	0.41
(2,3557)	1:141:A:TYR:HD1	1:136:A:ASN:HB2	4	0.41
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD11	6	0.41
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	6	0.41
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG21	10	0.41
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	14	0.41
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	1	0.41
(2,3289)	1:21:A:LEU:HD13	1:21:A:LEU:H	11	0.41
(2,3289)	1:21:A:LEU:HD12	1:21:A:LEU:H	13	0.41
(2,3289)	1:21:A:LEU:HD12	1:21:A:LEU:H	14	0.41
(2,3264)	1:94:A:VAL:HG22	1:172:A:ASP:H	4	0.41
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	15	0.41
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	5	0.41
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	14	0.41
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	2	0.41
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	15	0.41
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	3	0.41
(2,2675)	1:117:A:ILE:HD13	1:113:A:SER:H	8	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG21	8	0.41
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	4	0.41
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	14	0.41
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG12	11	0.41
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG12	14	0.41
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	4	0.41
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	10	0.41
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG23	14	0.41
(2,2151)	1:105:A:THR:HG21	1:105:A:THR:H	9	0.41
(2,2151)	1:105:A:THR:HG22	1:105:A:THR:H	12	0.41
(2,1953)	1:141:A:TYR:HE1	1:30:A:ASP:H	9	0.41
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	1	0.41
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	14	0.41
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG23	14	0.41
(2,1711)	1:63:A:ASN:H	1:105:A:THR:HG23	7	0.41
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	5	0.41
(2,1630)	1:178:A:LEU:HD23	1:153:A:GLN:H	14	0.41
(2,1547)	1:95:A:THR:HG22	1:78:A:GLU:HB2	12	0.41
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD23	1	0.41
(2,1522)	1:76:A:LEU:HD13	1:68:A:TYR:HE1	6	0.41
(2,1520)	1:76:A:LEU:HD13	1:29:A:ARG:H	14	0.41
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	14	0.41
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	5	0.41
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD12	14	0.41
(2,1384)	1:33:A:GLU:HG2	1:141:A:TYR:HE2	5	0.41
(2,1351)	1:94:A:VAL:HG13	1:96:A:TRP:H	4	0.41
(2,1351)	1:94:A:VAL:HG13	1:96:A:TRP:H	5	0.41
(2,1351)	1:94:A:VAL:HG11	1:96:A:TRP:H	10	0.41
(2,1351)	1:94:A:VAL:HG13	1:96:A:TRP:H	11	0.41
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	13	0.41
(2,1351)	1:94:A:VAL:HG13	1:96:A:TRP:H	14	0.41
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	3	0.41
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	7	0.41
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG21	7	0.41
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	7	0.41
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	14	0.41
(2,1280)	1:35:A:LEU:HD23	1:31:A:LEU:HA	2	0.41
(2,1280)	1:35:A:LEU:HD21	1:31:A:LEU:HA	9	0.41
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	9	0.41
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	13	0.41
(2,1163)	1:105:A:THR:HB	1:104:A:VAL:HG22	15	0.41
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	8	0.41
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD13	6	0.41
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD12	13	0.41
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD21	12	0.41
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	4	0.41
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG22	10	0.41
(2,851)	1:134:A:LEU:HD22	1:129:A:GLN:HB3	11	0.41
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	4	0.41
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	13	0.41
(2,654)	1:177:A:MET:HE3	1:174:A:LEU:HA	1	0.41
(2,652)	1:177:A:MET:HE2	1:179:A:SER:H	8	0.41
(2,638)	1:150:A:THR:HG23	1:153:A:GLN:HE21	10	0.41
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG22	1	0.41
(2,618)	1:43:A:THR:HG22	1:45:A:GLY:H	9	0.41
(2,500)	1:142:A:LEU:HD23	1:142:A:LEU:HD11	1	0.41
(2,500)	1:142:A:LEU:HD21	1:142:A:LEU:HD13	4	0.41
(2,500)	1:142:A:LEU:HD23	1:142:A:LEU:HD13	5	0.41
(2,500)	1:142:A:LEU:HD21	1:142:A:LEU:HD13	6	0.41
(2,500)	1:142:A:LEU:HD23	1:142:A:LEU:HD11	11	0.41
(2,468)	1:178:A:LEU:HD22	1:175:A:GLU:HA	7	0.41
(2,438)	1:39:A:LEU:HD11	1:42:A:MET:HB2	6	0.41
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	7	0.41
(2,438)	1:39:A:LEU:HD12	1:42:A:MET:HB2	13	0.41
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	3	0.41
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	7	0.41
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	1	0.41
(2,425)	1:35:A:LEU:HD11	1:35:A:LEU:H	7	0.41
(2,406)	1:156:A:LEU:HD12	1:93:A:PHE:HZ	8	0.41
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD22	7	0.41
(2,340)	1:102:A:MET:HE1	1:99:A:LYS:HE3	4	0.41
(2,336)	1:102:A:MET:HE1	1:100:A:PHE:HA	2	0.41
(2,328)	1:42:A:MET:HE2	1:60:A:ILE:HB	3	0.41
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD13	15	0.41
(2,130)	1:23:A:THR:HG22	1:23:A:THR:HG1	7	0.41
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD11	15	0.41
(2,77)	1:76:A:LEU:HD12	1:80:A:GLU:HG3	11	0.41
(2,43)	1:128:A:ILE:HG22	1:38:A:TYR:H	4	0.41
(2,43)	1:128:A:ILE:HG22	1:38:A:TYR:H	5	0.41
(2,43)	1:128:A:ILE:HG22	1:38:A:TYR:H	10	0.41
(2,43)	1:128:A:ILE:HG23	1:38:A:TYR:H	15	0.41
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	12	0.4
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	11	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	12	0.4
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	3	0.4
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	1	0.4
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	10	0.4
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	2	0.4
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	7	0.4
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD23	1	0.4
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD21	3	0.4
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	8	0.4
(2,4518)	1:128:A:ILE:HG22	1:124:A:PHE:HZ	5	0.4
(2,4495)	1:154:A:LEU:HD12	1:154:A:LEU:HG	6	0.4
(2,4495)	1:154:A:LEU:HD12	1:154:A:LEU:HG	9	0.4
(2,4410)	1:22:A:GLN:HG3	1:21:A:LEU:HD13	2	0.4
(2,4356)	1:180:A:VAL:HG12	1:180:A:VAL:H	8	0.4
(2,4347)	1:174:A:LEU:HD12	1:157:A:LYS:HE2	7	0.4
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	1	0.4
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	3	0.4
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	5	0.4
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	8	0.4
(2,4325)	1:188:A:MET:HE1	1:108:A:LYS:HE3	3	0.4
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	13	0.4
(2,4307)	1:56:A:LYS:HE3	1:59:A:ILE:HD13	6	0.4
(2,4307)	1:56:A:LYS:HE2	1:59:A:ILE:HD12	7	0.4
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG22	12	0.4
(2,4287)	1:13:A:LYS:HD2	1:15:A:PHE:HD2	6	0.4
(2,4264)	1:16:A:ILE:HD11	1:19:A:GLU:HB3	9	0.4
(2,4216)	1:157:A:LYS:H	1:160:A:LEU:HD22	2	0.4
(2,4197)	1:16:A:ILE:HG23	1:158:A:GLU:H	6	0.4
(2,4186)	1:178:A:LEU:HD21	1:179:A:SER:H	6	0.4
(2,4186)	1:178:A:LEU:HD23	1:179:A:SER:H	7	0.4
(2,4186)	1:178:A:LEU:HD22	1:179:A:SER:H	9	0.4
(2,4185)	1:178:A:LEU:HD11	1:179:A:SER:H	12	0.4
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD11	8	0.4
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	2	0.4
(2,4064)	1:17:A:MET:HE1	1:20:A:LEU:H	8	0.4
(2,4064)	1:17:A:MET:HE3	1:20:A:LEU:H	15	0.4
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	6	0.4
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	2	0.4
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	8	0.4
(2,3904)	1:31:A:LEU:HD22	1:72:A:ASN:H	13	0.4
(2,3889)	1:85:A:LEU:HD23	1:84:A:GLN:H	3	0.4
(2,3889)	1:85:A:LEU:HD23	1:84:A:GLN:H	11	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3872)	1:60:A:ILE:HD13	1:62:A:GLY:H	3	0.4
(2,3872)	1:60:A:ILE:HD13	1:62:A:GLY:H	11	0.4
(2,3833)	1:178:A:LEU:HD11	1:178:A:LEU:H	2	0.4
(2,3833)	1:178:A:LEU:HD13	1:178:A:LEU:H	8	0.4
(2,3833)	1:178:A:LEU:HD11	1:178:A:LEU:H	14	0.4
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	8	0.4
(2,3816)	1:156:A:LEU:HD21	1:156:A:LEU:H	9	0.4
(2,3816)	1:156:A:LEU:HD22	1:156:A:LEU:H	11	0.4
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD21	13	0.4
(2,3768)	1:117:A:ILE:HD11	1:117:A:ILE:H	12	0.4
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG22	7	0.4
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG22	14	0.4
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	13	0.4
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	3	0.4
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD21	10	0.4
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG21	13	0.4
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD12	9	0.4
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG22	10	0.4
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG23	14	0.4
(2,3289)	1:21:A:LEU:HD13	1:21:A:LEU:H	2	0.4
(2,3289)	1:21:A:LEU:HD11	1:21:A:LEU:H	15	0.4
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG23	5	0.4
(2,3032)	1:20:A:LEU:HD22	1:20:A:LEU:H	5	0.4
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	12	0.4
(2,2853)	1:150:A:THR:H	1:153:A:GLN:HE21	14	0.4
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG21	2	0.4
(2,2835)	1:146:A:VAL:HG12	1:148:A:ARG:H	6	0.4
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	7	0.4
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG21	2	0.4
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	12	0.4
(2,2288)	1:21:A:LEU:HD11	1:22:A:GLN:H	12	0.4
(2,2288)	1:21:A:LEU:HD12	1:22:A:GLN:H	13	0.4
(2,2275)	1:190:A:VAL:H	1:189:A:HIS:HB3	13	0.4
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD23	8	0.4
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	3	0.4
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG21	9	0.4
(2,2171)	1:174:A:LEU:HD22	1:174:A:LEU:H	11	0.4
(2,2151)	1:105:A:THR:HG22	1:105:A:THR:H	3	0.4
(2,2151)	1:105:A:THR:HG22	1:105:A:THR:H	15	0.4
(2,2116)	1:97:A:ALA:HB2	1:100:A:PHE:H	9	0.4
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD13	5	0.4
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD12	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1805)	1:185:A:ASN:HD21	1:182:A:LYS:HA	2	0.4
(2,1752)	1:76:A:LEU:HD21	1:78:A:GLU:H	4	0.4
(2,1752)	1:76:A:LEU:HD22	1:78:A:GLU:H	13	0.4
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG23	8	0.4
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG13	14	0.4
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD23	5	0.4
(2,1516)	1:39:A:LEU:HD11	1:61:A:PHE:HB3	13	0.4
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD13	1	0.4
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD13	2	0.4
(2,1421)	1:116:A:LEU:HD22	1:116:A:LEU:H	9	0.4
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD13	4	0.4
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD13	7	0.4
(2,1402)	1:35:A:LEU:HD11	1:65:A:GLN:HB2	10	0.4
(2,1402)	1:35:A:LEU:HD12	1:65:A:GLN:HB2	12	0.4
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	15	0.4
(2,1350)	1:35:A:LEU:HD12	1:36:A:GLU:H	5	0.4
(2,1317)	1:43:A:THR:HG22	1:57:A:GLU:HB3	9	0.4
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	4	0.4
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	6	0.4
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	8	0.4
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	9	0.4
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	15	0.4
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD21	10	0.4
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	1	0.4
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	12	0.4
(2,1280)	1:35:A:LEU:HD22	1:31:A:LEU:HA	13	0.4
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	12	0.4
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	3	0.4
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	11	0.4
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD12	8	0.4
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD13	12	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB3	3	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB1	9	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	11	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB1	12	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB1	13	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB1	14	0.4
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB1	15	0.4
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD11	4	0.4
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD13	11	0.4
(2,1037)	1:143:A:ILE:HG23	1:140:A:SER:HB2	2	0.4
(2,1037)	1:143:A:ILE:HG23	1:140:A:SER:HB2	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD13	8	0.4
(2,836)	1:64:A:ILE:HG23	1:65:A:GLN:HG3	14	0.4
(2,729)	1:97:A:ALA:HB1	1:100:A:PHE:HE1	9	0.4
(2,709)	1:49:A:ILE:HB	1:42:A:MET:HE2	7	0.4
(2,704)	1:18:A:ALA:HB1	1:21:A:LEU:HB3	11	0.4
(2,703)	1:18:A:ALA:HB3	1:15:A:PHE:HD2	8	0.4
(2,623)	1:146:A:VAL:HG23	1:146:A:VAL:HB	2	0.4
(2,623)	1:146:A:VAL:HG23	1:146:A:VAL:HB	11	0.4
(2,623)	1:146:A:VAL:HG21	1:146:A:VAL:HB	14	0.4
(2,623)	1:146:A:VAL:HG21	1:146:A:VAL:HB	15	0.4
(2,589)	1:64:A:ILE:HD11	1:35:A:LEU:HB3	1	0.4
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	2	0.4
(2,438)	1:39:A:LEU:HD11	1:42:A:MET:HB2	2	0.4
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	8	0.4
(2,438)	1:39:A:LEU:HD11	1:42:A:MET:HB2	10	0.4
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	5	0.4
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	7	0.4
(2,427)	1:35:A:LEU:HD11	1:35:A:LEU:HA	5	0.4
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	9	0.4
(2,419)	1:53:A:ILE:HD13	1:49:A:ILE:HB	1	0.4
(2,406)	1:156:A:LEU:HD12	1:93:A:PHE:HZ	9	0.4
(2,387)	1:31:A:LEU:HD22	1:67:A:ILE:HD12	14	0.4
(2,380)	1:31:A:LEU:HD21	1:70:A:PHE:H	9	0.4
(2,362)	1:156:A:LEU:HD23	1:152:A:TYR:HB2	15	0.4
(2,346)	1:102:A:MET:HE2	1:67:A:ILE:HD13	3	0.4
(2,328)	1:42:A:MET:HE1	1:60:A:ILE:HB	8	0.4
(2,318)	1:20:A:LEU:HD21	1:152:A:TYR:HD1	8	0.4
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	5	0.4
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	15	0.4
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	3	0.4
(2,171)	1:74:A:ILE:HG23	1:78:A:GLU:HG3	7	0.4
(2,168)	1:33:A:GLU:HG3	1:37:A:THR:H	2	0.4
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD22	7	0.4
(2,145)	1:36:A:GLU:HG2	1:35:A:LEU:HD23	15	0.4
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD21	2	0.4
(2,103)	1:28:A:VAL:HG13	1:31:A:LEU:HD21	5	0.4
(2,103)	1:28:A:VAL:HG13	1:31:A:LEU:HD22	8	0.4
(2,89)	1:116:A:LEU:HD11	1:117:A:ILE:H	7	0.4
(2,55)	1:142:A:LEU:HD12	1:106:A:TYR:HH	11	0.4
(2,43)	1:128:A:ILE:HG21	1:38:A:TYR:H	1	0.4
(2,40)	1:31:A:LEU:HD11	1:67:A:ILE:HB	13	0.4
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	6	0.39
(2,4803)	1:167:A:LYS:H	1:167:A:LYS:HE2	3	0.39
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG3	3	0.39
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG23	12	0.39
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	4	0.39
(2,4687)	1:11:A:ARG:HG2	1:12:A:LYS:H	15	0.39
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	2	0.39
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	14	0.39
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB2	1	0.39
(2,4654)	1:83:A:GLU:HG2	1:84:A:GLN:HE21	10	0.39
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	1	0.39
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	10	0.39
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	14	0.39
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	15	0.39
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD22	14	0.39
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD12	13	0.39
(2,4553)	1:64:A:ILE:HG21	1:65:A:GLN:HE21	9	0.39
(2,4547)	1:102:A:MET:HE3	1:64:A:ILE:HA	2	0.39
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD12	1	0.39
(2,4495)	1:154:A:LEU:HD11	1:154:A:LEU:HG	4	0.39
(2,4492)	1:79:A:LEU:HD21	1:25:A:LYS:HG3	9	0.39
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD3	11	0.39
(2,4338)	1:39:A:LEU:HD13	1:39:A:LEU:HG	2	0.39
(2,4338)	1:39:A:LEU:HD13	1:39:A:LEU:HG	6	0.39
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	9	0.39
(2,4338)	1:39:A:LEU:HD12	1:39:A:LEU:HG	14	0.39
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	14	0.39
(2,4304)	1:186:A:ASP:HB3	1:183:A:LYS:HG3	2	0.39
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG23	1	0.39
(2,4287)	1:13:A:LYS:HD2	1:15:A:PHE:HD1	8	0.39
(2,4264)	1:16:A:ILE:HD13	1:19:A:GLU:HB3	15	0.39
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	15	0.39
(2,4186)	1:178:A:LEU:HD23	1:179:A:SER:H	14	0.39
(2,4186)	1:178:A:LEU:HD21	1:179:A:SER:H	15	0.39
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD12	3	0.39
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD13	10	0.39
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD13	13	0.39
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	4	0.39
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	12	0.39
(2,4119)	1:7:A:GLU:HG2	1:7:A:GLU:H	15	0.39
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	9	0.39
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	4	0.39
(2,4021)	1:18:A:ALA:HB2	1:20:A:LEU:H	7	0.39
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	15	0.39
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD2	9	0.39
(2,3969)	1:184:A:ALA:HB3	1:108:A:LYS:H	4	0.39
(2,3969)	1:184:A:ALA:HB3	1:108:A:LYS:H	13	0.39
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	4	0.39
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD12	13	0.39
(2,3937)	1:184:A:ALA:HB1	1:182:A:LYS:H	4	0.39
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	6	0.39
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	13	0.39
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	10	0.39
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	14	0.39
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	15	0.39
(2,3889)	1:85:A:LEU:HD21	1:84:A:GLN:H	1	0.39
(2,3872)	1:60:A:ILE:HD13	1:62:A:GLY:H	14	0.39
(2,3768)	1:117:A:ILE:HD13	1:117:A:ILE:H	3	0.39
(2,3768)	1:117:A:ILE:HD11	1:117:A:ILE:H	8	0.39
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG22	13	0.39
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD13	4	0.39
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	7	0.39
(2,3652)	1:161:A:THR:HG23	1:162:A:CYS:H	9	0.39
(2,3652)	1:161:A:THR:HG23	1:162:A:CYS:H	10	0.39
(2,3652)	1:161:A:THR:HG21	1:162:A:CYS:H	14	0.39
(2,3599)	1:38:A:TYR:HE2	1:37:A:THR:HG23	7	0.39
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG11	9	0.39
(2,3372)	1:141:A:TYR:HE2	1:141:A:TYR:H	5	0.39
(2,3372)	1:141:A:TYR:HE1	1:141:A:TYR:H	11	0.39
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	1	0.39
(2,3182)	1:15:A:PHE:HB2	1:15:A:PHE:H	8	0.39
(2,3163)	1:42:A:MET:HE2	1:54:A:LEU:H	9	0.39
(2,3012)	1:12:A:LYS:H	1:12:A:LYS:HB2	10	0.39
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG21	7	0.39
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	4	0.39
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	8	0.39
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	12	0.39
(2,2763)	1:146:A:VAL:HG22	1:147:A:GLN:H	1	0.39
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG23	12	0.39
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	8	0.39
(2,2484)	1:17:A:MET:H	1:15:A:PHE:HB3	8	0.39
(2,2399)	1:117:A:ILE:HD13	1:116:A:LEU:H	4	0.39
(2,2288)	1:21:A:LEU:HD11	1:22:A:GLN:H	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	12	0.39
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD23	15	0.39
(2,2171)	1:174:A:LEU:HD22	1:174:A:LEU:H	7	0.39
(2,2151)	1:105:A:THR:HG23	1:105:A:THR:H	5	0.39
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	8	0.39
(2,1932)	1:10:A:GLY:H	1:11:A:ARG:HB3	13	0.39
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD11	12	0.39
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	15	0.39
(2,1752)	1:76:A:LEU:HD23	1:78:A:GLU:H	3	0.39
(2,1752)	1:76:A:LEU:HD21	1:78:A:GLU:H	6	0.39
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	2	0.39
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	4	0.39
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD11	1	0.39
(2,1590)	1:18:A:ALA:HB3	1:20:A:LEU:HA	10	0.39
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	13	0.39
(2,1547)	1:95:A:THR:HG22	1:78:A:GLU:HB2	6	0.39
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD22	7	0.39
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	15	0.39
(2,1519)	1:39:A:LEU:HD13	1:65:A:GLN:H	11	0.39
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	1	0.39
(2,1439)	1:102:A:MET:HE2	1:106:A:TYR:HD2	10	0.39
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	7	0.39
(2,1399)	1:7:A:GLU:HG3	1:8:A:PHE:HD2	2	0.39
(2,1385)	1:33:A:GLU:HG3	1:29:A:ARG:HD3	12	0.39
(2,1351)	1:94:A:VAL:HG12	1:96:A:TRP:H	6	0.39
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	2	0.39
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	3	0.39
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	10	0.39
(2,1292)	1:9:A:PRO:HB2	1:9:A:PRO:HD2	15	0.39
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD21	8	0.39
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	2	0.39
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	1	0.39
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB1	2	0.39
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	4	0.39
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	6	0.39
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	6	0.39
(2,1095)	1:190:A:VAL:HA	1:190:A:VAL:HB	5	0.39
(2,1095)	1:190:A:VAL:HA	1:190:A:VAL:HB	9	0.39
(2,1095)	1:190:A:VAL:HA	1:190:A:VAL:HB	12	0.39
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG23	15	0.39
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	3	0.39
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD12	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD13	11	0.39
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG22	5	0.39
(2,761)	1:37:A:THR:HG21	1:36:A:GLU:HG2	10	0.39
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG21	8	0.39
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG21	11	0.39
(2,652)	1:177:A:MET:HE3	1:179:A:SER:H	7	0.39
(2,652)	1:177:A:MET:HE3	1:179:A:SER:H	10	0.39
(2,652)	1:177:A:MET:HE2	1:179:A:SER:H	11	0.39
(2,644)	1:105:A:THR:HG21	1:108:A:LYS:HD3	10	0.39
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG22	10	0.39
(2,624)	1:39:A:LEU:HD12	1:43:A:THR:HG23	14	0.39
(2,623)	1:146:A:VAL:HG22	1:146:A:VAL:HB	1	0.39
(2,623)	1:146:A:VAL:HG21	1:146:A:VAL:HB	5	0.39
(2,623)	1:146:A:VAL:HG23	1:146:A:VAL:HB	6	0.39
(2,623)	1:146:A:VAL:HG21	1:146:A:VAL:HB	8	0.39
(2,623)	1:146:A:VAL:HG22	1:146:A:VAL:HB	9	0.39
(2,623)	1:146:A:VAL:HG22	1:146:A:VAL:HB	10	0.39
(2,623)	1:146:A:VAL:HG23	1:146:A:VAL:HB	13	0.39
(2,608)	1:28:A:VAL:HG13	1:75:A:PHE:H	12	0.39
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	5	0.39
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	7	0.39
(2,586)	1:180:A:VAL:HG22	1:183:A:LYS:HG2	15	0.39
(2,506)	1:155:A:LEU:HD22	1:148:A:ARG:HD3	14	0.39
(2,500)	1:142:A:LEU:HD23	1:142:A:LEU:HD11	9	0.39
(2,500)	1:142:A:LEU:HD23	1:142:A:LEU:HD11	10	0.39
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD13	12	0.39
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	14	0.39
(2,437)	1:39:A:LEU:HD11	1:42:A:MET:HG3	10	0.39
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	14	0.39
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	3	0.39
(2,419)	1:53:A:ILE:HD12	1:49:A:ILE:HB	6	0.39
(2,406)	1:156:A:LEU:HD11	1:93:A:PHE:HZ	4	0.39
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	10	0.39
(2,335)	1:102:A:MET:HE2	1:71:A:HIS:HE1	11	0.39
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD13	2	0.39
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG21	6	0.39
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB2	4	0.39
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD13	7	0.39
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD23	6	0.39
(2,94)	1:180:A:VAL:HG21	1:103:A:TYR:HA	3	0.39
(2,94)	1:180:A:VAL:HG23	1:103:A:TYR:HA	15	0.39
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	1	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:116:A:LEU:HD12	1:117:A:ILE:H	8	0.39
(2,86)	1:67:A:ILE:HG23	1:106:A:TYR:HD2	1	0.39
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	8	0.39
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	4	0.39
(2,4812)	1:162:A:CYS:H	1:160:A:LEU:HB2	1	0.38
(2,4812)	1:162:A:CYS:H	1:160:A:LEU:HB2	2	0.38
(2,4788)	1:99:A:LYS:H	1:98:A:ASP:HB3	2	0.38
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	14	0.38
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB2	14	0.38
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	6	0.38
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	9	0.38
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	13	0.38
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG2	9	0.38
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	3	0.38
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD22	11	0.38
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	4	0.38
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	5	0.38
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	6	0.38
(2,4430)	1:11:A:ARG:HG2	1:11:A:ARG:HD2	6	0.38
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	14	0.38
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	5	0.38
(2,4373)	1:167:A:LYS:HD2	1:167:A:LYS:HE2	1	0.38
(2,4325)	1:188:A:MET:HE1	1:108:A:LYS:HE3	9	0.38
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	12	0.38
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	15	0.38
(2,4287)	1:13:A:LYS:HD3	1:15:A:PHE:HD1	3	0.38
(2,4258)	1:95:A:THR:HG23	1:75:A:PHE:HD2	8	0.38
(2,4208)	1:64:A:ILE:HG22	1:66:A:GLU:H	8	0.38
(2,4172)	1:18:A:ALA:HB1	1:22:A:GLN:HE22	4	0.38
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	8	0.38
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	3	0.38
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD12	2	0.38
(2,4068)	1:26:A:ALA:HB3	1:24:A:GLU:H	8	0.38
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	9	0.38
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	10	0.38
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	13	0.38
(2,4064)	1:17:A:MET:HE3	1:20:A:LEU:H	12	0.38
(2,4058)	1:16:A:ILE:HD11	1:15:A:PHE:H	7	0.38
(2,4022)	1:143:A:ILE:HD13	1:147:A:GLN:HE22	1	0.38
(2,4021)	1:18:A:ALA:HB1	1:20:A:LEU:H	1	0.38
(2,4016)	1:64:A:ILE:HG22	1:61:A:PHE:H	13	0.38
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG21	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3956)	1:74:A:ILE:HG23	1:78:A:GLU:H	7	0.38
(2,3943)	1:18:A:ALA:HB2	1:17:A:MET:H	7	0.38
(2,3937)	1:184:A:ALA:HB1	1:182:A:LYS:H	7	0.38
(2,3937)	1:184:A:ALA:HB2	1:182:A:LYS:H	15	0.38
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD21	2	0.38
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	5	0.38
(2,3933)	1:94:A:VAL:HG22	1:95:A:THR:H	13	0.38
(2,3915)	1:121:A:ALA:HB3	1:119:A:GLU:H	7	0.38
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD21	8	0.38
(2,3816)	1:156:A:LEU:HD23	1:156:A:LEU:H	3	0.38
(2,3816)	1:156:A:LEU:HD22	1:156:A:LEU:H	14	0.38
(2,3768)	1:117:A:ILE:HD12	1:117:A:ILE:H	6	0.38
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG23	1	0.38
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG22	15	0.38
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	6	0.38
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	3	0.38
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	12	0.38
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD13	4	0.38
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD12	13	0.38
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	13	0.38
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG23	7	0.38
(2,3289)	1:21:A:LEU:HD11	1:21:A:LEU:H	8	0.38
(2,3289)	1:21:A:LEU:HD13	1:21:A:LEU:H	10	0.38
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	8	0.38
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG21	7	0.38
(2,3031)	1:20:A:LEU:HD11	1:20:A:LEU:H	11	0.38
(2,3031)	1:20:A:LEU:HD12	1:20:A:LEU:H	15	0.38
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	6	0.38
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD22	11	0.38
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG22	1	0.38
(2,2835)	1:146:A:VAL:HG12	1:148:A:ARG:H	10	0.38
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	3	0.38
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	5	0.38
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	10	0.38
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	13	0.38
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	14	0.38
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	8	0.38
(2,2783)	1:135:A:ALA:H	1:134:A:LEU:HA	6	0.38
(2,2763)	1:146:A:VAL:HG23	1:147:A:GLN:H	4	0.38
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG21	5	0.38
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG22	9	0.38
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG22	15	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	13	0.38
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	7	0.38
(2,2540)	1:185:A:ASN:HB2	1:185:A:ASN:HD21	5	0.38
(2,2399)	1:117:A:ILE:HD13	1:116:A:LEU:H	8	0.38
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	9	0.38
(2,2288)	1:21:A:LEU:HD12	1:22:A:GLN:H	3	0.38
(2,2288)	1:21:A:LEU:HD11	1:22:A:GLN:H	8	0.38
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	4	0.38
(2,2151)	1:105:A:THR:HG23	1:105:A:THR:H	1	0.38
(2,2151)	1:105:A:THR:HG23	1:105:A:THR:H	7	0.38
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	2	0.38
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	7	0.38
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG23	11	0.38
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	7	0.38
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG23	5	0.38
(2,1752)	1:76:A:LEU:HD21	1:78:A:GLU:H	9	0.38
(2,1752)	1:76:A:LEU:HD21	1:78:A:GLU:H	10	0.38
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	7	0.38
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	12	0.38
(2,1585)	1:154:A:LEU:HD13	1:148:A:ARG:HA	13	0.38
(2,1562)	1:13:A:LYS:HB3	1:13:A:LYS:H	1	0.38
(2,1562)	1:13:A:LYS:HB3	1:13:A:LYS:H	2	0.38
(2,1522)	1:76:A:LEU:HD11	1:68:A:TYR:HE1	8	0.38
(2,1516)	1:39:A:LEU:HD12	1:61:A:PHE:HB3	7	0.38
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	3	0.38
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	4	0.38
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD11	14	0.38
(2,1399)	1:7:A:GLU:HG3	1:8:A:PHE:HD1	8	0.38
(2,1351)	1:94:A:VAL:HG13	1:96:A:TRP:H	3	0.38
(2,1343)	1:17:A:MET:HE3	1:86:A:PRO:HA	10	0.38
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	1	0.38
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	5	0.38
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	11	0.38
(2,1297)	1:117:A:ILE:HA	1:117:A:ILE:HG13	13	0.38
(2,1254)	1:17:A:MET:HE2	1:82:A:TYR:H	3	0.38
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD23	10	0.38
(2,1202)	1:38:A:TYR:HA	1:128:A:ILE:HD12	13	0.38
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	3	0.38
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	10	0.38
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD12	1	0.38
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG21	14	0.38
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD11	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD12	9	0.38
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD22	5	0.38
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE1	4	0.38
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	1	0.38
(2,851)	1:134:A:LEU:HD21	1:129:A:GLN:HB3	3	0.38
(2,851)	1:134:A:LEU:HD22	1:129:A:GLN:HB3	7	0.38
(2,836)	1:64:A:ILE:HG21	1:65:A:GLN:HG3	3	0.38
(2,761)	1:37:A:THR:HG21	1:36:A:GLU:HG2	12	0.38
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	3	0.38
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	13	0.38
(2,666)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	5	0.38
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	9	0.38
(2,624)	1:39:A:LEU:HD11	1:43:A:THR:HG22	2	0.38
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG21	5	0.38
(2,623)	1:146:A:VAL:HG22	1:146:A:VAL:HB	3	0.38
(2,623)	1:146:A:VAL:HG23	1:146:A:VAL:HB	7	0.38
(2,592)	1:64:A:ILE:HD12	1:31:A:LEU:HD22	14	0.38
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	11	0.38
(2,577)	1:89:A:VAL:HG11	1:93:A:PHE:HE2	10	0.38
(2,500)	1:142:A:LEU:HD21	1:142:A:LEU:HD13	2	0.38
(2,500)	1:142:A:LEU:HD21	1:142:A:LEU:HD12	7	0.38
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD12	15	0.38
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	9	0.38
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	1	0.38
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	3	0.38
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	12	0.38
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD12	8	0.38
(2,359)	1:93:A:PHE:HZ	1:156:A:LEU:HD23	13	0.38
(2,346)	1:102:A:MET:HE1	1:67:A:ILE:HD13	6	0.38
(2,338)	1:102:A:MET:HE3	1:70:A:PHE:HB3	15	0.38
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	1	0.38
(2,318)	1:20:A:LEU:HD22	1:152:A:TYR:HD1	11	0.38
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	7	0.38
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	12	0.38
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB2	7	0.38
(2,112)	1:177:A:MET:HE2	1:100:A:PHE:HE2	15	0.38
(2,102)	1:28:A:VAL:HG11	1:72:A:ASN:HB3	5	0.38
(2,89)	1:116:A:LEU:HD11	1:117:A:ILE:H	4	0.38
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	11	0.38
(2,60)	1:174:A:LEU:HD21	1:178:A:LEU:H	15	0.38
(2,43)	1:128:A:ILE:HG21	1:38:A:TYR:H	11	0.38
(2,42)	1:53:A:ILE:HG21	1:120:A:HIS:HD2	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:53:A:ILE:HG23	1:120:A:HIS:HD2	15	0.38
(2,40)	1:31:A:LEU:HD11	1:67:A:ILE:HB	10	0.38
(2,40)	1:31:A:LEU:HD11	1:67:A:ILE:HB	15	0.38
(2,29)	1:35:A:LEU:HD13	1:33:A:GLU:H	12	0.38
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	10	0.37
(2,4778)	1:11:A:ARG:HD3	1:12:A:LYS:H	5	0.37
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	5	0.37
(2,4772)	1:32:A:HIS:HE1	1:69:A:ASP:HA	10	0.37
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	14	0.37
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	10	0.37
(2,4663)	1:108:A:LYS:H	1:109:A:ASN:HB3	3	0.37
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB2	9	0.37
(2,4603)	1:10:A:GLY:H	1:9:A:PRO:HG2	12	0.37
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD13	2	0.37
(2,4554)	1:146:A:VAL:HG21	1:110:A:LYS:HD3	10	0.37
(2,4553)	1:64:A:ILE:HG21	1:65:A:GLN:HE21	13	0.37
(2,4547)	1:102:A:MET:HE1	1:64:A:ILE:HA	15	0.37
(2,4518)	1:128:A:ILE:HG21	1:124:A:PHE:HZ	14	0.37
(2,4516)	1:141:A:TYR:HD2	1:138:A:ILE:HD12	4	0.37
(2,4489)	1:184:A:ALA:HB2	1:108:A:LYS:HE2	8	0.37
(2,4430)	1:11:A:ARG:HG2	1:11:A:ARG:HD2	1	0.37
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	4	0.37
(2,4423)	1:116:A:LEU:HD23	1:56:A:LYS:HE2	4	0.37
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG23	3	0.37
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	3	0.37
(2,4352)	1:28:A:VAL:HG23	1:25:A:LYS:HG2	2	0.37
(2,4340)	1:178:A:LEU:HD11	1:175:A:GLU:HG2	2	0.37
(2,4320)	1:188:A:MET:HA	1:108:A:LYS:HE2	9	0.37
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	5	0.37
(2,4305)	1:56:A:LYS:HE3	1:55:A:ASN:HD21	2	0.37
(2,4304)	1:186:A:ASP:HB2	1:183:A:LYS:HG3	7	0.37
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	12	0.37
(2,4232)	1:117:A:ILE:HG21	1:116:A:LEU:H	5	0.37
(2,4229)	1:28:A:VAL:HG13	1:73:A:ASN:H	12	0.37
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD22	10	0.37
(2,4193)	1:20:A:LEU:HD22	1:21:A:LEU:H	5	0.37
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	4	0.37
(2,4186)	1:178:A:LEU:HD22	1:179:A:SER:H	5	0.37
(2,4186)	1:178:A:LEU:HD21	1:179:A:SER:H	13	0.37
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG12	1	0.37
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG13	14	0.37
(2,4116)	1:79:A:LEU:HD13	1:78:A:GLU:H	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	14	0.37
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	6	0.37
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	8	0.37
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	11	0.37
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG22	2	0.37
(2,3988)	1:21:A:LEU:HD12	1:83:A:GLU:H	4	0.37
(2,3979)	1:18:A:ALA:HB3	1:22:A:GLN:H	1	0.37
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD13	12	0.37
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD12	7	0.37
(2,3961)	1:155:A:LEU:HD12	1:155:A:LEU:H	4	0.37
(2,3933)	1:94:A:VAL:HG22	1:95:A:THR:H	3	0.37
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	9	0.37
(2,3889)	1:85:A:LEU:HD21	1:84:A:GLN:H	15	0.37
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD11	1	0.37
(2,3872)	1:60:A:ILE:HD11	1:62:A:GLY:H	5	0.37
(2,3872)	1:60:A:ILE:HD13	1:62:A:GLY:H	9	0.37
(2,3872)	1:60:A:ILE:HD12	1:62:A:GLY:H	12	0.37
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD13	13	0.37
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD23	12	0.37
(2,3768)	1:117:A:ILE:HD11	1:117:A:ILE:H	10	0.37
(2,3768)	1:117:A:ILE:HD12	1:117:A:ILE:H	14	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG23	3	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG21	4	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG22	5	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG23	10	0.37
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG21	11	0.37
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD12	10	0.37
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	15	0.37
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	8	0.37
(2,3652)	1:161:A:THR:HG22	1:162:A:CYS:H	3	0.37
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	15	0.37
(2,3624)	1:3:A:LEU:H	1:3:A:LEU:HB3	6	0.37
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD12	1	0.37
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD13	7	0.37
(2,3344)	1:170:A:LEU:HD13	1:171:A:LYS:H	8	0.37
(2,3289)	1:21:A:LEU:HD13	1:21:A:LEU:H	5	0.37
(2,3257)	1:170:A:LEU:HD23	1:160:A:LEU:H	8	0.37
(2,3257)	1:170:A:LEU:HD22	1:160:A:LEU:H	14	0.37
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD12	10	0.37
(2,3106)	1:43:A:THR:H	1:44:A:SER:HB3	15	0.37
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG23	3	0.37
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG21	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD23	15	0.37
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD21	13	0.37
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG21	15	0.37
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	1	0.37
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	6	0.37
(2,2763)	1:146:A:VAL:HG23	1:147:A:GLN:H	2	0.37
(2,2763)	1:146:A:VAL:HG23	1:147:A:GLN:H	7	0.37
(2,2763)	1:146:A:VAL:HG21	1:147:A:GLN:H	14	0.37
(2,2763)	1:146:A:VAL:HG22	1:147:A:GLN:H	15	0.37
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG22	5	0.37
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG22	10	0.37
(2,2567)	1:91:A:HIS:H	1:89:A:VAL:HG21	12	0.37
(2,2399)	1:117:A:ILE:HD13	1:116:A:LEU:H	5	0.37
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD13	2	0.37
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	6	0.37
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	11	0.37
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD22	4	0.37
(2,2204)	1:122:A:GLY:HA2	1:123:A:THR:H	8	0.37
(2,2171)	1:174:A:LEU:HD23	1:174:A:LEU:H	1	0.37
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	6	0.37
(2,2171)	1:174:A:LEU:HD22	1:174:A:LEU:H	10	0.37
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	12	0.37
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	13	0.37
(2,2151)	1:105:A:THR:HG21	1:105:A:THR:H	8	0.37
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB2	2	0.37
(2,2150)	1:105:A:THR:H	1:184:A:ALA:HB2	5	0.37
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	13	0.37
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG11	10	0.37
(2,1805)	1:185:A:ASN:HD21	1:182:A:LYS:HA	7	0.37
(2,1752)	1:76:A:LEU:HD21	1:78:A:GLU:H	1	0.37
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG22	9	0.37
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	10	0.37
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	7	0.37
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	2	0.37
(2,1630)	1:178:A:LEU:HD21	1:153:A:GLN:H	6	0.37
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD13	13	0.37
(2,1594)	1:135:A:ALA:HA	1:129:A:GLN:HE22	3	0.37
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	6	0.37
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	14	0.37
(2,1558)	1:20:A:LEU:HD23	1:89:A:VAL:HA	11	0.37
(2,1555)	1:18:A:ALA:HB1	1:22:A:GLN:HB3	11	0.37
(2,1547)	1:95:A:THR:HG21	1:78:A:GLU:HB2	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1543)	1:128:A:ILE:HD11	1:132:A:HIS:HD2	9	0.37
(2,1522)	1:76:A:LEU:HD11	1:68:A:TYR:HE1	3	0.37
(2,1522)	1:76:A:LEU:HD11	1:68:A:TYR:HE1	15	0.37
(2,1519)	1:39:A:LEU:HD13	1:65:A:GLN:H	15	0.37
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	13	0.37
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD22	8	0.37
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	13	0.37
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	14	0.37
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD12	9	0.37
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	3	0.37
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD11	3	0.37
(2,1402)	1:35:A:LEU:HD12	1:65:A:GLN:HB2	8	0.37
(2,1371)	1:31:A:LEU:HD13	1:29:A:ARG:H	5	0.37
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	6	0.37
(2,1280)	1:35:A:LEU:HD21	1:31:A:LEU:HA	7	0.37
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	10	0.37
(2,1210)	1:134:A:LEU:HD12	1:134:A:LEU:HA	2	0.37
(2,1210)	1:134:A:LEU:HD12	1:134:A:LEU:HA	7	0.37
(2,1210)	1:134:A:LEU:HD11	1:134:A:LEU:HA	11	0.37
(2,1170)	1:18:A:ALA:HB2	1:18:A:ALA:HA	2	0.37
(2,1146)	1:135:A:ALA:HA	1:135:A:ALA:HB2	7	0.37
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD12	3	0.37
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD11	8	0.37
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD11	14	0.37
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	2	0.37
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	7	0.37
(2,890)	1:73:A:ASN:HB2	1:74:A:ILE:HD13	12	0.37
(2,868)	1:18:A:ALA:HB1	1:22:A:GLN:HG3	3	0.37
(2,761)	1:37:A:THR:HG22	1:36:A:GLU:HG2	13	0.37
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	6	0.37
(2,644)	1:105:A:THR:HG23	1:108:A:LYS:HD3	11	0.37
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	1	0.37
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	8	0.37
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG21	15	0.37
(2,623)	1:146:A:VAL:HG23	1:146:A:VAL:HB	4	0.37
(2,623)	1:146:A:VAL:HG22	1:146:A:VAL:HB	12	0.37
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD23	8	0.37
(2,592)	1:64:A:ILE:HD13	1:31:A:LEU:HD23	9	0.37
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	7	0.37
(2,577)	1:89:A:VAL:HG13	1:93:A:PHE:HE2	12	0.37
(2,500)	1:142:A:LEU:HD21	1:142:A:LEU:HD13	3	0.37
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD11	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD11	14	0.37
(2,469)	1:178:A:LEU:HD22	1:153:A:GLN:HA	4	0.37
(2,438)	1:39:A:LEU:HD11	1:42:A:MET:HB2	11	0.37
(2,437)	1:39:A:LEU:HD11	1:42:A:MET:HG3	2	0.37
(2,437)	1:39:A:LEU:HD11	1:42:A:MET:HG3	15	0.37
(2,427)	1:35:A:LEU:HD13	1:35:A:LEU:HA	15	0.37
(2,387)	1:31:A:LEU:HD22	1:67:A:ILE:HD11	12	0.37
(2,362)	1:156:A:LEU:HD23	1:152:A:TYR:HB2	1	0.37
(2,351)	1:188:A:MET:HE1	1:108:A:LYS:HA	4	0.37
(2,343)	1:99:A:LYS:HD2	1:102:A:MET:HE1	2	0.37
(2,328)	1:42:A:MET:HE1	1:60:A:ILE:HB	14	0.37
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG23	15	0.37
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	8	0.37
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB3	15	0.37
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG23	5	0.37
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	6	0.37
(2,94)	1:180:A:VAL:HG23	1:103:A:TYR:HA	1	0.37
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD13	8	0.37
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	5	0.37
(2,89)	1:116:A:LEU:HD11	1:117:A:ILE:H	9	0.37
(2,89)	1:116:A:LEU:HD11	1:117:A:ILE:H	12	0.37
(2,89)	1:116:A:LEU:HD12	1:117:A:ILE:H	15	0.37
(2,43)	1:128:A:ILE:HG23	1:38:A:TYR:H	9	0.37
(2,43)	1:128:A:ILE:HG21	1:38:A:TYR:H	12	0.37
(2,17)	1:39:A:LEU:HD23	1:42:A:MET:HG2	7	0.37
(2,16)	1:79:A:LEU:HD12	1:75:A:PHE:HA	2	0.37
(2,16)	1:79:A:LEU:HD11	1:75:A:PHE:HA	6	0.37
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	1	0.36
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	9	0.36
(2,4778)	1:11:A:ARG:HD2	1:12:A:LYS:H	13	0.36
(2,4687)	1:11:A:ARG:HG2	1:12:A:LYS:H	8	0.36
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB2	6	0.36
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG23	14	0.36
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	11	0.36
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	4	0.36
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	10	0.36
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD21	5	0.36
(2,4565)	1:72:A:ASN:H	1:76:A:LEU:HD11	4	0.36
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	1	0.36
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD3	15	0.36
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	3	0.36
(2,4373)	1:167:A:LYS:HD3	1:167:A:LYS:HE2	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4352)	1:28:A:VAL:HG22	1:25:A:LYS:HG2	11	0.36
(2,4348)	1:60:A:ILE:HD12	1:113:A:SER:H	15	0.36
(2,4329)	1:156:A:LEU:HD23	1:175:A:GLU:HG3	9	0.36
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG21	8	0.36
(2,4292)	1:48:A:GLU:HB3	1:49:A:ILE:HG22	11	0.36
(2,4232)	1:117:A:ILE:HG22	1:116:A:LEU:H	1	0.36
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	3	0.36
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	9	0.36
(2,4193)	1:20:A:LEU:HD22	1:21:A:LEU:H	4	0.36
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	7	0.36
(2,4193)	1:20:A:LEU:HD23	1:21:A:LEU:H	10	0.36
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	13	0.36
(2,4135)	1:94:A:VAL:H	1:176:A:VAL:HG11	10	0.36
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	8	0.36
(2,4078)	1:28:A:VAL:HG21	1:30:A:ASP:H	7	0.36
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	12	0.36
(2,4069)	1:23:A:THR:HG21	1:24:A:GLU:H	5	0.36
(2,4068)	1:26:A:ALA:HB2	1:24:A:GLU:H	5	0.36
(2,4068)	1:26:A:ALA:HB3	1:24:A:GLU:H	11	0.36
(2,4068)	1:26:A:ALA:HB3	1:24:A:GLU:H	14	0.36
(2,4064)	1:17:A:MET:HE3	1:20:A:LEU:H	2	0.36
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD21	2	0.36
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	2	0.36
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	9	0.36
(2,4021)	1:18:A:ALA:HB1	1:20:A:LEU:H	2	0.36
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG23	8	0.36
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG23	10	0.36
(2,3988)	1:21:A:LEU:HD11	1:83:A:GLU:H	5	0.36
(2,3969)	1:184:A:ALA:HB3	1:108:A:LYS:H	2	0.36
(2,3969)	1:184:A:ALA:HB3	1:108:A:LYS:H	5	0.36
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	12	0.36
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	10	0.36
(2,3943)	1:18:A:ALA:HB1	1:17:A:MET:H	1	0.36
(2,3943)	1:18:A:ALA:HB2	1:17:A:MET:H	4	0.36
(2,3943)	1:18:A:ALA:HB3	1:17:A:MET:H	5	0.36
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	3	0.36
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	14	0.36
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	11	0.36
(2,3913)	1:176:A:VAL:HG22	1:100:A:PHE:H	3	0.36
(2,3904)	1:31:A:LEU:HD23	1:72:A:ASN:H	14	0.36
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD13	1	0.36
(2,3872)	1:60:A:ILE:HD12	1:62:A:GLY:H	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD21	5	0.36
(2,3816)	1:156:A:LEU:HD23	1:156:A:LEU:H	15	0.36
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD23	7	0.36
(2,3768)	1:117:A:ILE:HD12	1:117:A:ILE:H	9	0.36
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG21	2	0.36
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG23	9	0.36
(2,3740)	1:95:A:THR:HG21	1:96:A:TRP:H	2	0.36
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD13	7	0.36
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD12	14	0.36
(2,3686)	1:60:A:ILE:HG21	1:60:A:ILE:H	3	0.36
(2,3686)	1:60:A:ILE:HG23	1:60:A:ILE:H	7	0.36
(2,3686)	1:60:A:ILE:HG21	1:60:A:ILE:H	8	0.36
(2,3635)	1:12:A:LYS:HA	1:13:A:LYS:H	3	0.36
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	8	0.36
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	1	0.36
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD12	15	0.36
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG22	13	0.36
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	2	0.36
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	5	0.36
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG11	13	0.36
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	9	0.36
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD12	12	0.36
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	7	0.36
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	14	0.36
(2,3031)	1:20:A:LEU:HD13	1:20:A:LEU:H	13	0.36
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG22	9	0.36
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG23	13	0.36
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	11	0.36
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	14	0.36
(2,2763)	1:146:A:VAL:HG23	1:147:A:GLN:H	11	0.36
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG21	4	0.36
(2,2643)	1:108:A:LYS:H	1:107:A:CYS:HB2	9	0.36
(2,2643)	1:108:A:LYS:H	1:107:A:CYS:HB2	13	0.36
(2,2638)	1:180:A:VAL:HG21	1:104:A:VAL:H	5	0.36
(2,2638)	1:180:A:VAL:HG21	1:104:A:VAL:H	11	0.36
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	11	0.36
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG22	3	0.36
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG21	6	0.36
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG22	12	0.36
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	15	0.36
(2,2165)	1:151:A:LYS:H	1:151:A:LYS:HB2	9	0.36
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	13	0.36
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	14	0.36
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	7	0.36
(2,1838)	1:16:A:ILE:HD12	1:158:A:GLU:H	14	0.36
(2,1752)	1:76:A:LEU:HD22	1:78:A:GLU:H	2	0.36
(2,1752)	1:76:A:LEU:HD22	1:78:A:GLU:H	5	0.36
(2,1752)	1:76:A:LEU:HD22	1:78:A:GLU:H	11	0.36
(2,1752)	1:76:A:LEU:HD22	1:78:A:GLU:H	14	0.36
(2,1752)	1:76:A:LEU:HD22	1:78:A:GLU:H	15	0.36
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG23	6	0.36
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	6	0.36
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	1	0.36
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	3	0.36
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD12	7	0.36
(2,1590)	1:18:A:ALA:HB3	1:20:A:LEU:HA	2	0.36
(2,1555)	1:18:A:ALA:HB1	1:22:A:GLN:HB3	7	0.36
(2,1543)	1:128:A:ILE:HD13	1:132:A:HIS:HD2	4	0.36
(2,1543)	1:128:A:ILE:HD13	1:132:A:HIS:HD2	7	0.36
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG21	7	0.36
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	7	0.36
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD22	5	0.36
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	10	0.36
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD22	11	0.36
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	15	0.36
(2,1476)	1:134:A:LEU:HD22	1:34:A:CYS:HA	1	0.36
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	10	0.36
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	1	0.36
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG11	1	0.36
(2,1371)	1:31:A:LEU:HD11	1:29:A:ARG:H	2	0.36
(2,1371)	1:31:A:LEU:HD12	1:29:A:ARG:H	8	0.36
(2,1321)	1:23:A:THR:HG21	1:22:A:GLN:HB3	3	0.36
(2,1279)	1:59:A:ILE:HG23	1:112:A:ASP:HB3	3	0.36
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE2	14	0.36
(2,1210)	1:134:A:LEU:HD12	1:134:A:LEU:HA	10	0.36
(2,1210)	1:134:A:LEU:HD13	1:134:A:LEU:HA	14	0.36
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	8	0.36
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	9	0.36
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG21	14	0.36
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD13	10	0.36
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD12	10	0.36
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD12	14	0.36
(2,935)	1:29:A:ARG:HG2	1:29:A:ARG:HD3	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	6	0.36
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD23	4	0.36
(2,836)	1:64:A:ILE:HG22	1:65:A:GLN:HG3	15	0.36
(2,761)	1:37:A:THR:HG22	1:36:A:GLU:HG2	15	0.36
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG23	5	0.36
(2,733)	1:97:A:ALA:HB2	1:176:A:VAL:HG12	7	0.36
(2,630)	1:64:A:ILE:HG23	1:35:A:LEU:HG	14	0.36
(2,589)	1:64:A:ILE:HD11	1:35:A:LEU:HB3	4	0.36
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	6	0.36
(2,528)	1:46:A:VAL:HG23	1:41:A:GLU:HB3	13	0.36
(2,500)	1:142:A:LEU:HD22	1:142:A:LEU:HD12	8	0.36
(2,438)	1:39:A:LEU:HD13	1:42:A:MET:HB2	5	0.36
(2,437)	1:39:A:LEU:HD11	1:42:A:MET:HG3	11	0.36
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	12	0.36
(2,415)	1:37:A:THR:HG21	1:36:A:GLU:HG3	11	0.36
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD12	4	0.36
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD12	10	0.36
(2,313)	1:20:A:LEU:HD13	1:22:A:GLN:H	7	0.36
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG21	9	0.36
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	1	0.36
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	14	0.36
(2,131)	1:23:A:THR:HG21	1:148:A:ARG:HD3	2	0.36
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD22	4	0.36
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD23	13	0.36
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD12	1	0.36
(2,89)	1:116:A:LEU:HD11	1:117:A:ILE:H	2	0.36
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	14	0.36
(2,87)	1:67:A:ILE:HG21	1:31:A:LEU:HD13	12	0.36
(2,40)	1:31:A:LEU:HD11	1:67:A:ILE:HB	1	0.36
(2,40)	1:31:A:LEU:HD11	1:67:A:ILE:HB	8	0.36
(2,40)	1:31:A:LEU:HD13	1:67:A:ILE:HB	9	0.36
(2,36)	1:39:A:LEU:HD12	1:65:A:GLN:HG2	6	0.36
(2,17)	1:39:A:LEU:HD23	1:42:A:MET:HG2	12	0.36
(2,4841)	1:171:A:LYS:HG2	1:170:A:LEU:H	1	0.35
(2,4841)	1:171:A:LYS:HG2	1:170:A:LEU:H	6	0.35
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	3	0.35
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	13	0.35
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	3	0.35
(2,4780)	1:47:A:GLU:HG3	1:47:A:GLU:H	6	0.35
(2,4687)	1:11:A:ARG:HG3	1:12:A:LYS:H	9	0.35
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG22	13	0.35
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG22	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	4	0.35
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG23	1	0.35
(2,4539)	1:95:A:THR:HG23	1:91:A:HIS:HB2	14	0.35
(2,4518)	1:128:A:ILE:HG21	1:124:A:PHE:HZ	1	0.35
(2,4518)	1:128:A:ILE:HG22	1:124:A:PHE:HZ	4	0.35
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	13	0.35
(2,4373)	1:167:A:LYS:HD3	1:167:A:LYS:HE2	6	0.35
(2,4331)	1:95:A:THR:HG21	1:92:A:CYS:HG	8	0.35
(2,4325)	1:188:A:MET:HE3	1:108:A:LYS:HE3	13	0.35
(2,4299)	1:101:A:GLN:HG2	1:104:A:VAL:HG11	15	0.35
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG22	4	0.35
(2,4282)	1:146:A:VAL:HG12	1:103:A:TYR:HE1	1	0.35
(2,4265)	1:142:A:LEU:HD13	1:110:A:LYS:HB2	8	0.35
(2,4258)	1:95:A:THR:HG21	1:75:A:PHE:HD2	6	0.35
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	9	0.35
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	7	0.35
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	5	0.35
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	9	0.35
(2,4172)	1:18:A:ALA:HB3	1:22:A:GLN:HE22	12	0.35
(2,4119)	1:7:A:GLU:HG2	1:7:A:GLU:H	1	0.35
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD11	11	0.35
(2,4084)	1:162:A:CYS:H	1:162:A:CYS:HB2	2	0.35
(2,4078)	1:28:A:VAL:HG21	1:30:A:ASP:H	1	0.35
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	3	0.35
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG23	4	0.35
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG21	11	0.35
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD13	3	0.35
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	15	0.35
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	10	0.35
(2,3937)	1:184:A:ALA:HB1	1:182:A:LYS:H	11	0.35
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD22	7	0.35
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	11	0.35
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	7	0.35
(2,3880)	1:166:A:GLY:H	1:170:A:LEU:HD11	9	0.35
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD13	2	0.35
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	4	0.35
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG23	8	0.35
(2,3744)	1:97:A:ALA:H	1:95:A:THR:HG21	12	0.35
(2,3740)	1:95:A:THR:HG21	1:96:A:TRP:H	6	0.35
(2,3686)	1:60:A:ILE:HG23	1:60:A:ILE:H	1	0.35
(2,3686)	1:60:A:ILE:HG22	1:60:A:ILE:H	5	0.35
(2,3686)	1:60:A:ILE:HG23	1:60:A:ILE:H	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3686)	1:60:A:ILE:HG22	1:60:A:ILE:H	9	0.35
(2,3686)	1:60:A:ILE:HG22	1:60:A:ILE:H	10	0.35
(2,3686)	1:60:A:ILE:HG21	1:60:A:ILE:H	11	0.35
(2,3686)	1:60:A:ILE:HG21	1:60:A:ILE:H	13	0.35
(2,3686)	1:60:A:ILE:HG22	1:60:A:ILE:H	14	0.35
(2,3686)	1:60:A:ILE:HG22	1:60:A:ILE:H	15	0.35
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD23	2	0.35
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	9	0.35
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	4	0.35
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	9	0.35
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD22	4	0.35
(2,3257)	1:170:A:LEU:HD23	1:160:A:LEU:H	13	0.35
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD12	11	0.35
(2,3130)	1:49:A:ILE:HD12	1:49:A:ILE:H	2	0.35
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	13	0.35
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG23	6	0.35
(2,3012)	1:12:A:LYS:H	1:12:A:LYS:HB2	9	0.35
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG22	8	0.35
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG21	11	0.35
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	12	0.35
(2,2818)	1:143:A:ILE:H	1:142:A:LEU:HB3	9	0.35
(2,2763)	1:146:A:VAL:HG21	1:147:A:GLN:H	8	0.35
(2,2644)	1:108:A:LYS:H	1:109:A:ASN:HB2	12	0.35
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG23	4	0.35
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG22	14	0.35
(2,2171)	1:174:A:LEU:HD21	1:174:A:LEU:H	8	0.35
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	9	0.35
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	10	0.35
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	6	0.35
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	11	0.35
(2,1937)	1:34:A:CYS:H	1:61:A:PHE:HD1	11	0.35
(2,1910)	1:177:A:MET:H	1:93:A:PHE:HD1	5	0.35
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	1	0.35
(2,1744)	1:76:A:LEU:HD21	1:77:A:LYS:H	8	0.35
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD13	2	0.35
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD11	11	0.35
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	15	0.35
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	4	0.35
(2,1522)	1:76:A:LEU:HD12	1:68:A:TYR:HE1	10	0.35
(2,1519)	1:39:A:LEU:HD11	1:65:A:GLN:H	13	0.35
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD22	6	0.35
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1463)	1:16:A:ILE:HG22	1:158:A:GLU:HG3	2	0.35
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD12	2	0.35
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	14	0.35
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD13	9	0.35
(2,1402)	1:35:A:LEU:HD12	1:65:A:GLN:HB2	13	0.35
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	2	0.35
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE1	12	0.35
(2,1254)	1:17:A:MET:HE3	1:82:A:TYR:H	9	0.35
(2,1202)	1:38:A:TYR:HA	1:128:A:ILE:HD11	14	0.35
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD13	2	0.35
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD13	2	0.35
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG23	9	0.35
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD22	12	0.35
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD23	3	0.35
(2,824)	1:134:A:LEU:HD22	1:33:A:GLU:HG3	4	0.35
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	15	0.35
(2,644)	1:105:A:THR:HG22	1:108:A:LYS:HD3	2	0.35
(2,644)	1:105:A:THR:HG23	1:108:A:LYS:HD3	9	0.35
(2,630)	1:64:A:ILE:HG21	1:35:A:LEU:HG	3	0.35
(2,630)	1:64:A:ILE:HG21	1:35:A:LEU:HG	7	0.35
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	15	0.35
(2,624)	1:39:A:LEU:HD13	1:43:A:THR:HG22	3	0.35
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	10	0.35
(2,567)	1:116:A:LEU:HD12	1:116:A:LEU:HG	2	0.35
(2,567)	1:116:A:LEU:HD13	1:116:A:LEU:HG	3	0.35
(2,567)	1:116:A:LEU:HD12	1:116:A:LEU:HG	4	0.35
(2,567)	1:116:A:LEU:HD12	1:116:A:LEU:HG	7	0.35
(2,567)	1:116:A:LEU:HD13	1:116:A:LEU:HG	8	0.35
(2,567)	1:116:A:LEU:HD12	1:116:A:LEU:HG	9	0.35
(2,567)	1:116:A:LEU:HD11	1:116:A:LEU:HG	10	0.35
(2,567)	1:116:A:LEU:HD11	1:116:A:LEU:HG	11	0.35
(2,567)	1:116:A:LEU:HD11	1:116:A:LEU:HG	13	0.35
(2,567)	1:116:A:LEU:HD11	1:116:A:LEU:HG	14	0.35
(2,567)	1:116:A:LEU:HD13	1:116:A:LEU:HG	15	0.35
(2,535)	1:76:A:LEU:HD22	1:71:A:HIS:HB3	12	0.35
(2,467)	1:178:A:LEU:HD23	1:175:A:GLU:H	15	0.35
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	13	0.35
(2,441)	1:31:A:LEU:HD13	1:61:A:PHE:HE1	1	0.35
(2,438)	1:39:A:LEU:HD11	1:42:A:MET:HB2	4	0.35
(2,387)	1:31:A:LEU:HD21	1:67:A:ILE:HD11	6	0.35
(2,387)	1:31:A:LEU:HD22	1:67:A:ILE:HD12	11	0.35
(2,362)	1:156:A:LEU:HD23	1:152:A:TYR:HB2	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,346)	1:102:A:MET:HE2	1:67:A:ILE:HD11	14	0.35
(2,328)	1:42:A:MET:HE2	1:60:A:ILE:HB	11	0.35
(2,316)	1:20:A:LEU:HD12	1:152:A:TYR:HB3	13	0.35
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	7	0.35
(2,313)	1:20:A:LEU:HD11	1:22:A:GLN:H	12	0.35
(2,313)	1:20:A:LEU:HD12	1:22:A:GLN:H	15	0.35
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD12	1	0.35
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD13	5	0.35
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	2	0.35
(2,112)	1:177:A:MET:HE1	1:100:A:PHE:HE1	5	0.35
(2,94)	1:180:A:VAL:HG22	1:103:A:TYR:HA	5	0.35
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	10	0.35
(2,73)	1:76:A:LEU:HD23	1:80:A:GLU:H	7	0.35
(2,19)	1:79:A:LEU:HD13	1:92:A:CYS:HG	13	0.35
(2,17)	1:39:A:LEU:HD23	1:42:A:MET:HG2	3	0.35
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	4	0.34
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	5	0.34
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD3	6	0.34
(2,4803)	1:167:A:LYS:H	1:167:A:LYS:HE3	4	0.34
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	2	0.34
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	7	0.34
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	5	0.34
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	8	0.34
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	8	0.34
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	12	0.34
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	4	0.34
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	10	0.34
(2,4561)	1:23:A:THR:HG21	1:16:A:ILE:HA	3	0.34
(2,4561)	1:23:A:THR:HG22	1:16:A:ILE:HA	14	0.34
(2,4553)	1:64:A:ILE:HG22	1:36:A:GLU:H	6	0.34
(2,4529)	1:60:A:ILE:HG21	1:113:A:SER:HB2	3	0.34
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD3	1	0.34
(2,4486)	1:104:A:VAL:HG12	1:183:A:LYS:HD3	2	0.34
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	10	0.34
(2,4430)	1:11:A:ARG:HG2	1:11:A:ARG:HD2	12	0.34
(2,4429)	1:11:A:ARG:HB3	1:11:A:ARG:HD3	5	0.34
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG21	15	0.34
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD23	1	0.34
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	7	0.34
(2,4348)	1:60:A:ILE:HD13	1:113:A:SER:H	8	0.34
(2,4325)	1:188:A:MET:HE3	1:108:A:LYS:HE3	11	0.34
(2,4272)	1:174:A:LEU:HD22	1:175:A:GLU:HB2	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4258)	1:95:A:THR:HG23	1:75:A:PHE:HD2	1	0.34
(2,4223)	1:159:A:LEU:HD11	1:156:A:LEU:H	15	0.34
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	8	0.34
(2,4170)	1:127:A:GLU:H	1:128:A:ILE:HD12	15	0.34
(2,4160)	1:53:A:ILE:HG21	1:122:A:GLY:H	7	0.34
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD13	4	0.34
(2,4046)	1:159:A:LEU:HD21	1:159:A:LEU:H	4	0.34
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	12	0.34
(2,3988)	1:21:A:LEU:HD13	1:83:A:GLU:H	9	0.34
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG22	9	0.34
(2,3979)	1:18:A:ALA:HB2	1:22:A:GLN:H	14	0.34
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	9	0.34
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	1	0.34
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	3	0.34
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	1	0.34
(2,3934)	1:42:A:MET:HE3	1:60:A:ILE:H	2	0.34
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	12	0.34
(2,3889)	1:85:A:LEU:HD23	1:84:A:GLN:H	10	0.34
(2,3886)	1:161:A:THR:H	1:162:A:CYS:HB2	8	0.34
(2,3872)	1:60:A:ILE:HD11	1:62:A:GLY:H	2	0.34
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	10	0.34
(2,3743)	1:97:A:ALA:HB1	1:97:A:ALA:H	7	0.34
(2,3740)	1:95:A:THR:HG22	1:96:A:TRP:H	5	0.34
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD11	9	0.34
(2,3708)	1:74:A:ILE:H	1:74:A:ILE:HD12	11	0.34
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	11	0.34
(2,3686)	1:60:A:ILE:HG23	1:60:A:ILE:H	2	0.34
(2,3686)	1:60:A:ILE:HG21	1:60:A:ILE:H	4	0.34
(2,3686)	1:60:A:ILE:HG22	1:60:A:ILE:H	12	0.34
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	3	0.34
(2,3624)	1:3:A:LEU:H	1:3:A:LEU:HB3	9	0.34
(2,3624)	1:3:A:LEU:H	1:3:A:LEU:HB3	15	0.34
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG21	6	0.34
(2,3585)	1:100:A:PHE:HD1	1:97:A:ALA:HB3	14	0.34
(2,3569)	1:141:A:TYR:HE2	1:136:A:ASN:HB3	1	0.34
(2,3569)	1:141:A:TYR:HE2	1:136:A:ASN:HB3	14	0.34
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG22	12	0.34
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG23	8	0.34
(2,3289)	1:21:A:LEU:HD11	1:21:A:LEU:H	4	0.34
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	4	0.34
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD13	6	0.34
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG21	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	13	0.34
(2,2893)	1:161:A:THR:H	1:162:A:CYS:HB3	8	0.34
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD22	14	0.34
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG22	3	0.34
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG22	5	0.34
(2,2763)	1:146:A:VAL:HG21	1:147:A:GLN:H	5	0.34
(2,2675)	1:117:A:ILE:HD12	1:113:A:SER:H	11	0.34
(2,2644)	1:108:A:LYS:H	1:109:A:ASN:HB2	13	0.34
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG22	7	0.34
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	9	0.34
(2,2446)	1:74:A:ILE:HG21	1:73:A:ASN:H	3	0.34
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD12	12	0.34
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	5	0.34
(2,2288)	1:21:A:LEU:HD13	1:22:A:GLN:H	11	0.34
(2,2275)	1:190:A:VAL:H	1:189:A:HIS:HB3	9	0.34
(2,2171)	1:174:A:LEU:HD22	1:174:A:LEU:H	14	0.34
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	15	0.34
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	4	0.34
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG11	11	0.34
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	5	0.34
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	10	0.34
(2,1860)	1:136:A:ASN:H	1:129:A:GLN:HE22	13	0.34
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG23	12	0.34
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	6	0.34
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG22	14	0.34
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	11	0.34
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	9	0.34
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	9	0.34
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	3	0.34
(2,1520)	1:76:A:LEU:HD13	1:29:A:ARG:H	7	0.34
(2,1516)	1:39:A:LEU:HD13	1:61:A:PHE:HB3	2	0.34
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	14	0.34
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD22	2	0.34
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	7	0.34
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD13	7	0.34
(2,1371)	1:31:A:LEU:HD13	1:29:A:ARG:H	4	0.34
(2,1321)	1:23:A:THR:HG21	1:22:A:GLN:HB3	12	0.34
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	10	0.34
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	12	0.34
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE3	11	0.34
(2,1245)	1:20:A:LEU:HD13	1:24:A:GLU:H	4	0.34
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1210)	1:134:A:LEU:HD13	1:134:A:LEU:HA	9	0.34
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	6	0.34
(2,1170)	1:18:A:ALA:HB3	1:18:A:ALA:HA	7	0.34
(2,1170)	1:18:A:ALA:HB2	1:18:A:ALA:HA	10	0.34
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	13	0.34
(2,1037)	1:143:A:ILE:HG21	1:140:A:SER:HB2	8	0.34
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	14	0.34
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD22	10	0.34
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD22	15	0.34
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG23	9	0.34
(2,761)	1:37:A:THR:HG23	1:36:A:GLU:HG2	5	0.34
(2,752)	1:11:A:ARG:HB3	1:12:A:LYS:H	12	0.34
(2,654)	1:177:A:MET:HE1	1:174:A:LEU:HA	14	0.34
(2,652)	1:177:A:MET:HE2	1:179:A:SER:H	13	0.34
(2,644)	1:105:A:THR:HG22	1:108:A:LYS:HD3	7	0.34
(2,644)	1:105:A:THR:HG21	1:108:A:LYS:HD3	15	0.34
(2,643)	1:105:A:THR:HG21	1:106:A:TYR:HD2	11	0.34
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	1	0.34
(2,577)	1:89:A:VAL:HG13	1:93:A:PHE:HE2	2	0.34
(2,567)	1:116:A:LEU:HD13	1:116:A:LEU:HG	1	0.34
(2,567)	1:116:A:LEU:HD11	1:116:A:LEU:HG	5	0.34
(2,567)	1:116:A:LEU:HD12	1:116:A:LEU:HG	6	0.34
(2,468)	1:178:A:LEU:HD21	1:175:A:GLU:HA	9	0.34
(2,468)	1:178:A:LEU:HD22	1:175:A:GLU:HA	11	0.34
(2,449)	1:53:A:ILE:HG22	1:125:A:PHE:HZ	10	0.34
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	8	0.34
(2,422)	1:49:A:ILE:HG21	1:124:A:PHE:HB3	8	0.34
(2,422)	1:49:A:ILE:HG21	1:124:A:PHE:HB3	13	0.34
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	14	0.34
(2,418)	1:53:A:ILE:HD12	1:124:A:PHE:HB3	13	0.34
(2,394)	1:39:A:LEU:HD21	1:39:A:LEU:HB3	4	0.34
(2,394)	1:39:A:LEU:HD21	1:39:A:LEU:HB3	6	0.34
(2,394)	1:39:A:LEU:HD22	1:39:A:LEU:HB3	9	0.34
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	9	0.34
(2,313)	1:20:A:LEU:HD11	1:22:A:GLN:H	10	0.34
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD12	14	0.34
(2,160)	1:177:A:MET:HB3	1:156:A:LEU:HD23	1	0.34
(2,131)	1:23:A:THR:HG22	1:148:A:ARG:HD3	8	0.34
(2,116)	1:177:A:MET:HE1	1:100:A:PHE:HB2	10	0.34
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD21	12	0.34
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD11	11	0.34
(2,89)	1:116:A:LEU:HD11	1:117:A:ILE:H	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:116:A:LEU:HD13	1:117:A:ILE:H	13	0.34
(2,40)	1:31:A:LEU:HD12	1:67:A:ILE:HB	5	0.34
(2,40)	1:31:A:LEU:HD11	1:67:A:ILE:HB	11	0.34
(2,40)	1:31:A:LEU:HD13	1:67:A:ILE:HB	12	0.34
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	9	0.34
(2,36)	1:39:A:LEU:HD12	1:65:A:GLN:HG2	10	0.34
(2,17)	1:39:A:LEU:HD21	1:42:A:MET:HG2	11	0.34
(2,4841)	1:171:A:LYS:HG2	1:170:A:LEU:H	7	0.33
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	9	0.33
(2,4818)	1:7:A:GLU:H	1:5:A:SER:HB2	7	0.33
(2,4815)	1:165:A:GLU:HG2	1:167:A:LYS:H	5	0.33
(2,4803)	1:167:A:LYS:H	1:167:A:LYS:HE2	5	0.33
(2,4778)	1:11:A:ARG:HD2	1:12:A:LYS:H	11	0.33
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	11	0.33
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	1	0.33
(2,4750)	1:120:A:HIS:HD2	1:121:A:ALA:HA	7	0.33
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	15	0.33
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG2	2	0.33
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG21	9	0.33
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	9	0.33
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	9	0.33
(2,4553)	1:64:A:ILE:HG23	1:65:A:GLN:HE21	4	0.33
(2,4539)	1:95:A:THR:HG22	1:91:A:HIS:HB2	12	0.33
(2,4521)	1:54:A:LEU:HD13	1:54:A:LEU:HA	8	0.33
(2,4521)	1:54:A:LEU:HD13	1:54:A:LEU:HA	11	0.33
(2,4502)	1:14:A:GLU:HB2	1:15:A:PHE:HE1	5	0.33
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	8	0.33
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG21	7	0.33
(2,4409)	1:172:A:ASP:HB2	1:94:A:VAL:HB	2	0.33
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG13	3	0.33
(2,4353)	1:43:A:THR:HG23	1:39:A:LEU:HB3	7	0.33
(2,4348)	1:60:A:ILE:HD13	1:113:A:SER:H	9	0.33
(2,4348)	1:60:A:ILE:HD12	1:113:A:SER:H	13	0.33
(2,4264)	1:16:A:ILE:HD12	1:19:A:GLU:HB3	5	0.33
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD12	6	0.33
(2,4258)	1:95:A:THR:HG22	1:75:A:PHE:HD1	7	0.33
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	12	0.33
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	6	0.33
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD23	8	0.33
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	11	0.33
(2,4210)	1:69:A:ASP:HA	1:73:A:ASN:HD22	3	0.33
(2,4193)	1:20:A:LEU:HD23	1:21:A:LEU:H	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4193)	1:20:A:LEU:HD23	1:21:A:LEU:H	8	0.33
(2,4116)	1:79:A:LEU:HD11	1:78:A:GLU:H	1	0.33
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	12	0.33
(2,4084)	1:162:A:CYS:H	1:162:A:CYS:HB2	14	0.33
(2,4083)	1:163:A:CYS:HB2	1:162:A:CYS:H	9	0.33
(2,4078)	1:28:A:VAL:HG22	1:30:A:ASP:H	11	0.33
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	12	0.33
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	12	0.33
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	3	0.33
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	6	0.33
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD1	5	0.33
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG21	6	0.33
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG23	9	0.33
(2,3937)	1:184:A:ALA:HB3	1:182:A:LYS:H	14	0.33
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD21	4	0.33
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD22	9	0.33
(2,3915)	1:121:A:ALA:HB1	1:119:A:GLU:H	2	0.33
(2,3910)	1:156:A:LEU:HD21	1:153:A:GLN:H	7	0.33
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD21	10	0.33
(2,3889)	1:85:A:LEU:HD22	1:84:A:GLN:H	9	0.33
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD21	2	0.33
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD22	3	0.33
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD21	10	0.33
(2,3740)	1:95:A:THR:HG23	1:96:A:TRP:H	1	0.33
(2,3728)	1:87:A:GLU:HG3	1:87:A:GLU:H	12	0.33
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	9	0.33
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	6	0.33
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD21	8	0.33
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	1	0.33
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG11	4	0.33
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD21	5	0.33
(2,3264)	1:94:A:VAL:HG23	1:172:A:ASP:H	6	0.33
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD13	2	0.33
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	10	0.33
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	6	0.33
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD13	8	0.33
(2,3042)	1:22:A:GLN:HB2	1:23:A:THR:H	5	0.33
(2,3031)	1:20:A:LEU:HD13	1:20:A:LEU:H	5	0.33
(2,2923)	1:170:A:LEU:H	1:168:A:GLY:HA2	8	0.33
(2,2922)	1:170:A:LEU:H	1:159:A:LEU:HD13	1	0.33
(2,2902)	1:166:A:GLY:HA3	1:167:A:LYS:H	2	0.33
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD23	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	15	0.33
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	4	0.33
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	15	0.33
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	12	0.33
(2,2763)	1:146:A:VAL:HG21	1:147:A:GLN:H	6	0.33
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG22	8	0.33
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG21	10	0.33
(2,2675)	1:117:A:ILE:HD11	1:113:A:SER:H	9	0.33
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	5	0.33
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	8	0.33
(2,2399)	1:117:A:ILE:HD13	1:116:A:LEU:H	13	0.33
(2,2288)	1:21:A:LEU:HD13	1:22:A:GLN:H	10	0.33
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG23	5	0.33
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	3	0.33
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	11	0.33
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	4	0.33
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	5	0.33
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	10	0.33
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	12	0.33
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	8	0.33
(2,1928)	1:185:A:ASN:HD22	1:182:A:LYS:HA	3	0.33
(2,1860)	1:136:A:ASN:H	1:129:A:GLN:HE22	10	0.33
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG21	2	0.33
(2,1744)	1:76:A:LEU:HD23	1:77:A:LYS:H	13	0.33
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	6	0.33
(2,1726)	1:101:A:GLN:H	1:101:A:GLN:HG3	2	0.33
(2,1630)	1:178:A:LEU:HD23	1:153:A:GLN:H	7	0.33
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD12	3	0.33
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD13	6	0.33
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD11	8	0.33
(2,1592)	1:135:A:ALA:HB2	1:129:A:GLN:HE22	2	0.33
(2,1590)	1:18:A:ALA:HB1	1:20:A:LEU:HA	7	0.33
(2,1562)	1:13:A:LYS:HB3	1:13:A:LYS:H	6	0.33
(2,1543)	1:128:A:ILE:HD11	1:132:A:HIS:HD2	15	0.33
(2,1530)	1:172:A:ASP:HA	1:174:A:LEU:HD21	12	0.33
(2,1522)	1:76:A:LEU:HD11	1:68:A:TYR:HE1	13	0.33
(2,1508)	1:105:A:THR:HG22	1:63:A:ASN:HB3	13	0.33
(2,1476)	1:134:A:LEU:HD22	1:34:A:CYS:HA	10	0.33
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD13	1	0.33
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD12	5	0.33
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD12	8	0.33
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD13	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	15	0.33
(2,1397)	1:188:A:MET:HE3	1:190:A:VAL:HG13	3	0.33
(2,1371)	1:31:A:LEU:HD11	1:29:A:ARG:H	6	0.33
(2,1369)	1:156:A:LEU:HD11	1:170:A:LEU:HB3	3	0.33
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	2	0.33
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	9	0.33
(2,1321)	1:23:A:THR:HG22	1:22:A:GLN:HB3	13	0.33
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG22	14	0.33
(2,1254)	1:17:A:MET:HE1	1:82:A:TYR:H	7	0.33
(2,1245)	1:20:A:LEU:HD13	1:24:A:GLU:H	5	0.33
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD22	2	0.33
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD23	6	0.33
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	7	0.33
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	15	0.33
(2,1210)	1:134:A:LEU:HD13	1:134:A:LEU:HA	15	0.33
(2,1200)	1:9:A:PRO:HB2	1:9:A:PRO:HA	15	0.33
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	3	0.33
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	13	0.33
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	14	0.33
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD11	12	0.33
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD13	13	0.33
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG23	8	0.33
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG23	10	0.33
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	9	0.33
(2,630)	1:64:A:ILE:HG21	1:35:A:LEU:HG	9	0.33
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	11	0.33
(2,577)	1:89:A:VAL:HG13	1:93:A:PHE:HE2	3	0.33
(2,567)	1:116:A:LEU:HD12	1:116:A:LEU:HG	12	0.33
(2,441)	1:31:A:LEU:HD13	1:61:A:PHE:HE1	11	0.33
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	9	0.33
(2,423)	1:42:A:MET:HE3	1:49:A:ILE:HG21	14	0.33
(2,394)	1:39:A:LEU:HD22	1:39:A:LEU:HB3	1	0.33
(2,394)	1:39:A:LEU:HD23	1:39:A:LEU:HB3	3	0.33
(2,394)	1:39:A:LEU:HD23	1:39:A:LEU:HB3	8	0.33
(2,394)	1:39:A:LEU:HD21	1:39:A:LEU:HB3	11	0.33
(2,394)	1:39:A:LEU:HD22	1:39:A:LEU:HB3	14	0.33
(2,394)	1:39:A:LEU:HD22	1:39:A:LEU:HB3	15	0.33
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD11	1	0.33
(2,343)	1:99:A:LYS:HD2	1:102:A:MET:HE1	4	0.33
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG22	6	0.33
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	5	0.33
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	9	0.33
(2,116)	1:177:A:MET:HE3	1:100:A:PHE:HB2	11	0.33
(2,87)	1:67:A:ILE:HG23	1:31:A:LEU:HD12	14	0.33
(2,61)	1:155:A:LEU:HD21	1:21:A:LEU:H	7	0.33
(2,61)	1:155:A:LEU:HD22	1:21:A:LEU:H	8	0.33
(2,55)	1:142:A:LEU:HD11	1:106:A:TYR:HH	2	0.33
(2,43)	1:128:A:ILE:HG21	1:38:A:TYR:H	6	0.33
(2,40)	1:31:A:LEU:HD12	1:67:A:ILE:HB	3	0.33
(2,40)	1:31:A:LEU:HD12	1:67:A:ILE:HB	4	0.33
(2,36)	1:39:A:LEU:HD13	1:65:A:GLN:HG2	13	0.33
(2,35)	1:39:A:LEU:HD11	1:65:A:GLN:HG3	9	0.33
(2,29)	1:35:A:LEU:HD13	1:33:A:GLU:H	13	0.33
(2,18)	1:79:A:LEU:HD13	1:92:A:CYS:HB2	4	0.33
(2,18)	1:79:A:LEU:HD13	1:92:A:CYS:HB2	5	0.33
(2,18)	1:79:A:LEU:HD13	1:92:A:CYS:HB2	8	0.33
(2,17)	1:39:A:LEU:HD21	1:42:A:MET:HG2	2	0.33
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	7	0.32
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	14	0.32
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	2	0.32
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	11	0.32
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	9	0.32
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	5	0.32
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	14	0.32
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG23	5	0.32
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG22	6	0.32
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	1	0.32
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD22	12	0.32
(2,4603)	1:10:A:GLY:H	1:9:A:PRO:HG2	13	0.32
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	7	0.32
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	8	0.32
(2,4558)	1:99:A:LYS:HD2	1:98:A:ASP:HB2	14	0.32
(2,4460)	1:19:A:GLU:HA	1:23:A:THR:HG21	5	0.32
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG3	3	0.32
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	15	0.32
(2,4423)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	2	0.32
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	9	0.32
(2,4304)	1:186:A:ASP:HB2	1:183:A:LYS:HG3	4	0.32
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG23	5	0.32
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG21	7	0.32
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG22	14	0.32
(2,4277)	1:16:A:ILE:HG22	1:158:A:GLU:HB2	9	0.32
(2,4234)	1:54:A:LEU:HD23	1:53:A:ILE:H	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	4	0.32
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	13	0.32
(2,4218)	1:85:A:LEU:HD13	1:84:A:GLN:H	12	0.32
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD23	4	0.32
(2,4193)	1:20:A:LEU:HD23	1:21:A:LEU:H	6	0.32
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	9	0.32
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	12	0.32
(2,4068)	1:26:A:ALA:HB3	1:24:A:GLU:H	15	0.32
(2,4064)	1:17:A:MET:HE2	1:20:A:LEU:H	9	0.32
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	8	0.32
(2,4021)	1:18:A:ALA:HB3	1:20:A:LEU:H	9	0.32
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD2	15	0.32
(2,4016)	1:64:A:ILE:HG22	1:61:A:PHE:H	7	0.32
(2,3995)	1:17:A:MET:HE3	1:85:A:LEU:H	11	0.32
(2,3988)	1:21:A:LEU:HD13	1:83:A:GLU:H	1	0.32
(2,3988)	1:21:A:LEU:HD11	1:83:A:GLU:H	11	0.32
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	14	0.32
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG23	4	0.32
(2,3942)	1:102:A:MET:HE2	1:102:A:MET:H	4	0.32
(2,3937)	1:184:A:ALA:HB1	1:182:A:LYS:H	5	0.32
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	6	0.32
(2,3933)	1:94:A:VAL:HG21	1:95:A:THR:H	6	0.32
(2,3931)	1:156:A:LEU:HD21	1:177:A:MET:H	13	0.32
(2,3913)	1:176:A:VAL:HG21	1:100:A:PHE:H	12	0.32
(2,3904)	1:31:A:LEU:HD23	1:72:A:ASN:H	12	0.32
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD23	11	0.32
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD12	4	0.32
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	3	0.32
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	5	0.32
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	4	0.32
(2,3844)	1:184:A:ALA:HB1	1:185:A:ASN:H	5	0.32
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD23	14	0.32
(2,3740)	1:95:A:THR:HG23	1:96:A:TRP:H	3	0.32
(2,3740)	1:95:A:THR:HG23	1:96:A:TRP:H	9	0.32
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	6	0.32
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	15	0.32
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	2	0.32
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	8	0.32
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD21	6	0.32
(2,3652)	1:161:A:THR:HG21	1:162:A:CYS:H	15	0.32
(2,3646)	1:22:A:GLN:HB3	1:23:A:THR:H	5	0.32
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	12	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD11	14	0.32
(2,3491)	1:91:A:HIS:HE1	1:95:A:THR:HG21	1	0.32
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG22	8	0.32
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG23	9	0.32
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	8	0.32
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG11	14	0.32
(2,3377)	1:155:A:LEU:H	1:155:A:LEU:HG	13	0.32
(2,3344)	1:170:A:LEU:HD13	1:171:A:LYS:H	1	0.32
(2,3307)	1:31:A:LEU:H	1:29:A:ARG:HD3	2	0.32
(2,3289)	1:21:A:LEU:HD11	1:21:A:LEU:H	7	0.32
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG13	14	0.32
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD13	3	0.32
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	7	0.32
(2,3199)	1:5:A:SER:H	1:4:A:GLY:HA3	2	0.32
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD12	3	0.32
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	3	0.32
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	7	0.32
(2,3130)	1:49:A:ILE:HD12	1:49:A:ILE:H	12	0.32
(2,3130)	1:49:A:ILE:HD12	1:49:A:ILE:H	14	0.32
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	15	0.32
(2,3080)	1:34:A:CYS:H	1:37:A:THR:HG23	1	0.32
(2,3042)	1:22:A:GLN:HB2	1:23:A:THR:H	4	0.32
(2,3012)	1:12:A:LYS:H	1:12:A:LYS:HB2	1	0.32
(2,2904)	1:166:A:GLY:H	1:167:A:LYS:H	1	0.32
(2,2861)	1:155:A:LEU:H	1:155:A:LEU:HA	13	0.32
(2,2763)	1:146:A:VAL:HG22	1:147:A:GLN:H	3	0.32
(2,2763)	1:146:A:VAL:HG22	1:147:A:GLN:H	10	0.32
(2,2638)	1:180:A:VAL:HG21	1:104:A:VAL:H	13	0.32
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG23	2	0.32
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	4	0.32
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	5	0.32
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	2	0.32
(2,2399)	1:117:A:ILE:HD13	1:116:A:LEU:H	10	0.32
(2,2399)	1:117:A:ILE:HD13	1:116:A:LEU:H	12	0.32
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	7	0.32
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	15	0.32
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	1	0.32
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG12	15	0.32
(2,1744)	1:76:A:LEU:HD21	1:77:A:LYS:H	10	0.32
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG21	11	0.32
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	5	0.32
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	8	0.32
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	13	0.32
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	15	0.32
(2,1630)	1:178:A:LEU:HD21	1:153:A:GLN:H	1	0.32
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD12	4	0.32
(2,1590)	1:18:A:ALA:HB3	1:20:A:LEU:HA	1	0.32
(2,1547)	1:95:A:THR:HG21	1:78:A:GLU:HB2	10	0.32
(2,1533)	1:53:A:ILE:HG22	1:117:A:ILE:H	1	0.32
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	11	0.32
(2,1476)	1:134:A:LEU:HD23	1:34:A:CYS:HA	5	0.32
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	3	0.32
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	4	0.32
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	13	0.32
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	13	0.32
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD11	1	0.32
(2,1371)	1:31:A:LEU:HD13	1:29:A:ARG:H	7	0.32
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	1	0.32
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	8	0.32
(2,1350)	1:35:A:LEU:HD13	1:36:A:GLU:H	11	0.32
(2,1350)	1:35:A:LEU:HD12	1:36:A:GLU:H	14	0.32
(2,1281)	1:32:A:HIS:HA	1:35:A:LEU:HD22	13	0.32
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	11	0.32
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	6	0.32
(2,1210)	1:134:A:LEU:HD11	1:134:A:LEU:HA	5	0.32
(2,1210)	1:134:A:LEU:HD12	1:134:A:LEU:HA	8	0.32
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	15	0.32
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD13	11	0.32
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	9	0.32
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD12	11	0.32
(2,1099)	1:22:A:GLN:HA	1:22:A:GLN:HG2	3	0.32
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	4	0.32
(2,918)	1:99:A:LYS:HD2	1:99:A:LYS:HE2	5	0.32
(2,918)	1:99:A:LYS:HD2	1:99:A:LYS:HE2	6	0.32
(2,761)	1:37:A:THR:HG21	1:36:A:GLU:HG2	7	0.32
(2,761)	1:37:A:THR:HG22	1:36:A:GLU:HG2	8	0.32
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG13	2	0.32
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG13	14	0.32
(2,733)	1:97:A:ALA:HB2	1:176:A:VAL:HG12	15	0.32
(2,704)	1:18:A:ALA:HB1	1:21:A:LEU:HB3	4	0.32
(2,700)	1:23:A:THR:HG23	1:21:A:LEU:H	4	0.32
(2,644)	1:105:A:THR:HG21	1:108:A:LYS:HD3	12	0.32
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	12	0.32
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	4	0.32
(2,468)	1:178:A:LEU:HD22	1:175:A:GLU:HA	3	0.32
(2,467)	1:178:A:LEU:HD21	1:175:A:GLU:H	12	0.32
(2,438)	1:39:A:LEU:HD11	1:42:A:MET:HB2	15	0.32
(2,437)	1:39:A:LEU:HD11	1:42:A:MET:HG3	6	0.32
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG23	13	0.32
(2,422)	1:49:A:ILE:HG21	1:124:A:PHE:HB3	2	0.32
(2,422)	1:49:A:ILE:HG23	1:124:A:PHE:HB3	9	0.32
(2,394)	1:39:A:LEU:HD23	1:39:A:LEU:HB3	5	0.32
(2,394)	1:39:A:LEU:HD23	1:39:A:LEU:HB3	7	0.32
(2,318)	1:20:A:LEU:HD23	1:152:A:TYR:HD1	2	0.32
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD11	13	0.32
(2,132)	1:23:A:THR:HG23	1:148:A:ARG:HD2	15	0.32
(2,93)	1:89:A:VAL:HG12	1:79:A:LEU:HD13	2	0.32
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD13	10	0.32
(2,86)	1:67:A:ILE:HG22	1:106:A:TYR:HD2	3	0.32
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	12	0.32
(2,40)	1:31:A:LEU:HD12	1:67:A:ILE:HB	14	0.32
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	1	0.32
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	12	0.32
(2,19)	1:79:A:LEU:HD12	1:92:A:CYS:HG	1	0.32
(2,19)	1:79:A:LEU:HD12	1:92:A:CYS:HG	6	0.32
(2,17)	1:39:A:LEU:HD23	1:42:A:MET:HG2	5	0.32
(2,17)	1:39:A:LEU:HD22	1:42:A:MET:HG2	14	0.32
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	11	0.31
(2,4816)	1:98:A:ASP:HB3	1:101:A:GLN:H	9	0.31
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	7	0.31
(2,4642)	1:62:A:GLY:H	1:64:A:ILE:HB	13	0.31
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	7	0.31
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	13	0.31
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	10	0.31
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	10	0.31
(2,4543)	1:157:A:LYS:HB2	1:156:A:LEU:HD21	8	0.31
(2,4521)	1:54:A:LEU:HD12	1:54:A:LEU:HA	6	0.31
(2,4521)	1:54:A:LEU:HD12	1:52:A:GLY:HA2	12	0.31
(2,4489)	1:184:A:ALA:HB2	1:108:A:LYS:HE3	6	0.31
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG21	8	0.31
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	15	0.31
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG13	2	0.31
(2,4348)	1:60:A:ILE:HD13	1:113:A:SER:H	7	0.31
(2,4331)	1:95:A:THR:HG22	1:92:A:CYS:HG	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4322)	1:20:A:LEU:HD12	1:152:A:TYR:H	13	0.31
(2,4304)	1:186:A:ASP:HB3	1:183:A:LYS:HG3	10	0.31
(2,4265)	1:142:A:LEU:HD12	1:110:A:LYS:HB2	14	0.31
(2,4264)	1:16:A:ILE:HD11	1:19:A:GLU:HB3	3	0.31
(2,4264)	1:16:A:ILE:HD12	1:19:A:GLU:HB3	10	0.31
(2,4234)	1:54:A:LEU:HD23	1:53:A:ILE:H	5	0.31
(2,4229)	1:28:A:VAL:HG12	1:73:A:ASN:H	3	0.31
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD21	5	0.31
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	11	0.31
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	15	0.31
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	1	0.31
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	3	0.31
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	13	0.31
(2,4110)	1:64:A:ILE:HG22	1:62:A:GLY:H	7	0.31
(2,4110)	1:64:A:ILE:HG22	1:62:A:GLY:H	13	0.31
(2,4078)	1:28:A:VAL:HG21	1:30:A:ASP:H	4	0.31
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	8	0.31
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	7	0.31
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	14	0.31
(2,3988)	1:21:A:LEU:HD12	1:83:A:GLU:H	7	0.31
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	5	0.31
(2,3976)	1:37:A:THR:HG21	1:38:A:TYR:H	10	0.31
(2,3976)	1:37:A:THR:HG22	1:38:A:TYR:H	13	0.31
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	8	0.31
(2,3956)	1:74:A:ILE:HG22	1:78:A:GLU:H	9	0.31
(2,3934)	1:42:A:MET:HE3	1:60:A:ILE:H	3	0.31
(2,3915)	1:121:A:ALA:HB2	1:119:A:GLU:H	14	0.31
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD13	1	0.31
(2,3872)	1:60:A:ILE:HD13	1:62:A:GLY:H	8	0.31
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	5	0.31
(2,3866)	1:35:A:LEU:HD22	1:65:A:GLN:HE21	2	0.31
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	6	0.31
(2,3866)	1:35:A:LEU:HD23	1:65:A:GLN:HE21	9	0.31
(2,3864)	1:147:A:GLN:HE21	1:143:A:ILE:HD12	12	0.31
(2,3796)	1:135:A:ALA:HB3	1:136:A:ASN:HD22	2	0.31
(2,3796)	1:135:A:ALA:HB2	1:136:A:ASN:HD22	9	0.31
(2,3794)	1:135:A:ALA:HB1	1:135:A:ALA:H	2	0.31
(2,3794)	1:135:A:ALA:HB1	1:135:A:ALA:H	7	0.31
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD23	11	0.31
(2,3768)	1:117:A:ILE:HD13	1:117:A:ILE:H	7	0.31
(2,3740)	1:95:A:THR:HG22	1:96:A:TRP:H	7	0.31
(2,3740)	1:95:A:THR:HG23	1:96:A:TRP:H	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3740)	1:95:A:THR:HG23	1:96:A:TRP:H	10	0.31
(2,3740)	1:95:A:THR:HG22	1:96:A:TRP:H	13	0.31
(2,3740)	1:95:A:THR:HG22	1:96:A:TRP:H	15	0.31
(2,3719)	1:81:A:LYS:HE2	1:81:A:LYS:H	5	0.31
(2,3713)	1:76:A:LEU:HD12	1:77:A:LYS:H	14	0.31
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD12	9	0.31
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	13	0.31
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	15	0.31
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	5	0.31
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	2	0.31
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	5	0.31
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	6	0.31
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG21	7	0.31
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD13	3	0.31
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG11	1	0.31
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG12	6	0.31
(2,3427)	1:14:A:GLU:HA	1:14:A:GLU:H	7	0.31
(2,3257)	1:170:A:LEU:HD21	1:160:A:LEU:H	7	0.31
(2,3257)	1:170:A:LEU:HD22	1:160:A:LEU:H	10	0.31
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	11	0.31
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	14	0.31
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD13	15	0.31
(2,3223)	1:117:A:ILE:HD12	1:139:A:SER:H	5	0.31
(2,3163)	1:42:A:MET:HE1	1:54:A:LEU:H	10	0.31
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	9	0.31
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	12	0.31
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	4	0.31
(2,3106)	1:43:A:THR:H	1:44:A:SER:HB3	5	0.31
(2,3031)	1:20:A:LEU:HD11	1:20:A:LEU:H	2	0.31
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	7	0.31
(2,2904)	1:166:A:GLY:H	1:167:A:LYS:H	2	0.31
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	1	0.31
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD23	14	0.31
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	1	0.31
(2,2763)	1:146:A:VAL:HG22	1:147:A:GLN:H	9	0.31
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG22	3	0.31
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG23	6	0.31
(2,2675)	1:117:A:ILE:HD13	1:113:A:SER:H	10	0.31
(2,2638)	1:180:A:VAL:HG23	1:104:A:VAL:H	9	0.31
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	10	0.31
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG23	8	0.31
(2,2399)	1:117:A:ILE:HD11	1:116:A:LEU:H	2	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2399)	1:117:A:ILE:HD12	1:116:A:LEU:H	11	0.31
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG21	13	0.31
(2,2148)	1:42:A:MET:H	1:41:A:GLU:HG3	6	0.31
(2,2124)	1:154:A:LEU:H	1:155:A:LEU:H	13	0.31
(2,1994)	1:67:A:ILE:HG23	1:71:A:HIS:H	12	0.31
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	2	0.31
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	5	0.31
(2,1902)	1:170:A:LEU:H	1:156:A:LEU:HD13	14	0.31
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	13	0.31
(2,1887)	1:152:A:TYR:H	1:177:A:MET:HG2	4	0.31
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG22	15	0.31
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	14	0.31
(2,1838)	1:16:A:ILE:HD11	1:158:A:GLU:H	1	0.31
(2,1838)	1:16:A:ILE:HD11	1:158:A:GLU:H	8	0.31
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	9	0.31
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG23	7	0.31
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	11	0.31
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD13	9	0.31
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG23	9	0.31
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	12	0.31
(2,1526)	1:178:A:LEU:HD22	1:176:A:VAL:H	9	0.31
(2,1512)	1:142:A:LEU:HD13	1:117:A:ILE:H	6	0.31
(2,1442)	1:74:A:ILE:HD11	1:99:A:LYS:HE2	2	0.31
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD11	6	0.31
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD13	9	0.31
(2,1436)	1:85:A:LEU:HB3	1:85:A:LEU:HD13	10	0.31
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD11	1	0.31
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD11	6	0.31
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD11	9	0.31
(2,1369)	1:156:A:LEU:HD13	1:170:A:LEU:HB3	10	0.31
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	7	0.31
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	9	0.31
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	10	0.31
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	11	0.31
(2,1321)	1:23:A:THR:HG22	1:22:A:GLN:HB3	2	0.31
(2,1309)	1:134:A:LEU:HD22	1:132:A:HIS:HD2	6	0.31
(2,1302)	1:156:A:LEU:HD12	1:174:A:LEU:HB3	5	0.31
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE3	13	0.31
(2,1254)	1:17:A:MET:HE1	1:82:A:TYR:H	12	0.31
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	9	0.31
(2,1170)	1:18:A:ALA:HB2	1:18:A:ALA:HA	1	0.31
(2,1170)	1:18:A:ALA:HB2	1:18:A:ALA:HA	12	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	5	0.31
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD12	15	0.31
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	1	0.31
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	9	0.31
(2,1037)	1:143:A:ILE:HG21	1:140:A:SER:HB2	14	0.31
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	15	0.31
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG23	7	0.31
(2,851)	1:134:A:LEU:HD21	1:129:A:GLN:HB3	15	0.31
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	12	0.31
(2,827)	1:47:A:GLU:HG2	1:47:A:GLU:H	6	0.31
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD23	7	0.31
(2,761)	1:37:A:THR:HG23	1:36:A:GLU:HG2	1	0.31
(2,761)	1:37:A:THR:HG23	1:36:A:GLU:HG2	3	0.31
(2,733)	1:97:A:ALA:HB2	1:176:A:VAL:HG12	8	0.31
(2,730)	1:97:A:ALA:HB1	1:93:A:PHE:HB3	4	0.31
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	11	0.31
(2,666)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	2	0.31
(2,644)	1:105:A:THR:HG21	1:108:A:LYS:HD3	3	0.31
(2,638)	1:150:A:THR:HG23	1:153:A:GLN:HE21	12	0.31
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	2	0.31
(2,630)	1:64:A:ILE:HG23	1:35:A:LEU:HG	4	0.31
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	10	0.31
(2,618)	1:43:A:THR:HG22	1:45:A:GLY:H	5	0.31
(2,609)	1:28:A:VAL:HG12	1:29:A:ARG:H	8	0.31
(2,609)	1:28:A:VAL:HG13	1:29:A:ARG:H	9	0.31
(2,472)	1:178:A:LEU:HD23	1:178:A:LEU:HG	3	0.31
(2,472)	1:178:A:LEU:HD22	1:178:A:LEU:HG	14	0.31
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	6	0.31
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	12	0.31
(2,449)	1:53:A:ILE:HG23	1:125:A:PHE:HZ	14	0.31
(2,441)	1:31:A:LEU:HD11	1:61:A:PHE:HE1	14	0.31
(2,437)	1:39:A:LEU:HD13	1:42:A:MET:HG3	1	0.31
(2,394)	1:39:A:LEU:HD21	1:39:A:LEU:HB3	2	0.31
(2,394)	1:39:A:LEU:HD22	1:39:A:LEU:HB3	10	0.31
(2,394)	1:39:A:LEU:HD23	1:39:A:LEU:HB3	12	0.31
(2,387)	1:31:A:LEU:HD22	1:67:A:ILE:HD11	7	0.31
(2,369)	1:138:A:ILE:HD13	1:60:A:ILE:HG22	4	0.31
(2,362)	1:156:A:LEU:HD22	1:152:A:TYR:HB2	14	0.31
(2,351)	1:188:A:MET:HE1	1:108:A:LYS:HA	12	0.31
(2,313)	1:20:A:LEU:HD12	1:22:A:GLN:H	6	0.31
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	13	0.31
(2,186)	1:148:A:ARG:HD2	1:20:A:LEU:HD13	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	1:74:A:ILE:HG21	1:78:A:GLU:HG3	15	0.31
(2,116)	1:177:A:MET:HE1	1:100:A:PHE:HB2	5	0.31
(2,116)	1:177:A:MET:HE3	1:100:A:PHE:HB2	8	0.31
(2,103)	1:28:A:VAL:HG12	1:31:A:LEU:HD22	10	0.31
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD12	14	0.31
(2,55)	1:142:A:LEU:HD13	1:106:A:TYR:HH	1	0.31
(2,40)	1:31:A:LEU:HD12	1:67:A:ILE:HB	7	0.31
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	7	0.31
(2,29)	1:35:A:LEU:HD12	1:33:A:GLU:H	10	0.31
(2,19)	1:79:A:LEU:HD13	1:92:A:CYS:HG	8	0.31
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	11	0.31
(2,4841)	1:171:A:LYS:HG2	1:170:A:LEU:H	3	0.3
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	8	0.3
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	3	0.3
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	9	0.3
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	14	0.3
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	5	0.3
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	14	0.3
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	9	0.3
(2,4539)	1:95:A:THR:HG23	1:91:A:HIS:HB2	7	0.3
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	8	0.3
(2,4521)	1:54:A:LEU:HD13	1:52:A:GLY:HA2	3	0.3
(2,4518)	1:128:A:ILE:HG22	1:124:A:PHE:HZ	2	0.3
(2,4518)	1:128:A:ILE:HG21	1:124:A:PHE:HZ	11	0.3
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD3	6	0.3
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD3	12	0.3
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	7	0.3
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	12	0.3
(2,4430)	1:11:A:ARG:HG2	1:11:A:ARG:HD2	7	0.3
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	1	0.3
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	4	0.3
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	6	0.3
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	1	0.3
(2,4271)	1:116:A:LEU:HD22	1:56:A:LYS:HE2	5	0.3
(2,4265)	1:142:A:LEU:HD11	1:110:A:LYS:HB2	6	0.3
(2,4258)	1:95:A:THR:HG23	1:75:A:PHE:HD2	10	0.3
(2,4234)	1:54:A:LEU:HD23	1:53:A:ILE:H	10	0.3
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	2	0.3
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	11	0.3
(2,4197)	1:16:A:ILE:HG21	1:158:A:GLU:H	10	0.3
(2,4193)	1:20:A:LEU:HD22	1:21:A:LEU:H	2	0.3
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4172)	1:18:A:ALA:HB1	1:22:A:GLN:HE22	11	0.3
(2,4064)	1:17:A:MET:HE3	1:20:A:LEU:H	14	0.3
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	5	0.3
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	15	0.3
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG22	14	0.3
(2,3988)	1:21:A:LEU:HD13	1:83:A:GLU:H	6	0.3
(2,3969)	1:184:A:ALA:HB3	1:108:A:LYS:H	7	0.3
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD23	15	0.3
(2,3934)	1:42:A:MET:HE2	1:60:A:ILE:H	8	0.3
(2,3933)	1:94:A:VAL:HG23	1:95:A:THR:H	9	0.3
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	7	0.3
(2,3915)	1:121:A:ALA:HB1	1:119:A:GLU:H	4	0.3
(2,3915)	1:121:A:ALA:HB1	1:119:A:GLU:H	13	0.3
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD22	3	0.3
(2,3872)	1:60:A:ILE:HD13	1:62:A:GLY:H	7	0.3
(2,3866)	1:35:A:LEU:HD22	1:65:A:GLN:HE21	4	0.3
(2,3796)	1:135:A:ALA:HB1	1:136:A:ASN:HD22	4	0.3
(2,3796)	1:135:A:ALA:HB3	1:136:A:ASN:HD22	10	0.3
(2,3768)	1:117:A:ILE:HD12	1:117:A:ILE:H	15	0.3
(2,3740)	1:95:A:THR:HG21	1:96:A:TRP:H	4	0.3
(2,3719)	1:81:A:LYS:HE2	1:81:A:LYS:H	15	0.3
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	12	0.3
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD11	4	0.3
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	6	0.3
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	12	0.3
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD23	8	0.3
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD22	9	0.3
(2,3639)	1:18:A:ALA:HB1	1:18:A:ALA:H	2	0.3
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	9	0.3
(2,3633)	1:9:A:PRO:HB2	1:10:A:GLY:H	4	0.3
(2,3569)	1:141:A:TYR:HE2	1:136:A:ASN:HB3	12	0.3
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD12	3	0.3
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD12	11	0.3
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD13	14	0.3
(2,3481)	1:100:A:PHE:HD2	1:176:A:VAL:HG23	4	0.3
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG21	10	0.3
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD12	7	0.3
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG22	2	0.3
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	7	0.3
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD11	11	0.3
(2,3447)	1:40:A:TRP:HZ3	1:46:A:VAL:HG21	9	0.3
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG12	10	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3399)	1:109:A:ASN:H	1:105:A:THR:HG21	13	0.3
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG23	1	0.3
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	15	0.3
(2,3289)	1:21:A:LEU:HD12	1:21:A:LEU:H	9	0.3
(2,3257)	1:170:A:LEU:HD21	1:160:A:LEU:H	3	0.3
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG13	10	0.3
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD12	5	0.3
(2,3223)	1:117:A:ILE:HD12	1:139:A:SER:H	4	0.3
(2,3200)	1:5:A:SER:H	1:6:A:PRO:HA	10	0.3
(2,3200)	1:5:A:SER:H	1:6:A:PRO:HA	11	0.3
(2,3130)	1:49:A:ILE:HD11	1:49:A:ILE:H	6	0.3
(2,3130)	1:49:A:ILE:HD11	1:49:A:ILE:H	8	0.3
(2,3031)	1:20:A:LEU:HD12	1:20:A:LEU:H	1	0.3
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	7	0.3
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG21	4	0.3
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG23	10	0.3
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	11	0.3
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	7	0.3
(2,2737)	1:127:A:GLU:H	1:128:A:ILE:HG23	11	0.3
(2,2643)	1:108:A:LYS:H	1:107:A:CYS:HB2	7	0.3
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG21	12	0.3
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG22	13	0.3
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG22	11	0.3
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	4	0.3
(2,2329)	1:57:A:GLU:H	1:57:A:GLU:HB3	13	0.3
(2,2165)	1:151:A:LYS:H	1:151:A:LYS:HB2	10	0.3
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	2	0.3
(2,2056)	1:72:A:ASN:H	1:73:A:ASN:HB3	1	0.3
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	1	0.3
(2,1930)	1:11:A:ARG:H	1:11:A:ARG:HB2	1	0.3
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG12	3	0.3
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG12	5	0.3
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG12	11	0.3
(2,1744)	1:76:A:LEU:HD21	1:77:A:LYS:H	1	0.3
(2,1744)	1:76:A:LEU:HD23	1:77:A:LYS:H	15	0.3
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	4	0.3
(2,1704)	1:57:A:GLU:H	1:49:A:ILE:HG21	11	0.3
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	14	0.3
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD11	10	0.3
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD11	15	0.3
(2,1590)	1:18:A:ALA:HB1	1:20:A:LEU:HA	11	0.3
(2,1590)	1:18:A:ALA:HB3	1:20:A:LEU:HA	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1547)	1:95:A:THR:HG21	1:78:A:GLU:HB2	1	0.3
(2,1547)	1:95:A:THR:HG21	1:78:A:GLU:HB2	9	0.3
(2,1543)	1:128:A:ILE:HD12	1:132:A:HIS:HD2	6	0.3
(2,1543)	1:128:A:ILE:HD13	1:132:A:HIS:HD2	8	0.3
(2,1525)	1:143:A:ILE:HG21	1:144:A:LYS:HE3	14	0.3
(2,1520)	1:76:A:LEU:HD11	1:29:A:ARG:H	3	0.3
(2,1520)	1:76:A:LEU:HD11	1:29:A:ARG:H	4	0.3
(2,1500)	1:49:A:ILE:HG23	1:53:A:ILE:HB	9	0.3
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD12	10	0.3
(2,1371)	1:31:A:LEU:HD11	1:29:A:ARG:H	12	0.3
(2,1371)	1:31:A:LEU:HD12	1:29:A:ARG:H	13	0.3
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	2	0.3
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	14	0.3
(2,1322)	1:74:A:ILE:HG23	1:78:A:GLU:HG2	7	0.3
(2,1321)	1:23:A:THR:HG21	1:22:A:GLN:HB3	1	0.3
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE2	8	0.3
(2,1254)	1:17:A:MET:HE1	1:82:A:TYR:H	14	0.3
(2,1253)	1:190:A:VAL:HG22	1:190:A:VAL:HA	13	0.3
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	14	0.3
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB3	12	0.3
(2,1170)	1:18:A:ALA:HB3	1:18:A:ALA:HA	4	0.3
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	15	0.3
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	4	0.3
(2,1103)	1:127:A:GLU:HA	1:128:A:ILE:HD11	7	0.3
(2,1093)	1:77:A:LYS:HG3	1:77:A:LYS:HA	7	0.3
(2,1088)	1:161:A:THR:HG23	1:158:A:GLU:HA	6	0.3
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD13	8	0.3
(2,935)	1:29:A:ARG:HG2	1:29:A:ARG:HD3	10	0.3
(2,935)	1:29:A:ARG:HG2	1:29:A:ARG:HD3	13	0.3
(2,859)	1:130:A:GLN:HG2	1:131:A:ARG:H	12	0.3
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG13	6	0.3
(2,700)	1:23:A:THR:HG21	1:21:A:LEU:H	5	0.3
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	1	0.3
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	4	0.3
(2,632)	1:64:A:ILE:HG23	1:39:A:LEU:HB2	7	0.3
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	10	0.3
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD22	7	0.3
(2,589)	1:64:A:ILE:HD11	1:35:A:LEU:HB3	15	0.3
(2,530)	1:49:A:ILE:HD13	1:124:A:PHE:HZ	11	0.3
(2,505)	1:174:A:LEU:HD22	1:157:A:LYS:HE3	13	0.3
(2,473)	1:59:A:ILE:HG21	1:112:A:ASP:HB2	1	0.3
(2,473)	1:59:A:ILE:HG23	1:112:A:ASP:HB2	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,472)	1:178:A:LEU:HD23	1:178:A:LEU:HG	1	0.3
(2,472)	1:178:A:LEU:HD21	1:178:A:LEU:HG	2	0.3
(2,472)	1:178:A:LEU:HD21	1:178:A:LEU:HG	5	0.3
(2,472)	1:178:A:LEU:HD22	1:178:A:LEU:HG	8	0.3
(2,472)	1:178:A:LEU:HD21	1:178:A:LEU:HG	9	0.3
(2,472)	1:178:A:LEU:HD22	1:178:A:LEU:HG	11	0.3
(2,472)	1:178:A:LEU:HD23	1:178:A:LEU:HG	13	0.3
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	4	0.3
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	8	0.3
(2,448)	1:31:A:LEU:HD13	1:31:A:LEU:HG	11	0.3
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	13	0.3
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	14	0.3
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	4	0.3
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	6	0.3
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	10	0.3
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	11	0.3
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	2	0.3
(2,418)	1:53:A:ILE:HD12	1:124:A:PHE:HB3	6	0.3
(2,394)	1:39:A:LEU:HD21	1:39:A:LEU:HB3	13	0.3
(2,340)	1:102:A:MET:HE3	1:99:A:LYS:HE3	10	0.3
(2,338)	1:102:A:MET:HE2	1:70:A:PHE:HB3	3	0.3
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD11	6	0.3
(2,283)	1:179:A:SER:HA	1:182:A:LYS:HB2	3	0.3
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD13	8	0.3
(2,171)	1:74:A:ILE:HG22	1:78:A:GLU:HG3	14	0.3
(2,116)	1:177:A:MET:HE1	1:100:A:PHE:HB2	7	0.3
(2,116)	1:177:A:MET:HE3	1:100:A:PHE:HB2	13	0.3
(2,116)	1:177:A:MET:HE3	1:100:A:PHE:HB2	14	0.3
(2,103)	1:28:A:VAL:HG13	1:31:A:LEU:HD21	11	0.3
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD21	14	0.3
(2,74)	1:54:A:LEU:HD12	1:51:A:PRO:HB2	4	0.3
(2,61)	1:155:A:LEU:HD21	1:21:A:LEU:H	10	0.3
(2,43)	1:128:A:ILE:HG23	1:38:A:TYR:H	3	0.3
(2,39)	1:31:A:LEU:HD12	1:34:A:CYS:H	12	0.3
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	14	0.3
(2,18)	1:79:A:LEU:HD11	1:92:A:CYS:HB2	9	0.3
(2,17)	1:39:A:LEU:HD21	1:42:A:MET:HG2	4	0.3
(2,17)	1:39:A:LEU:HD23	1:42:A:MET:HG2	8	0.3
(2,17)	1:39:A:LEU:HD21	1:42:A:MET:HG2	13	0.3
(1,11)	1:19:A:GLU:O	1:23:A:THR:H	4	0.3
(1,11)	1:19:A:GLU:O	1:23:A:THR:H	5	0.3
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD3	8	0.29
(2,4799)	1:166:A:GLY:H	1:165:A:GLU:HG2	15	0.29
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	4	0.29
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	12	0.29
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD23	8	0.29
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG22	1	0.29
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	2	0.29
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	8	0.29
(2,4545)	1:67:A:ILE:HD12	1:145:A:PRO:HG3	4	0.29
(2,4521)	1:54:A:LEU:HD13	1:54:A:LEU:HA	9	0.29
(2,4521)	1:54:A:LEU:HD11	1:52:A:GLY:HA2	13	0.29
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	13	0.29
(2,4409)	1:172:A:ASP:HB2	1:94:A:VAL:HB	13	0.29
(2,4396)	1:48:A:GLU:HG3	1:49:A:ILE:HG21	7	0.29
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	11	0.29
(2,4329)	1:156:A:LEU:HD22	1:175:A:GLU:HG2	1	0.29
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG21	2	0.29
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG23	3	0.29
(2,4272)	1:174:A:LEU:HD22	1:175:A:GLU:HB2	7	0.29
(2,4234)	1:54:A:LEU:HD22	1:53:A:ILE:H	13	0.29
(2,4234)	1:54:A:LEU:HD22	1:53:A:ILE:H	15	0.29
(2,4229)	1:28:A:VAL:HG12	1:73:A:ASN:H	7	0.29
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	1	0.29
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	13	0.29
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	11	0.29
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	6	0.29
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	6	0.29
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	11	0.29
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG23	7	0.29
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG21	12	0.29
(2,3988)	1:21:A:LEU:HD13	1:83:A:GLU:H	3	0.29
(2,3988)	1:21:A:LEU:HD13	1:83:A:GLU:H	14	0.29
(2,3979)	1:18:A:ALA:HB1	1:22:A:GLN:H	11	0.29
(2,3979)	1:18:A:ALA:HB2	1:22:A:GLN:H	13	0.29
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	2	0.29
(2,3976)	1:37:A:THR:HG22	1:38:A:TYR:H	8	0.29
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	9	0.29
(2,3976)	1:37:A:THR:HG21	1:38:A:TYR:H	12	0.29
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	7	0.29
(2,3915)	1:121:A:ALA:HB2	1:119:A:GLU:H	3	0.29
(2,3905)	1:28:A:VAL:HG12	1:72:A:ASN:H	7	0.29
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD13	12	0.29
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	11	0.29
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	12	0.29
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD22	5	0.29
(2,3740)	1:95:A:THR:HG21	1:96:A:TRP:H	12	0.29
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	9	0.29
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD21	4	0.29
(2,3646)	1:22:A:GLN:HB3	1:23:A:THR:H	4	0.29
(2,3639)	1:18:A:ALA:HB2	1:18:A:ALA:H	7	0.29
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	8	0.29
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG23	15	0.29
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD13	3	0.29
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD11	8	0.29
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD21	15	0.29
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	12	0.29
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD22	12	0.29
(2,3493)	1:124:A:PHE:HD1	1:128:A:ILE:HD11	6	0.29
(2,3481)	1:100:A:PHE:HD2	1:176:A:VAL:HG23	1	0.29
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG23	1	0.29
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG21	11	0.29
(2,3453)	1:58:A:HIS:HE1	1:59:A:ILE:HD12	6	0.29
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG11	2	0.29
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG13	3	0.29
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG13	11	0.29
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG13	12	0.29
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG22	11	0.29
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	10	0.29
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	13	0.29
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD13	1	0.29
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD13	13	0.29
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD13	13	0.29
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	15	0.29
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	5	0.29
(2,3130)	1:49:A:ILE:HD11	1:49:A:ILE:H	10	0.29
(2,3014)	1:16:A:ILE:H	1:14:A:GLU:HB3	10	0.29
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD21	10	0.29
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	6	0.29
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	1	0.29
(2,2835)	1:146:A:VAL:HG13	1:148:A:ARG:H	2	0.29
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	1	0.29
(2,2583)	1:94:A:VAL:H	1:177:A:MET:HE3	6	0.29
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG23	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG22	15	0.29
(2,2556)	1:89:A:VAL:H	1:88:A:ASP:HB3	3	0.29
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	13	0.29
(2,2527)	1:87:A:GLU:H	1:88:A:ASP:HB3	6	0.29
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	14	0.29
(2,2399)	1:117:A:ILE:HD12	1:116:A:LEU:H	7	0.29
(2,2288)	1:21:A:LEU:HD13	1:22:A:GLN:H	2	0.29
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	3	0.29
(2,2148)	1:42:A:MET:H	1:41:A:GLU:HG3	9	0.29
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	1	0.29
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD11	2	0.29
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD11	13	0.29
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	13	0.29
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	9	0.29
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	4	0.29
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG21	15	0.29
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	4	0.29
(2,1592)	1:135:A:ALA:HB3	1:129:A:GLN:HE22	11	0.29
(2,1533)	1:53:A:ILE:HG23	1:117:A:ILE:H	14	0.29
(2,1526)	1:178:A:LEU:HD22	1:176:A:VAL:H	8	0.29
(2,1520)	1:76:A:LEU:HD12	1:29:A:ARG:H	8	0.29
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	9	0.29
(2,1478)	1:114:A:ASN:HA	1:118:A:LEU:HD21	12	0.29
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD12	2	0.29
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	1	0.29
(2,1402)	1:35:A:LEU:HD11	1:65:A:GLN:HB2	14	0.29
(2,1386)	1:33:A:GLU:HG2	1:29:A:ARG:HD3	3	0.29
(2,1384)	1:33:A:GLU:HG2	1:141:A:TYR:HE2	6	0.29
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	3	0.29
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	5	0.29
(2,1343)	1:17:A:MET:HE3	1:86:A:PRO:HA	11	0.29
(2,1321)	1:23:A:THR:HG22	1:22:A:GLN:HB3	15	0.29
(2,1308)	1:142:A:LEU:HD22	1:61:A:PHE:HD2	4	0.29
(2,1282)	1:64:A:ILE:HG23	1:35:A:LEU:H	14	0.29
(2,1264)	1:60:A:ILE:HG21	1:42:A:MET:HE3	1	0.29
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE1	9	0.29
(2,1255)	1:17:A:MET:HE2	1:82:A:TYR:HE2	15	0.29
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	10	0.29
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG23	2	0.29
(2,1170)	1:18:A:ALA:HB1	1:18:A:ALA:HA	5	0.29
(2,1170)	1:18:A:ALA:HB3	1:18:A:ALA:HA	11	0.29
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD12	1	0.29
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD12	14	0.29
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG22	4	0.29
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	6	0.29
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	15	0.29
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	2	0.29
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD22	1	0.29
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD22	11	0.29
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE3	5	0.29
(2,851)	1:134:A:LEU:HD21	1:129:A:GLN:HB3	5	0.29
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	6	0.29
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	10	0.29
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD23	7	0.29
(2,630)	1:64:A:ILE:HG21	1:35:A:LEU:HG	13	0.29
(2,619)	1:40:A:TRP:HD1	1:43:A:THR:HG21	9	0.29
(2,609)	1:28:A:VAL:HG13	1:29:A:ARG:H	13	0.29
(2,609)	1:28:A:VAL:HG13	1:29:A:ARG:H	14	0.29
(2,603)	1:28:A:VAL:HG22	1:72:A:ASN:HB3	14	0.29
(2,589)	1:64:A:ILE:HD13	1:35:A:LEU:HB3	14	0.29
(2,535)	1:76:A:LEU:HD23	1:71:A:HIS:HB3	15	0.29
(2,472)	1:178:A:LEU:HD22	1:178:A:LEU:HG	7	0.29
(2,468)	1:178:A:LEU:HD21	1:175:A:GLU:HA	2	0.29
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	7	0.29
(2,448)	1:31:A:LEU:HD13	1:31:A:LEU:HG	2	0.29
(2,448)	1:31:A:LEU:HD12	1:31:A:LEU:HG	5	0.29
(2,448)	1:31:A:LEU:HD12	1:31:A:LEU:HG	6	0.29
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	7	0.29
(2,448)	1:31:A:LEU:HD13	1:31:A:LEU:HG	9	0.29
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	15	0.29
(2,433)	1:35:A:LEU:HD13	1:35:A:LEU:HG	5	0.29
(2,433)	1:35:A:LEU:HD13	1:35:A:LEU:HG	8	0.29
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	9	0.29
(2,425)	1:35:A:LEU:HD12	1:35:A:LEU:H	10	0.29
(2,422)	1:49:A:ILE:HG21	1:124:A:PHE:HB3	6	0.29
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	15	0.29
(2,408)	1:156:A:LEU:HD13	1:156:A:LEU:HB3	5	0.29
(2,379)	1:142:A:LEU:HD23	1:138:A:ILE:HD11	12	0.29
(2,332)	1:42:A:MET:HE3	1:60:A:ILE:HG13	10	0.29
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD11	1	0.29
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD11	3	0.29
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD13	8	0.29
(2,313)	1:20:A:LEU:HD13	1:22:A:GLN:H	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,170)	1:37:A:THR:HG21	1:33:A:GLU:HG3	12	0.29
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG11	13	0.29
(2,116)	1:177:A:MET:HE1	1:100:A:PHE:HB2	3	0.29
(2,114)	1:177:A:MET:HE3	1:93:A:PHE:HE1	2	0.29
(2,114)	1:177:A:MET:HE3	1:93:A:PHE:HE1	14	0.29
(2,93)	1:89:A:VAL:HG13	1:79:A:LEU:HD13	5	0.29
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	7	0.29
(2,36)	1:39:A:LEU:HD12	1:65:A:GLN:HG2	2	0.29
(2,19)	1:79:A:LEU:HD13	1:92:A:CYS:HG	2	0.29
(2,4836)	1:68:A:TYR:HE1	1:28:A:VAL:H	8	0.28
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	13	0.28
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	15	0.28
(2,4802)	1:167:A:LYS:HD3	1:167:A:LYS:H	2	0.28
(2,4788)	1:98:A:ASP:HB2	1:99:A:LYS:H	8	0.28
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	2	0.28
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	5	0.28
(2,4749)	1:15:A:PHE:HD2	1:14:A:GLU:HG2	13	0.28
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	5	0.28
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG21	8	0.28
(2,4651)	1:82:A:TYR:H	1:21:A:LEU:HD11	2	0.28
(2,4639)	1:56:A:LYS:H	1:42:A:MET:HB3	6	0.28
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	3	0.28
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	11	0.28
(2,4486)	1:104:A:VAL:HG13	1:183:A:LYS:HD3	10	0.28
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	7	0.28
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD2	7	0.28
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG21	15	0.28
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	2	0.28
(2,4319)	1:187:A:ALA:HA	1:183:A:LYS:HD3	7	0.28
(2,4282)	1:146:A:VAL:HG12	1:103:A:TYR:HE1	14	0.28
(2,4271)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	13	0.28
(2,4267)	1:134:A:LEU:HD11	1:132:A:HIS:H	6	0.28
(2,4234)	1:54:A:LEU:HD21	1:53:A:ILE:H	4	0.28
(2,4234)	1:54:A:LEU:HD21	1:53:A:ILE:H	7	0.28
(2,4234)	1:54:A:LEU:HD22	1:53:A:ILE:H	11	0.28
(2,4229)	1:28:A:VAL:HG11	1:73:A:ASN:H	8	0.28
(2,4229)	1:28:A:VAL:HG13	1:73:A:ASN:H	15	0.28
(2,4211)	1:156:A:LEU:H	1:155:A:LEU:HD22	2	0.28
(2,4172)	1:18:A:ALA:HB3	1:22:A:GLN:HE22	1	0.28
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	6	0.28
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	2	0.28
(2,4128)	1:81:A:LYS:H	1:82:A:TYR:HE2	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	15	0.28
(2,4064)	1:17:A:MET:HE3	1:20:A:LEU:H	5	0.28
(2,4064)	1:17:A:MET:HE2	1:20:A:LEU:H	6	0.28
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD23	1	0.28
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	9	0.28
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	5	0.28
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	12	0.28
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG21	1	0.28
(2,3995)	1:17:A:MET:HE1	1:85:A:LEU:H	5	0.28
(2,3988)	1:21:A:LEU:HD12	1:83:A:GLU:H	8	0.28
(2,3988)	1:21:A:LEU:HD13	1:83:A:GLU:H	13	0.28
(2,3979)	1:18:A:ALA:HB2	1:22:A:GLN:H	8	0.28
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	3	0.28
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	6	0.28
(2,3976)	1:37:A:THR:HG22	1:38:A:TYR:H	15	0.28
(2,3935)	1:36:A:GLU:H	1:35:A:LEU:HD21	5	0.28
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG23	1	0.28
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG22	2	0.28
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG22	5	0.28
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD22	5	0.28
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD12	10	0.28
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	14	0.28
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	10	0.28
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD22	4	0.28
(2,3796)	1:135:A:ALA:HB1	1:136:A:ASN:HD22	5	0.28
(2,3794)	1:135:A:ALA:HB2	1:135:A:ALA:H	3	0.28
(2,3794)	1:135:A:ALA:HB2	1:135:A:ALA:H	11	0.28
(2,3740)	1:95:A:THR:HG21	1:96:A:TRP:H	11	0.28
(2,3713)	1:76:A:LEU:HD13	1:77:A:LYS:H	11	0.28
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	4	0.28
(2,3701)	1:68:A:TYR:H	1:67:A:ILE:HD13	1	0.28
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	7	0.28
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	15	0.28
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD22	10	0.28
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD22	14	0.28
(2,3652)	1:161:A:THR:HG23	1:162:A:CYS:H	2	0.28
(2,3639)	1:18:A:ALA:HB1	1:18:A:ALA:H	10	0.28
(2,3624)	1:3:A:LEU:H	1:3:A:LEU:HB3	14	0.28
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	8	0.28
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	12	0.28
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG22	4	0.28
(2,3310)	1:69:A:ASP:H	1:64:A:ILE:HD13	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3130)	1:49:A:ILE:HD12	1:49:A:ILE:H	1	0.28
(2,3130)	1:49:A:ILE:HD13	1:49:A:ILE:H	9	0.28
(2,3130)	1:49:A:ILE:HD12	1:49:A:ILE:H	11	0.28
(2,3031)	1:20:A:LEU:HD13	1:20:A:LEU:H	7	0.28
(2,2904)	1:166:A:GLY:H	1:167:A:LYS:H	15	0.28
(2,2852)	1:150:A:THR:H	1:149:A:VAL:HG21	12	0.28
(2,2638)	1:180:A:VAL:HG21	1:104:A:VAL:H	6	0.28
(2,2630)	1:150:A:THR:HG22	1:154:A:LEU:H	15	0.28
(2,2585)	1:94:A:VAL:HG13	1:95:A:THR:H	8	0.28
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG23	1	0.28
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG23	10	0.28
(2,2556)	1:89:A:VAL:H	1:88:A:ASP:HB3	11	0.28
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG11	3	0.28
(2,2527)	1:87:A:GLU:H	1:88:A:ASP:HB3	3	0.28
(2,2455)	1:73:A:ASN:HB2	1:74:A:ILE:H	2	0.28
(2,2446)	1:74:A:ILE:HG23	1:73:A:ASN:H	2	0.28
(2,2446)	1:74:A:ILE:HG23	1:73:A:ASN:H	10	0.28
(2,2446)	1:74:A:ILE:HG23	1:73:A:ASN:H	12	0.28
(2,2399)	1:117:A:ILE:HD11	1:116:A:LEU:H	14	0.28
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD12	3	0.28
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD13	8	0.28
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG21	13	0.28
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	14	0.28
(2,2269)	1:141:A:TYR:H	1:142:A:LEU:HD23	12	0.28
(2,2247)	1:132:A:HIS:H	1:130:A:GLN:HG3	12	0.28
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG23	1	0.28
(2,2128)	1:163:A:CYS:H	1:163:A:CYS:HA	10	0.28
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB2	4	0.28
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	14	0.28
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	12	0.28
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG21	7	0.28
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	14	0.28
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD12	5	0.28
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD12	14	0.28
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	6	0.28
(2,1533)	1:53:A:ILE:HG22	1:117:A:ILE:H	15	0.28
(2,1526)	1:178:A:LEU:HD23	1:176:A:VAL:H	3	0.28
(2,1526)	1:178:A:LEU:HD22	1:176:A:VAL:H	5	0.28
(2,1526)	1:178:A:LEU:HD23	1:176:A:VAL:H	14	0.28
(2,1520)	1:76:A:LEU:HD12	1:29:A:ARG:H	13	0.28
(2,1519)	1:39:A:LEU:HD13	1:65:A:GLN:H	6	0.28
(2,1512)	1:142:A:LEU:HD12	1:117:A:ILE:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1510)	1:116:A:LEU:HD22	1:54:A:LEU:H	1	0.28
(2,1476)	1:134:A:LEU:HD21	1:34:A:CYS:HA	7	0.28
(2,1476)	1:134:A:LEU:HD21	1:34:A:CYS:HA	9	0.28
(2,1444)	1:43:A:THR:HG22	1:39:A:LEU:HB2	9	0.28
(2,1442)	1:74:A:ILE:HD11	1:99:A:LYS:HE2	11	0.28
(2,1439)	1:102:A:MET:HE3	1:106:A:TYR:HD2	2	0.28
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD12	3	0.28
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD11	13	0.28
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	3	0.28
(2,1384)	1:33:A:GLU:HG2	1:141:A:TYR:HE2	12	0.28
(2,1371)	1:31:A:LEU:HD13	1:29:A:ARG:H	14	0.28
(2,1369)	1:156:A:LEU:HD13	1:170:A:LEU:HB3	1	0.28
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	4	0.28
(2,1321)	1:23:A:THR:HG22	1:22:A:GLN:HB3	14	0.28
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG22	1	0.28
(2,1279)	1:59:A:ILE:HG22	1:112:A:ASP:HB3	11	0.28
(2,1278)	1:54:A:LEU:HA	1:42:A:MET:HE1	10	0.28
(2,1254)	1:17:A:MET:HE3	1:82:A:TYR:H	4	0.28
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	14	0.28
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	2	0.28
(2,1165)	1:161:A:THR:HG22	1:161:A:THR:HA	12	0.28
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	5	0.28
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	14	0.28
(2,1097)	1:78:A:GLU:HA	1:81:A:LYS:HG3	2	0.28
(2,1088)	1:161:A:THR:HG23	1:158:A:GLU:HA	5	0.28
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD13	12	0.28
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	12	0.28
(2,851)	1:134:A:LEU:HD23	1:129:A:GLN:HB3	2	0.28
(2,761)	1:37:A:THR:HG21	1:36:A:GLU:HG2	2	0.28
(2,761)	1:37:A:THR:HG23	1:36:A:GLU:HG2	9	0.28
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG13	13	0.28
(2,729)	1:97:A:ALA:HB2	1:100:A:PHE:HE1	5	0.28
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	1	0.28
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	3	0.28
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	12	0.28
(2,644)	1:105:A:THR:HG23	1:108:A:LYS:HD3	13	0.28
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	2	0.28
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	3	0.28
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	12	0.28
(2,615)	1:28:A:VAL:HG13	1:28:A:VAL:HB	4	0.28
(2,615)	1:28:A:VAL:HG12	1:28:A:VAL:HB	9	0.28
(2,609)	1:28:A:VAL:HG11	1:29:A:ARG:H	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,609)	1:28:A:VAL:HG13	1:29:A:ARG:H	6	0.28
(2,609)	1:28:A:VAL:HG12	1:29:A:ARG:H	11	0.28
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG21	5	0.28
(2,475)	1:59:A:ILE:HG23	1:116:A:LEU:HB3	9	0.28
(2,475)	1:59:A:ILE:HG23	1:116:A:LEU:HB3	15	0.28
(2,473)	1:59:A:ILE:HG21	1:112:A:ASP:HB2	11	0.28
(2,472)	1:178:A:LEU:HD21	1:178:A:LEU:HG	6	0.28
(2,449)	1:53:A:ILE:HG22	1:125:A:PHE:HZ	15	0.28
(2,448)	1:31:A:LEU:HD12	1:31:A:LEU:HG	3	0.28
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	10	0.28
(2,448)	1:31:A:LEU:HD13	1:31:A:LEU:HG	12	0.28
(2,437)	1:39:A:LEU:HD11	1:42:A:MET:HG3	4	0.28
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	1	0.28
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	2	0.28
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	3	0.28
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	7	0.28
(2,433)	1:35:A:LEU:HD11	1:35:A:LEU:HG	11	0.28
(2,433)	1:35:A:LEU:HD13	1:35:A:LEU:HG	12	0.28
(2,433)	1:35:A:LEU:HD13	1:35:A:LEU:HG	13	0.28
(2,433)	1:35:A:LEU:HD13	1:35:A:LEU:HG	14	0.28
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	4	0.28
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	10	0.28
(2,418)	1:53:A:ILE:HD11	1:124:A:PHE:HB3	10	0.28
(2,408)	1:156:A:LEU:HD12	1:156:A:LEU:HB3	12	0.28
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	11	0.28
(2,387)	1:31:A:LEU:HD23	1:67:A:ILE:HD11	3	0.28
(2,379)	1:142:A:LEU:HD23	1:138:A:ILE:HD12	15	0.28
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG21	13	0.28
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	13	0.28
(2,285)	1:19:A:GLU:HA	1:22:A:GLN:HB3	4	0.28
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG13	14	0.28
(2,63)	1:174:A:LEU:HD21	1:175:A:GLU:HA	6	0.28
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	9	0.28
(2,42)	1:53:A:ILE:HG23	1:120:A:HIS:HD2	1	0.28
(2,40)	1:31:A:LEU:HD13	1:67:A:ILE:HB	2	0.28
(2,36)	1:39:A:LEU:HD12	1:65:A:GLN:HG2	11	0.28
(2,17)	1:39:A:LEU:HD22	1:42:A:MET:HG2	1	0.28
(2,17)	1:39:A:LEU:HD22	1:42:A:MET:HG2	10	0.28
(2,4823)	1:13:A:LYS:H	1:13:A:LYS:HE2	1	0.27
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	9	0.27
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	12	0.27
(2,4812)	1:162:A:CYS:H	1:160:A:LEU:HB2	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4772)	1:32:A:HIS:HE1	1:69:A:ASP:HA	12	0.27
(2,4699)	1:7:A:GLU:H	1:5:A:SER:HB2	7	0.27
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	4	0.27
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	6	0.27
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG2	8	0.27
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	1	0.27
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	14	0.27
(2,4624)	1:98:A:ASP:HB2	1:100:A:PHE:H	15	0.27
(2,4611)	1:37:A:THR:H	1:134:A:LEU:HD21	8	0.27
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	1	0.27
(2,4486)	1:104:A:VAL:HG12	1:183:A:LYS:HG2	12	0.27
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	15	0.27
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	10	0.27
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG13	4	0.27
(2,4331)	1:95:A:THR:HG21	1:92:A:CYS:HG	9	0.27
(2,4325)	1:188:A:MET:HE1	1:108:A:LYS:HE3	6	0.27
(2,4305)	1:56:A:LYS:HE2	1:55:A:ASN:HD21	10	0.27
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	7	0.27
(2,4243)	1:94:A:VAL:HG22	1:92:A:CYS:H	12	0.27
(2,4236)	1:33:A:GLU:HG3	1:34:A:CYS:H	15	0.27
(2,4234)	1:54:A:LEU:HD23	1:53:A:ILE:H	3	0.27
(2,4229)	1:28:A:VAL:HG12	1:73:A:ASN:H	6	0.27
(2,4119)	1:7:A:GLU:HG2	1:7:A:GLU:H	7	0.27
(2,4078)	1:28:A:VAL:HG22	1:30:A:ASP:H	13	0.27
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	3	0.27
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD23	6	0.27
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	3	0.27
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	14	0.27
(2,4046)	1:159:A:LEU:HD21	1:159:A:LEU:H	10	0.27
(2,4029)	1:183:A:LYS:HG2	1:183:A:LYS:H	1	0.27
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	5	0.27
(2,3995)	1:17:A:MET:HE2	1:85:A:LEU:H	3	0.27
(2,3995)	1:17:A:MET:HE3	1:85:A:LEU:H	9	0.27
(2,3995)	1:17:A:MET:HE1	1:85:A:LEU:H	14	0.27
(2,3988)	1:21:A:LEU:HD11	1:83:A:GLU:H	10	0.27
(2,3988)	1:21:A:LEU:HD12	1:83:A:GLU:H	12	0.27
(2,3988)	1:21:A:LEU:HD12	1:83:A:GLU:H	15	0.27
(2,3979)	1:18:A:ALA:HB2	1:22:A:GLN:H	6	0.27
(2,3979)	1:18:A:ALA:HB3	1:22:A:GLN:H	10	0.27
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	7	0.27
(2,3956)	1:74:A:ILE:HG23	1:78:A:GLU:H	11	0.27
(2,3956)	1:74:A:ILE:HG23	1:78:A:GLU:H	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3934)	1:42:A:MET:HE3	1:60:A:ILE:H	15	0.27
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	11	0.27
(2,3923)	1:49:A:ILE:HD11	1:42:A:MET:H	7	0.27
(2,3923)	1:49:A:ILE:HD12	1:42:A:MET:H	8	0.27
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD11	15	0.27
(2,3889)	1:85:A:LEU:HD23	1:84:A:GLN:H	4	0.27
(2,3886)	1:161:A:THR:H	1:162:A:CYS:HB2	14	0.27
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD13	11	0.27
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	15	0.27
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	1	0.27
(2,3866)	1:35:A:LEU:HD23	1:65:A:GLN:HE21	7	0.27
(2,3796)	1:135:A:ALA:HB1	1:136:A:ASN:HD22	11	0.27
(2,3794)	1:135:A:ALA:HB2	1:135:A:ALA:H	4	0.27
(2,3794)	1:135:A:ALA:HB2	1:135:A:ALA:H	5	0.27
(2,3794)	1:135:A:ALA:HB3	1:135:A:ALA:H	9	0.27
(2,3794)	1:135:A:ALA:HB3	1:135:A:ALA:H	12	0.27
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD23	9	0.27
(2,3728)	1:87:A:GLU:HG3	1:87:A:GLU:H	2	0.27
(2,3713)	1:76:A:LEU:HD12	1:77:A:LYS:H	10	0.27
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	4	0.27
(2,3657)	1:33:A:GLU:HB3	1:33:A:GLU:H	2	0.27
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	6	0.27
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG22	4	0.27
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG22	15	0.27
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD21	15	0.27
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG23	14	0.27
(2,3257)	1:170:A:LEU:HD21	1:160:A:LEU:H	5	0.27
(2,3257)	1:170:A:LEU:HD21	1:160:A:LEU:H	12	0.27
(2,3238)	1:185:A:ASN:H	1:104:A:VAL:HG12	5	0.27
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD12	8	0.27
(2,3223)	1:117:A:ILE:HD11	1:139:A:SER:H	1	0.27
(2,3200)	1:5:A:SER:H	1:6:A:PRO:HA	7	0.27
(2,3163)	1:42:A:MET:HE1	1:54:A:LEU:H	15	0.27
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	1	0.27
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD11	3	0.27
(2,2904)	1:166:A:GLY:H	1:167:A:LYS:H	3	0.27
(2,2899)	1:165:A:GLU:H	1:164:A:GLU:H	2	0.27
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	9	0.27
(2,2718)	1:11:A:ARG:H	1:11:A:ARG:HB3	15	0.27
(2,2585)	1:94:A:VAL:HG11	1:95:A:THR:H	9	0.27
(2,2556)	1:89:A:VAL:H	1:88:A:ASP:HB3	6	0.27
(2,2446)	1:74:A:ILE:HG21	1:73:A:ASN:H	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2446)	1:74:A:ILE:HG23	1:73:A:ASN:H	7	0.27
(2,2399)	1:117:A:ILE:HD12	1:116:A:LEU:H	1	0.27
(2,2399)	1:117:A:ILE:HD11	1:116:A:LEU:H	6	0.27
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG21	7	0.27
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	11	0.27
(2,2247)	1:132:A:HIS:H	1:130:A:GLN:HG3	6	0.27
(2,2187)	1:107:A:CYS:H	1:104:A:VAL:HG21	4	0.27
(2,2113)	1:100:A:PHE:H	1:101:A:GLN:HB2	2	0.27
(2,2004)	1:162:A:CYS:H	1:163:A:CYS:HA	12	0.27
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	3	0.27
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	8	0.27
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	9	0.27
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	11	0.27
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	14	0.27
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	15	0.27
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG22	7	0.27
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD12	10	0.27
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD13	13	0.27
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG21	10	0.27
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	12	0.27
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	1	0.27
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	4	0.27
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	10	0.27
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG21	10	0.27
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	3	0.27
(2,1611)	1:68:A:TYR:H	1:31:A:LEU:HD13	12	0.27
(2,1592)	1:135:A:ALA:HB1	1:129:A:GLN:HE22	15	0.27
(2,1533)	1:53:A:ILE:HG22	1:117:A:ILE:H	3	0.27
(2,1526)	1:178:A:LEU:HD23	1:176:A:VAL:H	7	0.27
(2,1526)	1:178:A:LEU:HD21	1:176:A:VAL:H	13	0.27
(2,1520)	1:76:A:LEU:HD13	1:29:A:ARG:H	9	0.27
(2,1520)	1:76:A:LEU:HD11	1:29:A:ARG:H	11	0.27
(2,1519)	1:39:A:LEU:HD12	1:65:A:GLN:H	9	0.27
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	4	0.27
(2,1512)	1:142:A:LEU:HD12	1:117:A:ILE:H	10	0.27
(2,1500)	1:49:A:ILE:HG23	1:53:A:ILE:HB	12	0.27
(2,1500)	1:49:A:ILE:HG21	1:53:A:ILE:HB	14	0.27
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	15	0.27
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD12	3	0.27
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD12	7	0.27
(2,1422)	1:116:A:LEU:HD21	1:60:A:ILE:HA	5	0.27
(2,1399)	1:7:A:GLU:HG3	1:8:A:PHE:HD2	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1371)	1:31:A:LEU:HD12	1:29:A:ARG:H	1	0.27
(2,1371)	1:31:A:LEU:HD12	1:29:A:ARG:H	15	0.27
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	10	0.27
(2,1307)	1:114:A:ASN:HB3	1:114:A:ASN:HD21	1	0.27
(2,1302)	1:156:A:LEU:HD11	1:174:A:LEU:HB3	9	0.27
(2,1245)	1:20:A:LEU:HD12	1:24:A:GLU:H	3	0.27
(2,1223)	1:53:A:ILE:HA	1:56:A:LYS:HE2	4	0.27
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG23	1	0.27
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG22	12	0.27
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD11	8	0.27
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD11	10	0.27
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	6	0.27
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	7	0.27
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	11	0.27
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD23	10	0.27
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD23	13	0.27
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD21	12	0.27
(2,761)	1:37:A:THR:HG23	1:36:A:GLU:HG2	6	0.27
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG12	1	0.27
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG11	10	0.27
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG13	11	0.27
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	12	0.27
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	8	0.27
(2,615)	1:28:A:VAL:HG11	1:28:A:VAL:HB	7	0.27
(2,615)	1:28:A:VAL:HG12	1:28:A:VAL:HB	14	0.27
(2,592)	1:64:A:ILE:HD12	1:31:A:LEU:HD21	6	0.27
(2,589)	1:64:A:ILE:HD11	1:35:A:LEU:HB3	9	0.27
(2,577)	1:89:A:VAL:HG11	1:93:A:PHE:HE2	1	0.27
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	9	0.27
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE1	9	0.27
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE1	12	0.27
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	7	0.27
(2,472)	1:178:A:LEU:HD21	1:178:A:LEU:HG	15	0.27
(2,468)	1:178:A:LEU:HD21	1:175:A:GLU:HA	8	0.27
(2,468)	1:178:A:LEU:HD22	1:175:A:GLU:HA	14	0.27
(2,449)	1:53:A:ILE:HG22	1:125:A:PHE:HZ	1	0.27
(2,448)	1:31:A:LEU:HD11	1:31:A:LEU:HG	1	0.27
(2,433)	1:35:A:LEU:HD12	1:35:A:LEU:HG	15	0.27
(2,409)	1:156:A:LEU:HD11	1:156:A:LEU:HG	12	0.27
(2,409)	1:156:A:LEU:HD12	1:156:A:LEU:HG	13	0.27
(2,409)	1:156:A:LEU:HD12	1:156:A:LEU:HG	15	0.27
(2,408)	1:156:A:LEU:HD11	1:156:A:LEU:HB3	13	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,406)	1:156:A:LEU:HD11	1:93:A:PHE:HZ	13	0.27
(2,402)	1:35:A:LEU:HD23	1:35:A:LEU:HG	3	0.27
(2,402)	1:35:A:LEU:HD23	1:35:A:LEU:HG	5	0.27
(2,402)	1:35:A:LEU:HD21	1:35:A:LEU:HG	8	0.27
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	10	0.27
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	12	0.27
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	13	0.27
(2,402)	1:35:A:LEU:HD23	1:35:A:LEU:HG	14	0.27
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	15	0.27
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	4	0.27
(2,313)	1:20:A:LEU:HD12	1:22:A:GLN:H	1	0.27
(2,267)	1:183:A:LYS:HA	1:186:A:ASP:HB2	1	0.27
(2,236)	1:25:A:LYS:HA	1:76:A:LEU:HD13	7	0.27
(2,172)	1:169:A:GLU:HG2	1:94:A:VAL:HG23	6	0.27
(2,171)	1:74:A:ILE:HG23	1:78:A:GLU:HG3	13	0.27
(2,131)	1:23:A:THR:HG23	1:148:A:ARG:HD3	14	0.27
(2,98)	1:28:A:VAL:HG22	1:72:A:ASN:HD21	5	0.27
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD13	7	0.27
(2,92)	1:116:A:LEU:HD13	1:115:A:GLN:HB2	3	0.27
(2,19)	1:79:A:LEU:HD12	1:92:A:CYS:HG	3	0.27
(2,18)	1:79:A:LEU:HD13	1:92:A:CYS:HB2	2	0.27
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	8	0.26
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	8	0.26
(2,4812)	1:162:A:CYS:H	1:160:A:LEU:HB2	13	0.26
(2,4788)	1:98:A:ASP:HB2	1:99:A:LYS:H	11	0.26
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	6	0.26
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	10	0.26
(2,4732)	1:121:A:ALA:H	1:119:A:GLU:HA	7	0.26
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	1	0.26
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	11	0.26
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG2	13	0.26
(2,4687)	1:11:A:ARG:HG2	1:12:A:LYS:H	1	0.26
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	10	0.26
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	13	0.26
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	15	0.26
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD21	2	0.26
(2,4561)	1:23:A:THR:HG23	1:16:A:ILE:HA	10	0.26
(2,4529)	1:60:A:ILE:HG22	1:113:A:SER:HB2	5	0.26
(2,4525)	1:99:A:LYS:HG2	1:71:A:HIS:HE1	2	0.26
(2,4521)	1:54:A:LEU:HD13	1:52:A:GLY:HA2	10	0.26
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD13	2	0.26
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	8	0.26
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG3	11	0.26
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	14	0.26
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD2	14	0.26
(2,4422)	1:56:A:LYS:HE2	1:56:A:LYS:HG2	8	0.26
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	10	0.26
(2,4320)	1:188:A:MET:HA	1:108:A:LYS:HE2	2	0.26
(2,4320)	1:188:A:MET:HA	1:108:A:LYS:HE2	15	0.26
(2,4304)	1:186:A:ASP:HB2	1:183:A:LYS:HG3	13	0.26
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	9	0.26
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	12	0.26
(2,4234)	1:54:A:LEU:HD22	1:53:A:ILE:H	12	0.26
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	3	0.26
(2,4229)	1:28:A:VAL:HG12	1:73:A:ASN:H	9	0.26
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	6	0.26
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	9	0.26
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD11	9	0.26
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	4	0.26
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	6	0.26
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	8	0.26
(2,4047)	1:156:A:LEU:HD12	1:159:A:LEU:H	13	0.26
(2,4038)	1:29:A:ARG:HG2	1:29:A:ARG:H	12	0.26
(2,4016)	1:64:A:ILE:HG22	1:61:A:PHE:H	3	0.26
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	5	0.26
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	6	0.26
(2,4007)	1:40:A:TRP:HE1	1:44:A:SER:HB3	15	0.26
(2,3995)	1:17:A:MET:HE3	1:85:A:LEU:H	1	0.26
(2,3995)	1:17:A:MET:HE3	1:85:A:LEU:H	4	0.26
(2,3995)	1:17:A:MET:HE3	1:85:A:LEU:H	10	0.26
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG23	12	0.26
(2,3979)	1:18:A:ALA:HB3	1:22:A:GLN:H	12	0.26
(2,3979)	1:18:A:ALA:HB2	1:22:A:GLN:H	15	0.26
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	1	0.26
(2,3964)	1:64:A:ILE:H	1:67:A:ILE:HD13	11	0.26
(2,3961)	1:155:A:LEU:HD11	1:155:A:LEU:H	5	0.26
(2,3956)	1:74:A:ILE:HG22	1:78:A:GLU:H	5	0.26
(2,3934)	1:42:A:MET:HE3	1:60:A:ILE:H	11	0.26
(2,3915)	1:121:A:ALA:HB1	1:119:A:GLU:H	6	0.26
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD13	14	0.26
(2,3866)	1:35:A:LEU:HD23	1:65:A:GLN:HE21	8	0.26
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	14	0.26
(2,3796)	1:135:A:ALA:HB2	1:136:A:ASN:HD22	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3794)	1:135:A:ALA:HB3	1:135:A:ALA:H	15	0.26
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD22	8	0.26
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD22	15	0.26
(2,3740)	1:95:A:THR:HG22	1:96:A:TRP:H	14	0.26
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	14	0.26
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD21	11	0.26
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD22	15	0.26
(2,3652)	1:161:A:THR:HG21	1:162:A:CYS:H	1	0.26
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	13	0.26
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	14	0.26
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	15	0.26
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	14	0.26
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	14	0.26
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG21	6	0.26
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG21	13	0.26
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG11	8	0.26
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG13	9	0.26
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG13	14	0.26
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD21	11	0.26
(2,3370)	1:134:A:LEU:H	1:135:A:ALA:H	6	0.26
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG22	2	0.26
(2,3344)	1:170:A:LEU:HD11	1:171:A:LYS:H	7	0.26
(2,3264)	1:94:A:VAL:HG23	1:172:A:ASP:H	2	0.26
(2,3223)	1:117:A:ILE:HD13	1:139:A:SER:H	2	0.26
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD12	4	0.26
(2,3031)	1:20:A:LEU:HD12	1:20:A:LEU:H	3	0.26
(2,3031)	1:20:A:LEU:HD11	1:20:A:LEU:H	10	0.26
(2,2963)	1:179:A:SER:H	1:177:A:MET:HB3	1	0.26
(2,2907)	1:169:A:GLU:H	1:169:A:GLU:HA	1	0.26
(2,2896)	1:164:A:GLU:H	1:163:A:CYS:H	11	0.26
(2,2876)	1:155:A:LEU:H	1:156:A:LEU:H	13	0.26
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD23	10	0.26
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD23	12	0.26
(2,2835)	1:146:A:VAL:HG11	1:148:A:ARG:H	13	0.26
(2,2675)	1:117:A:ILE:HD11	1:113:A:SER:H	15	0.26
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	8	0.26
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	14	0.26
(2,2630)	1:150:A:THR:HG23	1:154:A:LEU:H	5	0.26
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG23	3	0.26
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG21	6	0.26
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	13	0.26
(2,2446)	1:74:A:ILE:HG21	1:73:A:ASN:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2446)	1:74:A:ILE:HG22	1:73:A:ASN:H	6	0.26
(2,2446)	1:74:A:ILE:HG22	1:73:A:ASN:H	9	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG21	2	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	5	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG21	8	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	9	0.26
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	10	0.26
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	15	0.26
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG23	7	0.26
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	4	0.26
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	8	0.26
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	6	0.26
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	10	0.26
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG22	7	0.26
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	12	0.26
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG21	4	0.26
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD13	5	0.26
(2,1838)	1:16:A:ILE:HD11	1:158:A:GLU:H	12	0.26
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG22	13	0.26
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG13	7	0.26
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	9	0.26
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	13	0.26
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	14	0.26
(2,1630)	1:178:A:LEU:HD21	1:153:A:GLN:H	15	0.26
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	3	0.26
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG23	7	0.26
(2,1547)	1:95:A:THR:HG21	1:78:A:GLU:HB2	3	0.26
(2,1536)	1:60:A:ILE:HD13	1:53:A:ILE:HG22	10	0.26
(2,1526)	1:178:A:LEU:HD23	1:176:A:VAL:H	11	0.26
(2,1512)	1:142:A:LEU:HD11	1:117:A:ILE:H	12	0.26
(2,1500)	1:49:A:ILE:HG21	1:53:A:ILE:HB	4	0.26
(2,1500)	1:49:A:ILE:HG22	1:53:A:ILE:HB	10	0.26
(2,1444)	1:43:A:THR:HG21	1:39:A:LEU:HB2	13	0.26
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD12	5	0.26
(2,1371)	1:31:A:LEU:HD12	1:29:A:ARG:H	10	0.26
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	6	0.26
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	6	0.26
(2,1321)	1:23:A:THR:HG21	1:22:A:GLN:HB3	6	0.26
(2,1309)	1:134:A:LEU:HD23	1:132:A:HIS:HD2	1	0.26
(2,1302)	1:156:A:LEU:HD11	1:174:A:LEU:HB3	1	0.26
(2,1302)	1:156:A:LEU:HD13	1:174:A:LEU:HB3	4	0.26
(2,1302)	1:156:A:LEU:HD13	1:174:A:LEU:HB3	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG22	6	0.26
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	1	0.26
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	5	0.26
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE1	7	0.26
(2,1254)	1:17:A:MET:HE3	1:82:A:TYR:H	6	0.26
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD11	4	0.26
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD23	8	0.26
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	14	0.26
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG21	6	0.26
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD13	13	0.26
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	5	0.26
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	8	0.26
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	10	0.26
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	15	0.26
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD22	15	0.26
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD21	9	0.26
(2,851)	1:134:A:LEU:HD22	1:129:A:GLN:HB3	9	0.26
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	1	0.26
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	4	0.26
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	6	0.26
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	7	0.26
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	14	0.26
(2,733)	1:97:A:ALA:HB2	1:176:A:VAL:HG12	3	0.26
(2,733)	1:97:A:ALA:HB1	1:176:A:VAL:HG13	9	0.26
(2,730)	1:97:A:ALA:HB2	1:93:A:PHE:HB3	8	0.26
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	9	0.26
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	13	0.26
(2,644)	1:105:A:THR:HG22	1:108:A:LYS:HD3	14	0.26
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	2	0.26
(2,622)	1:43:A:THR:HG22	1:42:A:MET:HG3	15	0.26
(2,618)	1:43:A:THR:HG22	1:45:A:GLY:H	11	0.26
(2,609)	1:28:A:VAL:HG11	1:29:A:ARG:H	10	0.26
(2,609)	1:28:A:VAL:HG11	1:29:A:ARG:H	12	0.26
(2,597)	1:28:A:VAL:HG22	1:72:A:ASN:HD22	8	0.26
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	3	0.26
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	13	0.26
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	8	0.26
(2,557)	1:60:A:ILE:HD13	1:42:A:MET:HE1	5	0.26
(2,533)	1:49:A:ILE:HD13	1:42:A:MET:HE2	10	0.26
(2,505)	1:174:A:LEU:HD21	1:157:A:LYS:HE3	1	0.26
(2,475)	1:59:A:ILE:HG23	1:116:A:LEU:HB3	11	0.26
(2,475)	1:59:A:ILE:HG22	1:116:A:LEU:HB3	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,475)	1:59:A:ILE:HG21	1:116:A:LEU:HB3	14	0.26
(2,473)	1:59:A:ILE:HG21	1:112:A:ASP:HB2	9	0.26
(2,472)	1:178:A:LEU:HD23	1:178:A:LEU:HG	4	0.26
(2,472)	1:178:A:LEU:HD21	1:178:A:LEU:HG	10	0.26
(2,468)	1:178:A:LEU:HD23	1:175:A:GLU:HA	6	0.26
(2,467)	1:178:A:LEU:HD22	1:175:A:GLU:H	4	0.26
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	5	0.26
(2,418)	1:53:A:ILE:HD11	1:124:A:PHE:HB3	4	0.26
(2,409)	1:156:A:LEU:HD13	1:156:A:LEU:HG	1	0.26
(2,409)	1:156:A:LEU:HD11	1:156:A:LEU:HG	2	0.26
(2,409)	1:156:A:LEU:HD11	1:156:A:LEU:HG	3	0.26
(2,409)	1:156:A:LEU:HD11	1:156:A:LEU:HG	5	0.26
(2,409)	1:156:A:LEU:HD13	1:156:A:LEU:HG	8	0.26
(2,409)	1:156:A:LEU:HD13	1:156:A:LEU:HG	9	0.26
(2,409)	1:156:A:LEU:HD13	1:156:A:LEU:HG	10	0.26
(2,409)	1:156:A:LEU:HD11	1:156:A:LEU:HG	11	0.26
(2,408)	1:156:A:LEU:HD13	1:156:A:LEU:HB3	2	0.26
(2,408)	1:156:A:LEU:HD12	1:156:A:LEU:HB3	8	0.26
(2,408)	1:156:A:LEU:HD12	1:156:A:LEU:HB3	9	0.26
(2,406)	1:156:A:LEU:HD12	1:93:A:PHE:HZ	12	0.26
(2,402)	1:35:A:LEU:HD23	1:35:A:LEU:HG	2	0.26
(2,402)	1:35:A:LEU:HD23	1:35:A:LEU:HG	4	0.26
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	6	0.26
(2,328)	1:42:A:MET:HE2	1:60:A:ILE:HB	6	0.26
(2,312)	1:3:A:LEU:HD21	1:3:A:LEU:HA	5	0.26
(2,307)	1:145:A:PRO:HA	1:144:A:LYS:HB2	13	0.26
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD13	6	0.26
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG13	14	0.26
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB2	13	0.26
(2,171)	1:74:A:ILE:HG22	1:78:A:GLU:HG3	9	0.26
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG12	7	0.26
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	12	0.26
(2,92)	1:116:A:LEU:HD13	1:115:A:GLN:HB2	11	0.26
(2,74)	1:54:A:LEU:HD13	1:51:A:PRO:HB2	2	0.26
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	8	0.26
(2,74)	1:54:A:LEU:HD13	1:51:A:PRO:HB2	10	0.26
(2,66)	1:118:A:LEU:HD23	1:114:A:ASN:HD21	6	0.26
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	3	0.26
(2,29)	1:35:A:LEU:HD13	1:33:A:GLU:H	8	0.26
(2,17)	1:39:A:LEU:HD21	1:42:A:MET:HG2	6	0.26
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	3	0.25
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4788)	1:99:A:LYS:H	1:98:A:ASP:HB3	6	0.25
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	4	0.25
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	2	0.25
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	7	0.25
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG21	7	0.25
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG23	10	0.25
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	5	0.25
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	9	0.25
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	15	0.25
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG21	3	0.25
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	5	0.25
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD23	12	0.25
(2,4584)	1:170:A:LEU:HD23	1:90:A:GLY:H	5	0.25
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	9	0.25
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	12	0.25
(2,4548)	1:49:A:ILE:HG21	1:55:A:ASN:HB3	4	0.25
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD13	8	0.25
(2,4529)	1:60:A:ILE:HG22	1:113:A:SER:HB2	11	0.25
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	5	0.25
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	9	0.25
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	13	0.25
(2,4395)	1:48:A:GLU:HB3	1:48:A:GLU:HG3	9	0.25
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD21	6	0.25
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	7	0.25
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	14	0.25
(2,4329)	1:156:A:LEU:HD23	1:175:A:GLU:HG3	6	0.25
(2,4299)	1:101:A:GLN:HG2	1:104:A:VAL:HG13	7	0.25
(2,4272)	1:174:A:LEU:HD21	1:175:A:GLU:HB2	8	0.25
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	2	0.25
(2,4236)	1:33:A:GLU:HG3	1:34:A:CYS:H	8	0.25
(2,4234)	1:54:A:LEU:HD21	1:53:A:ILE:H	8	0.25
(2,4234)	1:54:A:LEU:HD21	1:53:A:ILE:H	14	0.25
(2,4229)	1:28:A:VAL:HG11	1:73:A:ASN:H	11	0.25
(2,4197)	1:16:A:ILE:HG21	1:158:A:GLU:H	15	0.25
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	9	0.25
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	10	0.25
(2,4172)	1:18:A:ALA:HB1	1:22:A:GLN:HE22	7	0.25
(2,4112)	1:76:A:LEU:HD21	1:25:A:LYS:H	2	0.25
(2,4112)	1:76:A:LEU:HD21	1:25:A:LYS:H	11	0.25
(2,4084)	1:162:A:CYS:H	1:162:A:CYS:HB2	9	0.25
(2,4084)	1:162:A:CYS:H	1:162:A:CYS:HB2	10	0.25
(2,4078)	1:28:A:VAL:HG22	1:30:A:ASP:H	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	10	0.25
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	7	0.25
(2,4016)	1:64:A:ILE:HG21	1:61:A:PHE:H	4	0.25
(2,4015)	1:39:A:LEU:HD21	1:61:A:PHE:H	14	0.25
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	7	0.25
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	12	0.25
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG22	15	0.25
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG21	6	0.25
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	2	0.25
(2,3978)	1:23:A:THR:HG22	1:22:A:GLN:H	2	0.25
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG22	2	0.25
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	14	0.25
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	12	0.25
(2,3915)	1:121:A:ALA:HB2	1:119:A:GLU:H	1	0.25
(2,3915)	1:121:A:ALA:HB1	1:119:A:GLU:H	5	0.25
(2,3915)	1:121:A:ALA:HB3	1:119:A:GLU:H	15	0.25
(2,3913)	1:176:A:VAL:HG22	1:100:A:PHE:H	2	0.25
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD23	9	0.25
(2,3886)	1:161:A:THR:H	1:162:A:CYS:HB2	9	0.25
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD12	6	0.25
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG21	3	0.25
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	15	0.25
(2,3794)	1:135:A:ALA:HB1	1:135:A:ALA:H	1	0.25
(2,3794)	1:135:A:ALA:HB2	1:135:A:ALA:H	8	0.25
(2,3794)	1:135:A:ALA:HB3	1:135:A:ALA:H	13	0.25
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	10	0.25
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	1	0.25
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	10	0.25
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD22	1	0.25
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD23	3	0.25
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD23	5	0.25
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD23	12	0.25
(2,3647)	1:26:A:ALA:HB1	1:26:A:ALA:H	14	0.25
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD23	11	0.25
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD22	13	0.25
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	5	0.25
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG13	5	0.25
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG12	10	0.25
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG12	5	0.25
(2,3344)	1:170:A:LEU:HD12	1:171:A:LYS:H	14	0.25
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG23	1	0.25
(2,3264)	1:94:A:VAL:HG21	1:172:A:ASP:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3260)	1:161:A:THR:HG23	1:158:A:GLU:H	5	0.25
(2,3257)	1:170:A:LEU:HD23	1:160:A:LEU:H	1	0.25
(2,3223)	1:117:A:ILE:HD11	1:139:A:SER:H	11	0.25
(2,3119)	1:45:A:GLY:H	1:44:A:SER:HB2	15	0.25
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	1	0.25
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	11	0.25
(2,2835)	1:146:A:VAL:HG12	1:148:A:ARG:H	5	0.25
(2,2763)	1:146:A:VAL:HG23	1:147:A:GLN:H	13	0.25
(2,2638)	1:180:A:VAL:HG23	1:104:A:VAL:H	3	0.25
(2,2638)	1:180:A:VAL:HG21	1:104:A:VAL:H	4	0.25
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	15	0.25
(2,2630)	1:150:A:THR:HG23	1:154:A:LEU:H	8	0.25
(2,2630)	1:150:A:THR:HG23	1:154:A:LEU:H	9	0.25
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	1	0.25
(2,2585)	1:94:A:VAL:HG13	1:95:A:THR:H	11	0.25
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG21	11	0.25
(2,2556)	1:89:A:VAL:H	1:88:A:ASP:HB3	1	0.25
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	9	0.25
(2,2446)	1:74:A:ILE:HG23	1:73:A:ASN:H	11	0.25
(2,2399)	1:117:A:ILE:HD12	1:116:A:LEU:H	3	0.25
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD12	13	0.25
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD12	15	0.25
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG21	3	0.25
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	12	0.25
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG22	15	0.25
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	2	0.25
(2,2171)	1:174:A:LEU:HD23	1:174:A:LEU:H	5	0.25
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB2	7	0.25
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	6	0.25
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	10	0.25
(2,1923)	1:184:A:ALA:H	1:180:A:VAL:HG13	9	0.25
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG21	10	0.25
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD12	11	0.25
(2,1833)	1:13:A:LYS:H	1:13:A:LYS:HB2	5	0.25
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	6	0.25
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	7	0.25
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG22	11	0.25
(2,1534)	1:53:A:ILE:HG23	1:60:A:ILE:HA	7	0.25
(2,1533)	1:53:A:ILE:HG23	1:117:A:ILE:H	11	0.25
(2,1526)	1:178:A:LEU:HD22	1:176:A:VAL:H	2	0.25
(2,1500)	1:49:A:ILE:HG22	1:53:A:ILE:HB	7	0.25
(2,1444)	1:43:A:THR:HG22	1:39:A:LEU:HB2	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1349)	1:20:A:LEU:HD12	1:23:A:THR:H	8	0.25
(2,1343)	1:17:A:MET:HE1	1:86:A:PRO:HA	12	0.25
(2,1318)	1:177:A:MET:HE2	1:173:A:GLY:H	13	0.25
(2,1312)	1:127:A:GLU:HB2	1:128:A:ILE:HG23	13	0.25
(2,1302)	1:156:A:LEU:HD13	1:174:A:LEU:HB3	6	0.25
(2,1302)	1:156:A:LEU:HD11	1:174:A:LEU:HB3	10	0.25
(2,1302)	1:156:A:LEU:HD11	1:174:A:LEU:HB3	12	0.25
(2,1302)	1:156:A:LEU:HD13	1:174:A:LEU:HB3	14	0.25
(2,1302)	1:156:A:LEU:HD13	1:174:A:LEU:HB3	15	0.25
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG23	3	0.25
(2,1279)	1:59:A:ILE:HG22	1:112:A:ASP:HB3	1	0.25
(2,1279)	1:59:A:ILE:HG22	1:112:A:ASP:HB3	9	0.25
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE3	2	0.25
(2,1264)	1:60:A:ILE:HG22	1:42:A:MET:HE3	3	0.25
(2,1264)	1:60:A:ILE:HG21	1:42:A:MET:HE3	6	0.25
(2,1254)	1:17:A:MET:HE3	1:82:A:TYR:H	1	0.25
(2,1212)	1:167:A:LYS:HA	1:167:A:LYS:HB3	7	0.25
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	1	0.25
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG22	2	0.25
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	14	0.25
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG22	15	0.25
(2,1210)	1:134:A:LEU:HD12	1:134:A:LEU:HA	1	0.25
(2,1190)	1:19:A:GLU:HA	1:22:A:GLN:HG2	4	0.25
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	7	0.25
(2,1165)	1:161:A:THR:HG21	1:161:A:THR:HA	13	0.25
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	14	0.25
(2,1150)	1:43:A:THR:HA	1:49:A:ILE:HD11	7	0.25
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG23	4	0.25
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	3	0.25
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	2	0.25
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD11	7	0.25
(2,1088)	1:161:A:THR:HG23	1:158:A:GLU:HA	8	0.25
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG22	9	0.25
(2,1060)	1:36:A:GLU:HA	1:35:A:LEU:HD11	4	0.25
(2,918)	1:99:A:LYS:HD2	1:99:A:LYS:HE2	9	0.25
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	8	0.25
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD21	8	0.25
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD23	14	0.25
(2,859)	1:130:A:GLN:HG2	1:131:A:ARG:H	1	0.25
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	8	0.25
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	10	0.25
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG12	5	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,730)	1:97:A:ALA:HB1	1:93:A:PHE:HB3	15	0.25
(2,632)	1:64:A:ILE:HG22	1:39:A:LEU:HB2	4	0.25
(2,619)	1:40:A:TRP:HD1	1:43:A:THR:HG23	14	0.25
(2,615)	1:28:A:VAL:HG13	1:28:A:VAL:HB	2	0.25
(2,615)	1:28:A:VAL:HG12	1:28:A:VAL:HB	3	0.25
(2,615)	1:28:A:VAL:HG12	1:28:A:VAL:HB	6	0.25
(2,615)	1:28:A:VAL:HG13	1:28:A:VAL:HB	10	0.25
(2,615)	1:28:A:VAL:HG11	1:28:A:VAL:HB	11	0.25
(2,615)	1:28:A:VAL:HG13	1:28:A:VAL:HB	12	0.25
(2,615)	1:28:A:VAL:HG13	1:28:A:VAL:HB	15	0.25
(2,609)	1:28:A:VAL:HG11	1:29:A:ARG:H	2	0.25
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD23	3	0.25
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD22	11	0.25
(2,589)	1:64:A:ILE:HD12	1:35:A:LEU:HB3	8	0.25
(2,577)	1:89:A:VAL:HG11	1:93:A:PHE:HE2	5	0.25
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	15	0.25
(2,529)	1:176:A:VAL:HG23	1:97:A:ALA:HB1	14	0.25
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG23	3	0.25
(2,475)	1:59:A:ILE:HG22	1:116:A:LEU:HB3	6	0.25
(2,473)	1:59:A:ILE:HG21	1:112:A:ASP:HB2	4	0.25
(2,472)	1:178:A:LEU:HD22	1:178:A:LEU:HG	12	0.25
(2,449)	1:53:A:ILE:HG22	1:125:A:PHE:HZ	3	0.25
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG21	1	0.25
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG23	12	0.25
(2,418)	1:53:A:ILE:HD12	1:124:A:PHE:HB3	8	0.25
(2,409)	1:156:A:LEU:HD12	1:156:A:LEU:HG	4	0.25
(2,409)	1:156:A:LEU:HD12	1:156:A:LEU:HG	6	0.25
(2,409)	1:156:A:LEU:HD12	1:156:A:LEU:HG	7	0.25
(2,409)	1:156:A:LEU:HD12	1:156:A:LEU:HG	14	0.25
(2,408)	1:156:A:LEU:HD13	1:156:A:LEU:HB3	3	0.25
(2,408)	1:156:A:LEU:HD11	1:156:A:LEU:HB3	4	0.25
(2,408)	1:156:A:LEU:HD11	1:156:A:LEU:HB3	6	0.25
(2,408)	1:156:A:LEU:HD11	1:156:A:LEU:HB3	7	0.25
(2,408)	1:156:A:LEU:HD12	1:156:A:LEU:HB3	10	0.25
(2,408)	1:156:A:LEU:HD13	1:156:A:LEU:HB3	11	0.25
(2,406)	1:156:A:LEU:HD13	1:93:A:PHE:HZ	5	0.25
(2,402)	1:35:A:LEU:HD21	1:35:A:LEU:HG	9	0.25
(2,383)	1:31:A:LEU:HD21	1:31:A:LEU:HA	2	0.25
(2,383)	1:31:A:LEU:HD21	1:31:A:LEU:HA	7	0.25
(2,383)	1:31:A:LEU:HD21	1:31:A:LEU:HA	11	0.25
(2,377)	1:142:A:LEU:HD21	1:117:A:ILE:HD12	6	0.25
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD11	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,362)	1:156:A:LEU:HD23	1:152:A:TYR:HB2	3	0.25
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD13	10	0.25
(2,314)	1:93:A:PHE:HZ	1:20:A:LEU:HD12	14	0.25
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG23	13	0.25
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG21	4	0.25
(2,267)	1:183:A:LYS:HA	1:186:A:ASP:HB2	14	0.25
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB2	5	0.25
(2,171)	1:74:A:ILE:HG22	1:78:A:GLU:HG3	5	0.25
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG22	2	0.25
(2,121)	1:161:A:THR:HG23	1:158:A:GLU:HB3	8	0.25
(2,93)	1:89:A:VAL:HG12	1:79:A:LEU:HD12	3	0.25
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD11	9	0.25
(2,93)	1:89:A:VAL:HG12	1:79:A:LEU:HD13	12	0.25
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD13	13	0.25
(2,86)	1:67:A:ILE:HG23	1:106:A:TYR:HD2	4	0.25
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	9	0.25
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	11	0.25
(2,57)	1:142:A:LEU:HD13	1:61:A:PHE:HE1	11	0.25
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	6	0.25
(2,42)	1:53:A:ILE:HG21	1:120:A:HIS:HD2	11	0.25
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	13	0.25
(2,36)	1:39:A:LEU:HD12	1:65:A:GLN:HG2	4	0.25
(1,121)	1:153:A:GLN:O	1:157:A:LYS:H	4	0.25
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	5	0.24
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	10	0.24
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	14	0.24
(2,4816)	1:98:A:ASP:HB3	1:101:A:GLN:H	3	0.24
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	10	0.24
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	12	0.24
(2,4788)	1:99:A:LYS:H	1:98:A:ASP:HB3	14	0.24
(2,4778)	1:11:A:ARG:HD3	1:12:A:LYS:H	6	0.24
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG23	7	0.24
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG23	15	0.24
(2,4715)	1:7:A:GLU:H	1:9:A:PRO:HD3	13	0.24
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB2	8	0.24
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	3	0.24
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	11	0.24
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	8	0.24
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	5	0.24
(2,4553)	1:64:A:ILE:HG21	1:65:A:GLN:HE21	7	0.24
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	12	0.24
(2,4545)	1:67:A:ILE:HD11	1:145:A:PRO:HG3	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4521)	1:54:A:LEU:HD11	1:54:A:LEU:HA	1	0.24
(2,4521)	1:54:A:LEU:HD11	1:52:A:GLY:HA2	14	0.24
(2,4521)	1:54:A:LEU:HD13	1:54:A:LEU:HA	15	0.24
(2,4518)	1:128:A:ILE:HG22	1:124:A:PHE:HZ	13	0.24
(2,4489)	1:184:A:ALA:HB3	1:108:A:LYS:HE2	5	0.24
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD11	13	0.24
(2,4472)	1:20:A:LEU:HD21	1:155:A:LEU:HD11	10	0.24
(2,4472)	1:20:A:LEU:HD22	1:155:A:LEU:HD11	13	0.24
(2,4457)	1:164:A:GLU:HG2	1:164:A:GLU:HA	6	0.24
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	6	0.24
(2,4447)	1:179:A:SER:HB2	1:182:A:LYS:HD3	11	0.24
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG22	6	0.24
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG21	7	0.24
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD3	10	0.24
(2,4423)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	12	0.24
(2,4329)	1:156:A:LEU:HD21	1:175:A:GLU:HG3	4	0.24
(2,4258)	1:95:A:THR:HG23	1:75:A:PHE:HD1	9	0.24
(2,4258)	1:95:A:THR:HG21	1:75:A:PHE:HD2	11	0.24
(2,4234)	1:54:A:LEU:HD21	1:53:A:ILE:H	6	0.24
(2,4229)	1:28:A:VAL:HG13	1:73:A:ASN:H	1	0.24
(2,4193)	1:20:A:LEU:HD22	1:21:A:LEU:H	3	0.24
(2,4116)	1:79:A:LEU:HD12	1:78:A:GLU:H	8	0.24
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	2	0.24
(2,4078)	1:28:A:VAL:HG21	1:30:A:ASP:H	5	0.24
(2,4073)	1:131:A:ARG:HE	1:131:A:ARG:HG2	15	0.24
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	1	0.24
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	14	0.24
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG23	4	0.24
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	2	0.24
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	9	0.24
(2,3982)	1:53:A:ILE:HD12	1:121:A:ALA:H	11	0.24
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	12	0.24
(2,3978)	1:23:A:THR:HG23	1:22:A:GLN:H	8	0.24
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	1	0.24
(2,3974)	1:161:A:THR:HG22	1:160:A:LEU:H	3	0.24
(2,3974)	1:161:A:THR:HG23	1:160:A:LEU:H	10	0.24
(2,3974)	1:161:A:THR:HG22	1:160:A:LEU:H	13	0.24
(2,3942)	1:102:A:MET:HE3	1:102:A:MET:H	6	0.24
(2,3904)	1:31:A:LEU:HD21	1:72:A:ASN:H	15	0.24
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	4	0.24
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG23	6	0.24
(2,3866)	1:35:A:LEU:HD22	1:65:A:GLN:HE21	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	12	0.24
(2,3830)	1:177:A:MET:HE2	1:178:A:LEU:H	14	0.24
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD21	12	0.24
(2,3794)	1:135:A:ALA:HB1	1:135:A:ALA:H	14	0.24
(2,3713)	1:76:A:LEU:HD13	1:77:A:LYS:H	1	0.24
(2,3713)	1:76:A:LEU:HD11	1:77:A:LYS:H	15	0.24
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	11	0.24
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	6	0.24
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	13	0.24
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD21	2	0.24
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD21	13	0.24
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	1	0.24
(2,3647)	1:26:A:ALA:HB3	1:26:A:ALA:H	5	0.24
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	9	0.24
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	13	0.24
(2,3544)	1:68:A:TYR:HD1	1:31:A:LEU:HD11	9	0.24
(2,3536)	1:32:A:HIS:HD2	1:32:A:HIS:HA	3	0.24
(2,3464)	1:152:A:TYR:HE1	1:20:A:LEU:HD11	12	0.24
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG11	7	0.24
(2,3436)	1:82:A:TYR:HD1	1:85:A:LEU:HD21	12	0.24
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD22	12	0.24
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD23	13	0.24
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD22	14	0.24
(2,3344)	1:170:A:LEU:HD12	1:171:A:LYS:H	11	0.24
(2,3223)	1:117:A:ILE:HD12	1:139:A:SER:H	8	0.24
(2,3223)	1:117:A:ILE:HD12	1:139:A:SER:H	13	0.24
(2,3200)	1:5:A:SER:H	1:6:A:PRO:HA	15	0.24
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD11	2	0.24
(2,3119)	1:45:A:GLY:H	1:44:A:SER:HB2	5	0.24
(2,3031)	1:20:A:LEU:HD13	1:20:A:LEU:H	4	0.24
(2,3031)	1:20:A:LEU:HD13	1:20:A:LEU:H	9	0.24
(2,3031)	1:20:A:LEU:HD13	1:20:A:LEU:H	14	0.24
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	9	0.24
(2,2927)	1:156:A:LEU:HD22	1:173:A:GLY:H	15	0.24
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	1	0.24
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	10	0.24
(2,2527)	1:87:A:GLU:H	1:88:A:ASP:HB3	11	0.24
(2,2446)	1:74:A:ILE:HG21	1:73:A:ASN:H	8	0.24
(2,2446)	1:74:A:ILE:HG22	1:73:A:ASN:H	14	0.24
(2,2399)	1:117:A:ILE:HD11	1:116:A:LEU:H	9	0.24
(2,2399)	1:117:A:ILE:HD12	1:116:A:LEU:H	15	0.24
(2,2247)	1:132:A:HIS:H	1:130:A:GLN:HG3	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD11	1	0.24
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD12	10	0.24
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD12	4	0.24
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	9	0.24
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG21	3	0.24
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG21	3	0.24
(2,1543)	1:128:A:ILE:HD12	1:132:A:HIS:HD2	10	0.24
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG23	13	0.24
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	5	0.24
(2,1510)	1:116:A:LEU:HD23	1:54:A:LEU:H	5	0.24
(2,1500)	1:49:A:ILE:HG21	1:53:A:ILE:HB	3	0.24
(2,1444)	1:43:A:THR:HG23	1:39:A:LEU:HB2	1	0.24
(2,1439)	1:102:A:MET:HE1	1:106:A:TYR:HD2	5	0.24
(2,1439)	1:102:A:MET:HE2	1:106:A:TYR:HD2	9	0.24
(2,1422)	1:116:A:LEU:HD22	1:60:A:ILE:HA	4	0.24
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD12	11	0.24
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	7	0.24
(2,1369)	1:156:A:LEU:HD11	1:170:A:LEU:HB3	2	0.24
(2,1336)	1:46:A:VAL:HG13	1:46:A:VAL:HA	4	0.24
(2,1336)	1:46:A:VAL:HG11	1:46:A:VAL:HA	6	0.24
(2,1302)	1:156:A:LEU:HD12	1:174:A:LEU:HB3	2	0.24
(2,1302)	1:156:A:LEU:HD12	1:174:A:LEU:HB3	3	0.24
(2,1302)	1:156:A:LEU:HD13	1:174:A:LEU:HB3	7	0.24
(2,1300)	1:117:A:ILE:HG21	1:60:A:ILE:HG21	15	0.24
(2,1254)	1:17:A:MET:HE2	1:82:A:TYR:H	13	0.24
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	12	0.24
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG22	13	0.24
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	9	0.24
(2,1131)	1:183:A:LYS:HA	1:183:A:LYS:HG3	12	0.24
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	3	0.24
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	7	0.24
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	3	0.24
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	13	0.24
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	14	0.24
(2,1036)	1:140:A:SER:HB2	1:136:A:ASN:HB3	14	0.24
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD21	5	0.24
(2,918)	1:99:A:LYS:HD2	1:99:A:LYS:HE2	13	0.24
(2,872)	1:80:A:GLU:HG3	1:21:A:LEU:HD23	6	0.24
(2,851)	1:134:A:LEU:HD22	1:129:A:GLN:HB3	14	0.24
(2,788)	1:143:A:ILE:HG23	1:143:A:ILE:HB	5	0.24
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	6	0.24
(2,788)	1:143:A:ILE:HG22	1:143:A:ILE:HB	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,761)	1:37:A:THR:HG23	1:36:A:GLU:HG2	14	0.24
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG23	2	0.24
(2,730)	1:97:A:ALA:HB3	1:93:A:PHE:HB3	1	0.24
(2,729)	1:97:A:ALA:HB2	1:100:A:PHE:HE1	3	0.24
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	1	0.24
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	10	0.24
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	7	0.24
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	5	0.24
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	7	0.24
(2,696)	1:49:A:ILE:HD13	1:49:A:ILE:HG12	11	0.24
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	14	0.24
(2,658)	1:104:A:VAL:HG12	1:184:A:ALA:HA	5	0.24
(2,644)	1:105:A:THR:HG23	1:108:A:LYS:HD3	8	0.24
(2,643)	1:105:A:THR:HG23	1:106:A:TYR:HD2	2	0.24
(2,643)	1:105:A:THR:HG23	1:106:A:TYR:HD2	5	0.24
(2,630)	1:64:A:ILE:HG22	1:35:A:LEU:HG	6	0.24
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	3	0.24
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	12	0.24
(2,622)	1:43:A:THR:HG21	1:42:A:MET:HG3	13	0.24
(2,615)	1:28:A:VAL:HG11	1:28:A:VAL:HB	5	0.24
(2,615)	1:28:A:VAL:HG11	1:28:A:VAL:HB	8	0.24
(2,602)	1:28:A:VAL:HG21	1:28:A:VAL:HB	2	0.24
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	5	0.24
(2,602)	1:28:A:VAL:HG23	1:28:A:VAL:HB	11	0.24
(2,600)	1:28:A:VAL:HG21	1:28:A:VAL:HA	10	0.24
(2,592)	1:64:A:ILE:HD13	1:31:A:LEU:HD23	4	0.24
(2,589)	1:64:A:ILE:HD13	1:35:A:LEU:HB3	6	0.24
(2,577)	1:89:A:VAL:HG12	1:93:A:PHE:HE2	13	0.24
(2,557)	1:60:A:ILE:HD13	1:42:A:MET:HE3	2	0.24
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE2	8	0.24
(2,492)	1:159:A:LEU:HD21	1:160:A:LEU:H	15	0.24
(2,478)	1:59:A:ILE:HG23	1:60:A:ILE:HG22	1	0.24
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG22	6	0.24
(2,475)	1:59:A:ILE:HG21	1:116:A:LEU:HB3	7	0.24
(2,425)	1:35:A:LEU:HD13	1:35:A:LEU:H	8	0.24
(2,425)	1:35:A:LEU:HD13	1:35:A:LEU:H	12	0.24
(2,425)	1:35:A:LEU:HD13	1:35:A:LEU:H	13	0.24
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	9	0.24
(2,418)	1:53:A:ILE:HD11	1:124:A:PHE:HB3	11	0.24
(2,408)	1:156:A:LEU:HD12	1:156:A:LEU:HB3	1	0.24
(2,406)	1:156:A:LEU:HD11	1:93:A:PHE:HZ	7	0.24
(2,402)	1:35:A:LEU:HD22	1:35:A:LEU:HG	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,402)	1:35:A:LEU:HD21	1:35:A:LEU:HG	7	0.24
(2,313)	1:20:A:LEU:HD13	1:22:A:GLN:H	14	0.24
(2,312)	1:3:A:LEU:HD23	1:3:A:LEU:HA	14	0.24
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG23	15	0.24
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG23	3	0.24
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	1	0.24
(2,171)	1:74:A:ILE:HG22	1:78:A:GLU:HG3	6	0.24
(2,171)	1:74:A:ILE:HG23	1:78:A:GLU:HG3	12	0.24
(2,121)	1:161:A:THR:HG21	1:158:A:GLU:HB3	4	0.24
(2,74)	1:54:A:LEU:HD13	1:51:A:PRO:HB2	3	0.24
(2,74)	1:54:A:LEU:HD12	1:51:A:PRO:HB2	5	0.24
(2,74)	1:54:A:LEU:HD12	1:51:A:PRO:HB2	12	0.24
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	13	0.24
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	11	0.24
(2,57)	1:142:A:LEU:HD11	1:61:A:PHE:HE1	7	0.24
(2,57)	1:142:A:LEU:HD13	1:61:A:PHE:HE1	14	0.24
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	8	0.24
(2,39)	1:31:A:LEU:HD13	1:34:A:CYS:H	15	0.24
(2,18)	1:79:A:LEU:HD12	1:92:A:CYS:HB2	6	0.24
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD3	13	0.23
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	4	0.23
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	15	0.23
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	1	0.23
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	12	0.23
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	3	0.23
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	1	0.23
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	9	0.23
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	11	0.23
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	5	0.23
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	14	0.23
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	12	0.23
(2,4601)	1:186:A:ASP:HB2	1:186:A:ASP:H	7	0.23
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	1	0.23
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	14	0.23
(2,4489)	1:184:A:ALA:HB2	1:108:A:LYS:HE3	3	0.23
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD12	9	0.23
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD11	12	0.23
(2,4472)	1:20:A:LEU:HD23	1:155:A:LEU:HD13	5	0.23
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	4	0.23
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	5	0.23
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	10	0.23
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4447)	1:179:A:SER:HB3	1:182:A:LYS:HD3	4	0.23
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG21	9	0.23
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG22	9	0.23
(2,4423)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	1	0.23
(2,4422)	1:56:A:LYS:HE2	1:56:A:LYS:HG2	5	0.23
(2,4418)	1:185:A:ASN:HB3	1:182:A:LYS:HB3	3	0.23
(2,4331)	1:95:A:THR:HG23	1:92:A:CYS:HG	14	0.23
(2,4271)	1:116:A:LEU:HD22	1:56:A:LYS:HE2	11	0.23
(2,4267)	1:134:A:LEU:HD11	1:132:A:HIS:H	1	0.23
(2,4263)	1:178:A:LEU:HD23	1:175:A:GLU:HG2	13	0.23
(2,4236)	1:33:A:GLU:HG3	1:34:A:CYS:H	5	0.23
(2,4229)	1:28:A:VAL:HG13	1:73:A:ASN:H	2	0.23
(2,4193)	1:20:A:LEU:HD21	1:21:A:LEU:H	14	0.23
(2,4116)	1:79:A:LEU:HD13	1:78:A:GLU:H	15	0.23
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	3	0.23
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	7	0.23
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	11	0.23
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD11	3	0.23
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD13	5	0.23
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	6	0.23
(2,4064)	1:17:A:MET:HE1	1:20:A:LEU:H	3	0.23
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	15	0.23
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	5	0.23
(2,4046)	1:159:A:LEU:HD21	1:159:A:LEU:H	3	0.23
(2,4038)	1:29:A:ARG:HG2	1:29:A:ARG:H	10	0.23
(2,4015)	1:39:A:LEU:HD23	1:61:A:PHE:H	2	0.23
(2,3995)	1:17:A:MET:HE3	1:85:A:LEU:H	6	0.23
(2,3992)	1:35:A:LEU:HD21	1:65:A:GLN:H	3	0.23
(2,3982)	1:53:A:ILE:HD12	1:121:A:ALA:H	3	0.23
(2,3982)	1:53:A:ILE:HD12	1:121:A:ALA:H	4	0.23
(2,3982)	1:53:A:ILE:HD13	1:121:A:ALA:H	5	0.23
(2,3982)	1:53:A:ILE:HD13	1:121:A:ALA:H	6	0.23
(2,3982)	1:53:A:ILE:HD13	1:121:A:ALA:H	8	0.23
(2,3982)	1:53:A:ILE:HD13	1:121:A:ALA:H	13	0.23
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	5	0.23
(2,3976)	1:37:A:THR:HG23	1:38:A:TYR:H	14	0.23
(2,3974)	1:161:A:THR:HG21	1:160:A:LEU:H	1	0.23
(2,3974)	1:161:A:THR:HG21	1:160:A:LEU:H	14	0.23
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	3	0.23
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	12	0.23
(2,3937)	1:184:A:ALA:HB1	1:182:A:LYS:H	13	0.23
(2,3934)	1:42:A:MET:HE3	1:60:A:ILE:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3934)	1:42:A:MET:HE3	1:60:A:ILE:H	10	0.23
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	13	0.23
(2,3934)	1:42:A:MET:HE2	1:60:A:ILE:H	14	0.23
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	6	0.23
(2,3915)	1:121:A:ALA:HB1	1:119:A:GLU:H	8	0.23
(2,3910)	1:156:A:LEU:HD22	1:153:A:GLN:H	2	0.23
(2,3910)	1:156:A:LEU:HD21	1:153:A:GLN:H	5	0.23
(2,3905)	1:28:A:VAL:HG13	1:72:A:ASN:H	15	0.23
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD23	7	0.23
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD23	14	0.23
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD12	5	0.23
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD11	9	0.23
(2,3886)	1:161:A:THR:H	1:162:A:CYS:HB2	2	0.23
(2,3796)	1:135:A:ALA:HB2	1:136:A:ASN:HD22	13	0.23
(2,3794)	1:135:A:ALA:HB2	1:135:A:ALA:H	10	0.23
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	2	0.23
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	12	0.23
(2,3713)	1:76:A:LEU:HD13	1:77:A:LYS:H	2	0.23
(2,3682)	1:54:A:LEU:HD22	1:55:A:ASN:HD21	9	0.23
(2,3670)	1:43:A:THR:HG23	1:44:A:SER:H	7	0.23
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD22	9	0.23
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD22	15	0.23
(2,3662)	1:39:A:LEU:H	1:39:A:LEU:HD23	7	0.23
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	3	0.23
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	10	0.23
(2,3640)	1:18:A:ALA:HB2	1:19:A:GLU:H	4	0.23
(2,3636)	1:13:A:LYS:HA	1:14:A:GLU:H	2	0.23
(2,3636)	1:13:A:LYS:HA	1:14:A:GLU:H	5	0.23
(2,3622)	1:4:A:GLY:HA2	1:5:A:SER:H	10	0.23
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	3	0.23
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD12	9	0.23
(2,3569)	1:141:A:TYR:HE2	1:136:A:ASN:HB3	3	0.23
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD12	9	0.23
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG21	6	0.23
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG21	3	0.23
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG12	13	0.23
(2,3445)	1:40:A:TRP:HZ2	1:46:A:VAL:HG11	15	0.23
(2,3434)	1:22:A:GLN:HE22	1:21:A:LEU:HD12	3	0.23
(2,3223)	1:117:A:ILE:HD11	1:139:A:SER:H	3	0.23
(2,3223)	1:117:A:ILE:HD13	1:139:A:SER:H	9	0.23
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	2	0.23
(2,3031)	1:20:A:LEU:HD12	1:20:A:LEU:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2963)	1:179:A:SER:H	1:177:A:MET:HB3	14	0.23
(2,2882)	1:158:A:GLU:H	1:157:A:LYS:HG3	2	0.23
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD23	2	0.23
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	3	0.23
(2,2843)	1:149:A:VAL:H	1:146:A:VAL:HG12	7	0.23
(2,2762)	1:130:A:GLN:H	1:131:A:ARG:HG2	1	0.23
(2,2675)	1:117:A:ILE:HD13	1:113:A:SER:H	12	0.23
(2,2630)	1:150:A:THR:HG23	1:154:A:LEU:H	2	0.23
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	6	0.23
(2,2585)	1:94:A:VAL:HG13	1:95:A:THR:H	14	0.23
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	15	0.23
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG12	1	0.23
(2,2446)	1:74:A:ILE:HG23	1:73:A:ASN:H	13	0.23
(2,2446)	1:74:A:ILE:HG21	1:73:A:ASN:H	15	0.23
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD13	10	0.23
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	9	0.23
(2,2276)	1:190:A:VAL:H	1:188:A:MET:HA	5	0.23
(2,2128)	1:163:A:CYS:H	1:163:A:CYS:HA	3	0.23
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	5	0.23
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	6	0.23
(2,1984)	1:53:A:ILE:H	1:53:A:ILE:HG12	7	0.23
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD11	4	0.23
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	2	0.23
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	15	0.23
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG21	1	0.23
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG23	2	0.23
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG22	4	0.23
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	12	0.23
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	12	0.23
(2,1633)	1:33:A:GLU:H	1:68:A:TYR:HE1	9	0.23
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG23	3	0.23
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG21	6	0.23
(2,1526)	1:178:A:LEU:HD21	1:176:A:VAL:H	1	0.23
(2,1508)	1:105:A:THR:HG22	1:63:A:ASN:HB3	6	0.23
(2,1500)	1:49:A:ILE:HG23	1:53:A:ILE:HB	13	0.23
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	7	0.23
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD13	6	0.23
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	4	0.23
(2,1369)	1:156:A:LEU:HD12	1:170:A:LEU:HB3	7	0.23
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	12	0.23
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	13	0.23
(2,1357)	1:9:A:PRO:HB3	1:9:A:PRO:HA	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1343)	1:17:A:MET:HE3	1:86:A:PRO:HA	9	0.23
(2,1343)	1:17:A:MET:HE1	1:86:A:PRO:HA	14	0.23
(2,1336)	1:46:A:VAL:HG13	1:46:A:VAL:HA	2	0.23
(2,1336)	1:46:A:VAL:HG12	1:46:A:VAL:HA	12	0.23
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	9	0.23
(2,1321)	1:23:A:THR:HG21	1:22:A:GLN:HB3	11	0.23
(2,1279)	1:59:A:ILE:HG23	1:112:A:ASP:HB3	5	0.23
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD13	5	0.23
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	7	0.23
(2,1210)	1:134:A:LEU:HD11	1:134:A:LEU:HA	4	0.23
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG23	12	0.23
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	2	0.23
(2,1165)	1:161:A:THR:HG22	1:161:A:THR:HA	3	0.23
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	15	0.23
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG21	9	0.23
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG22	15	0.23
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD12	2	0.23
(2,1122)	1:7:A:GLU:HG2	1:7:A:GLU:HA	12	0.23
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	3	0.23
(2,1052)	1:104:A:VAL:HG21	1:180:A:VAL:HA	15	0.23
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	9	0.23
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	13	0.23
(2,874)	1:188:A:MET:HG3	1:108:A:LYS:HG2	11	0.23
(2,868)	1:18:A:ALA:HB2	1:22:A:GLN:HG3	9	0.23
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE1	13	0.23
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	2	0.23
(2,788)	1:143:A:ILE:HG23	1:143:A:ILE:HB	1	0.23
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	9	0.23
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	14	0.23
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD23	3	0.23
(2,733)	1:97:A:ALA:HB1	1:176:A:VAL:HG12	4	0.23
(2,733)	1:97:A:ALA:HB3	1:176:A:VAL:HG12	12	0.23
(2,730)	1:97:A:ALA:HB2	1:93:A:PHE:HB3	5	0.23
(2,727)	1:143:A:ILE:HD12	1:143:A:ILE:HG12	3	0.23
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	6	0.23
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	7	0.23
(2,727)	1:143:A:ILE:HD11	1:143:A:ILE:HG12	9	0.23
(2,727)	1:143:A:ILE:HD12	1:143:A:ILE:HG12	15	0.23
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD22	2	0.23
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	4	0.23
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD22	5	0.23
(2,704)	1:18:A:ALA:HB3	1:21:A:LEU:HB3	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,696)	1:49:A:ILE:HD13	1:49:A:ILE:HG12	1	0.23
(2,696)	1:49:A:ILE:HD13	1:49:A:ILE:HG12	2	0.23
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	3	0.23
(2,696)	1:49:A:ILE:HD12	1:49:A:ILE:HG12	8	0.23
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	13	0.23
(2,666)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	6	0.23
(2,643)	1:105:A:THR:HG21	1:106:A:TYR:HD2	9	0.23
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	5	0.23
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	10	0.23
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD23	1	0.23
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	1	0.23
(2,609)	1:28:A:VAL:HG11	1:29:A:ARG:H	1	0.23
(2,602)	1:28:A:VAL:HG23	1:28:A:VAL:HB	10	0.23
(2,602)	1:28:A:VAL:HG21	1:28:A:VAL:HB	15	0.23
(2,601)	1:28:A:VAL:HG22	1:71:A:HIS:HB2	4	0.23
(2,600)	1:28:A:VAL:HG22	1:28:A:VAL:HA	2	0.23
(2,553)	1:16:A:ILE:HG22	1:16:A:ILE:H	6	0.23
(2,492)	1:159:A:LEU:HD21	1:160:A:LEU:H	3	0.23
(2,492)	1:159:A:LEU:HD21	1:160:A:LEU:H	10	0.23
(2,475)	1:59:A:ILE:HG23	1:116:A:LEU:HB3	2	0.23
(2,473)	1:59:A:ILE:HG23	1:112:A:ASP:HB2	8	0.23
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG21	4	0.23
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG23	6	0.23
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG21	15	0.23
(2,418)	1:53:A:ILE:HD12	1:124:A:PHE:HB3	5	0.23
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	14	0.23
(2,408)	1:156:A:LEU:HD11	1:156:A:LEU:HB3	15	0.23
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	1	0.23
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	9	0.23
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	10	0.23
(2,379)	1:142:A:LEU:HD22	1:138:A:ILE:HD13	4	0.23
(2,379)	1:142:A:LEU:HD23	1:138:A:ILE:HD11	14	0.23
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD11	5	0.23
(2,377)	1:142:A:LEU:HD21	1:117:A:ILE:HD13	7	0.23
(2,377)	1:142:A:LEU:HD22	1:117:A:ILE:HD11	12	0.23
(2,377)	1:142:A:LEU:HD22	1:117:A:ILE:HD12	14	0.23
(2,369)	1:138:A:ILE:HD13	1:60:A:ILE:HG23	1	0.23
(2,369)	1:138:A:ILE:HD12	1:60:A:ILE:HG21	3	0.23
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	6	0.23
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	15	0.23
(2,312)	1:3:A:LEU:HD22	1:3:A:LEU:HA	4	0.23
(2,302)	1:136:A:ASN:HA	1:129:A:GLN:HE22	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG13	5	0.23
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG11	13	0.23
(2,179)	1:145:A:PRO:HB2	1:144:A:LYS:HB2	13	0.23
(2,171)	1:74:A:ILE:HG23	1:78:A:GLU:HG3	10	0.23
(2,170)	1:37:A:THR:HG23	1:33:A:GLU:HG3	2	0.23
(2,164)	1:127:A:GLU:HB3	1:128:A:ILE:HD11	6	0.23
(2,124)	1:187:A:ALA:HB3	1:183:A:LYS:HE2	13	0.23
(2,120)	1:161:A:THR:HG22	1:158:A:GLU:HG2	3	0.23
(2,112)	1:177:A:MET:HE3	1:100:A:PHE:HE1	12	0.23
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD13	4	0.23
(2,93)	1:89:A:VAL:HG11	1:79:A:LEU:HD12	6	0.23
(2,40)	1:31:A:LEU:HD13	1:67:A:ILE:HB	6	0.23
(2,25)	1:37:A:THR:HG22	1:33:A:GLU:HG2	1	0.23
(2,17)	1:39:A:LEU:HD22	1:42:A:MET:HG2	15	0.23
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	9	0.22
(2,4816)	1:98:A:ASP:HB3	1:101:A:GLN:H	5	0.22
(2,4781)	1:48:A:GLU:HG2	1:49:A:ILE:H	15	0.22
(2,4780)	1:47:A:GLU:HG3	1:47:A:GLU:H	5	0.22
(2,4766)	1:8:A:PHE:HD1	1:7:A:GLU:HB2	3	0.22
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	3	0.22
(2,4687)	1:11:A:ARG:HG3	1:12:A:LYS:H	5	0.22
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG2	1	0.22
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	7	0.22
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	10	0.22
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	4	0.22
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	6	0.22
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	8	0.22
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	4	0.22
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	13	0.22
(2,4561)	1:23:A:THR:HG21	1:16:A:ILE:HA	11	0.22
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD11	3	0.22
(2,4521)	1:54:A:LEU:HD12	1:52:A:GLY:HA2	5	0.22
(2,4492)	1:79:A:LEU:HD23	1:25:A:LYS:HG3	14	0.22
(2,4460)	1:19:A:GLU:HA	1:23:A:THR:HG23	4	0.22
(2,4435)	1:94:A:VAL:HG21	1:94:A:VAL:HA	11	0.22
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	5	0.22
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD3	5	0.22
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG21	1	0.22
(2,4422)	1:56:A:LYS:HE2	1:56:A:LYS:HG2	13	0.22
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG11	9	0.22
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG12	10	0.22
(2,4329)	1:156:A:LEU:HD21	1:175:A:GLU:HG3	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4272)	1:174:A:LEU:HD21	1:175:A:GLU:HB2	4	0.22
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	1	0.22
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	15	0.22
(2,4236)	1:33:A:GLU:HG3	1:34:A:CYS:H	3	0.22
(2,4234)	1:54:A:LEU:HD21	1:53:A:ILE:H	1	0.22
(2,4232)	1:117:A:ILE:HG22	1:116:A:LEU:H	14	0.22
(2,4229)	1:28:A:VAL:HG13	1:73:A:ASN:H	10	0.22
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	1	0.22
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	10	0.22
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	12	0.22
(2,4064)	1:17:A:MET:HE2	1:20:A:LEU:H	11	0.22
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	13	0.22
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	12	0.22
(2,4046)	1:159:A:LEU:HD21	1:159:A:LEU:H	14	0.22
(2,4030)	1:118:A:LEU:HD22	1:118:A:LEU:H	2	0.22
(2,4030)	1:118:A:LEU:HD22	1:118:A:LEU:H	6	0.22
(2,4030)	1:118:A:LEU:HD22	1:118:A:LEU:H	11	0.22
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	1	0.22
(2,4016)	1:64:A:ILE:HG22	1:61:A:PHE:H	9	0.22
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	10	0.22
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	11	0.22
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	15	0.22
(2,3998)	1:49:A:ILE:HD12	1:54:A:LEU:H	15	0.22
(2,3995)	1:17:A:MET:HE2	1:85:A:LEU:H	13	0.22
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	14	0.22
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	15	0.22
(2,3979)	1:18:A:ALA:HB2	1:22:A:GLN:H	9	0.22
(2,3976)	1:37:A:THR:HG21	1:38:A:TYR:H	11	0.22
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	3	0.22
(2,3969)	1:184:A:ALA:HB1	1:108:A:LYS:H	15	0.22
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	5	0.22
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG23	4	0.22
(2,3915)	1:121:A:ALA:HB3	1:119:A:GLU:H	12	0.22
(2,3910)	1:156:A:LEU:HD21	1:153:A:GLN:H	12	0.22
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD13	6	0.22
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG21	7	0.22
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG22	9	0.22
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG21	13	0.22
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	12	0.22
(2,3860)	1:149:A:VAL:HG11	1:153:A:GLN:HE21	9	0.22
(2,3856)	1:135:A:ALA:HB1	1:136:A:ASN:HD21	11	0.22
(2,3856)	1:135:A:ALA:HB2	1:136:A:ASN:HD21	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	2	0.22
(2,3830)	1:177:A:MET:HE1	1:178:A:LEU:H	12	0.22
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD21	1	0.22
(2,3691)	1:64:A:ILE:HG22	1:65:A:GLN:H	9	0.22
(2,3682)	1:54:A:LEU:HD21	1:55:A:ASN:HD21	15	0.22
(2,3652)	1:161:A:THR:HG23	1:162:A:CYS:H	12	0.22
(2,3647)	1:26:A:ALA:HB1	1:26:A:ALA:H	2	0.22
(2,3647)	1:26:A:ALA:HB1	1:26:A:ALA:H	8	0.22
(2,3647)	1:26:A:ALA:HB1	1:26:A:ALA:H	11	0.22
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	12	0.22
(2,3647)	1:26:A:ALA:HB1	1:26:A:ALA:H	15	0.22
(2,3640)	1:18:A:ALA:HB1	1:19:A:GLU:H	2	0.22
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD11	5	0.22
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD21	1	0.22
(2,3555)	1:96:A:TRP:HD1	1:95:A:THR:HG22	5	0.22
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD13	11	0.22
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG23	9	0.22
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	4	0.22
(2,3223)	1:117:A:ILE:HD12	1:139:A:SER:H	10	0.22
(2,3223)	1:117:A:ILE:HD13	1:139:A:SER:H	14	0.22
(2,3144)	1:52:A:GLY:H	1:53:A:ILE:HD13	5	0.22
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD11	2	0.22
(2,3012)	1:12:A:LYS:H	1:12:A:LYS:HB2	4	0.22
(2,2927)	1:156:A:LEU:HD22	1:173:A:GLY:H	3	0.22
(2,2927)	1:156:A:LEU:HD23	1:173:A:GLY:H	10	0.22
(2,2927)	1:156:A:LEU:HD23	1:173:A:GLY:H	12	0.22
(2,2909)	1:169:A:GLU:H	1:168:A:GLY:HA3	9	0.22
(2,2904)	1:166:A:GLY:H	1:167:A:LYS:H	13	0.22
(2,2812)	1:138:A:ILE:H	1:38:A:TYR:HD1	4	0.22
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	4	0.22
(2,2675)	1:117:A:ILE:HD11	1:113:A:SER:H	2	0.22
(2,2630)	1:150:A:THR:HG22	1:154:A:LEU:H	11	0.22
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	12	0.22
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	6	0.22
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	13	0.22
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	1	0.22
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	6	0.22
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	15	0.22
(2,2500)	1:81:A:LYS:H	1:79:A:LEU:HB3	7	0.22
(2,2446)	1:74:A:ILE:HG22	1:73:A:ASN:H	5	0.22
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG23	6	0.22
(2,2313)	1:54:A:LEU:HD23	1:55:A:ASN:HD22	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2288)	1:21:A:LEU:HD12	1:22:A:GLN:H	9	0.22
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	11	0.22
(2,2056)	1:72:A:ASN:H	1:73:A:ASN:HB3	2	0.22
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD11	3	0.22
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD12	8	0.22
(2,1991)	1:35:A:LEU:HD22	1:68:A:TYR:H	1	0.22
(2,1953)	1:141:A:TYR:HE1	1:30:A:ASP:H	4	0.22
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD13	1	0.22
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	11	0.22
(2,1547)	1:95:A:THR:HG22	1:78:A:GLU:HB2	4	0.22
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG22	3	0.22
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG22	14	0.22
(2,1533)	1:53:A:ILE:HG23	1:117:A:ILE:H	4	0.22
(2,1427)	1:19:A:GLU:HA	1:22:A:GLN:HG3	4	0.22
(2,1399)	1:7:A:GLU:HG3	1:8:A:PHE:HD1	13	0.22
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	1	0.22
(2,1343)	1:17:A:MET:HE3	1:86:A:PRO:HA	1	0.22
(2,1336)	1:46:A:VAL:HG13	1:46:A:VAL:HA	15	0.22
(2,1322)	1:74:A:ILE:HG23	1:78:A:GLU:HG2	11	0.22
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB2	7	0.22
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	8	0.22
(2,1309)	1:134:A:LEU:HD22	1:132:A:HIS:HD2	9	0.22
(2,1302)	1:156:A:LEU:HD11	1:174:A:LEU:HB3	8	0.22
(2,1302)	1:156:A:LEU:HD12	1:174:A:LEU:HB3	11	0.22
(2,1300)	1:117:A:ILE:HG22	1:60:A:ILE:HG21	14	0.22
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD12	9	0.22
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD11	15	0.22
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG22	3	0.22
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD13	5	0.22
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	10	0.22
(2,1084)	1:37:A:THR:HA	1:128:A:ILE:HG21	1	0.22
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	1	0.22
(2,1042)	1:171:A:LYS:HA	1:171:A:LYS:HB2	2	0.22
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD22	4	0.22
(2,928)	1:29:A:ARG:HD2	1:29:A:ARG:H	12	0.22
(2,918)	1:99:A:LYS:HD2	1:99:A:LYS:HE2	10	0.22
(2,851)	1:134:A:LEU:HD23	1:129:A:GLN:HB3	10	0.22
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	9	0.22
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	11	0.22
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	13	0.22
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	15	0.22
(2,788)	1:143:A:ILE:HG22	1:143:A:ILE:HB	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	10	0.22
(2,788)	1:143:A:ILE:HG23	1:143:A:ILE:HB	13	0.22
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD21	10	0.22
(2,761)	1:37:A:THR:HG21	1:36:A:GLU:HG2	4	0.22
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	1	0.22
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	2	0.22
(2,727)	1:143:A:ILE:HD11	1:143:A:ILE:HG12	4	0.22
(2,727)	1:143:A:ILE:HD11	1:143:A:ILE:HG12	5	0.22
(2,727)	1:143:A:ILE:HD11	1:143:A:ILE:HG12	11	0.22
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	13	0.22
(2,727)	1:143:A:ILE:HD13	1:143:A:ILE:HG12	14	0.22
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	14	0.22
(2,704)	1:18:A:ALA:HB1	1:21:A:LEU:HB3	5	0.22
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	5	0.22
(2,696)	1:49:A:ILE:HD12	1:49:A:ILE:HG12	10	0.22
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	15	0.22
(2,652)	1:177:A:MET:HE3	1:179:A:SER:H	5	0.22
(2,644)	1:105:A:THR:HG23	1:108:A:LYS:HD3	6	0.22
(2,622)	1:43:A:THR:HG22	1:42:A:MET:HG3	5	0.22
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	8	0.22
(2,615)	1:28:A:VAL:HG13	1:28:A:VAL:HB	1	0.22
(2,615)	1:28:A:VAL:HG12	1:28:A:VAL:HB	13	0.22
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	1	0.22
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	4	0.22
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	9	0.22
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD23	10	0.22
(2,577)	1:89:A:VAL:HG11	1:93:A:PHE:HE2	14	0.22
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE1	1	0.22
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE1	7	0.22
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE2	14	0.22
(2,512)	1:170:A:LEU:HD21	1:170:A:LEU:HG	2	0.22
(2,512)	1:170:A:LEU:HD23	1:170:A:LEU:HG	14	0.22
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	11	0.22
(2,478)	1:59:A:ILE:HG23	1:60:A:ILE:HG23	2	0.22
(2,478)	1:59:A:ILE:HG22	1:60:A:ILE:HG21	12	0.22
(2,478)	1:59:A:ILE:HG22	1:60:A:ILE:HG21	15	0.22
(2,475)	1:59:A:ILE:HG21	1:116:A:LEU:HB3	10	0.22
(2,468)	1:178:A:LEU:HD21	1:175:A:GLU:HA	5	0.22
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG21	11	0.22
(2,422)	1:49:A:ILE:HG21	1:124:A:PHE:HB3	12	0.22
(2,408)	1:156:A:LEU:HD11	1:156:A:LEU:HB3	14	0.22
(2,406)	1:156:A:LEU:HD11	1:93:A:PHE:HZ	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	4	0.22
(2,377)	1:142:A:LEU:HD21	1:117:A:ILE:HD12	2	0.22
(2,377)	1:142:A:LEU:HD22	1:117:A:ILE:HD11	8	0.22
(2,351)	1:188:A:MET:HE3	1:108:A:LYS:HA	8	0.22
(2,348)	1:70:A:PHE:HD2	1:102:A:MET:HE3	10	0.22
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	1	0.22
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	4	0.22
(2,312)	1:3:A:LEU:HD21	1:3:A:LEU:HA	10	0.22
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB1	9	0.22
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD13	4	0.22
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD11	9	0.22
(2,133)	1:23:A:THR:HG23	1:22:A:GLN:HB2	7	0.22
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	1	0.22
(2,106)	1:43:A:THR:HG23	1:42:A:MET:HG2	2	0.22
(2,103)	1:28:A:VAL:HG11	1:31:A:LEU:HD22	9	0.22
(2,74)	1:54:A:LEU:HD13	1:51:A:PRO:HB2	6	0.22
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	14	0.22
(2,63)	1:174:A:LEU:HD23	1:175:A:GLU:HA	9	0.22
(2,57)	1:142:A:LEU:HD12	1:61:A:PHE:HE1	4	0.22
(2,21)	1:39:A:LEU:HD23	1:138:A:ILE:HD13	4	0.22
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	12	0.22
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	1	0.21
(2,4788)	1:98:A:ASP:HB2	1:99:A:LYS:H	10	0.21
(2,4776)	1:11:A:ARG:HG2	1:11:A:ARG:H	1	0.21
(2,4767)	1:8:A:PHE:HD1	1:9:A:PRO:HG2	13	0.21
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG21	1	0.21
(2,4715)	1:7:A:GLU:H	1:6:A:PRO:HD2	3	0.21
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG3	10	0.21
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	12	0.21
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG23	2	0.21
(2,4653)	1:87:A:GLU:H	1:89:A:VAL:HG22	4	0.21
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	10	0.21
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	12	0.21
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	15	0.21
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	4	0.21
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	2	0.21
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	14	0.21
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	14	0.21
(2,4586)	1:93:A:PHE:H	1:176:A:VAL:HG12	8	0.21
(2,4576)	1:62:A:GLY:H	1:113:A:SER:H	7	0.21
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	2	0.21
(2,4489)	1:184:A:ALA:HB3	1:108:A:LYS:HE2	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD3	13	0.21
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	2	0.21
(2,4435)	1:94:A:VAL:HG21	1:94:A:VAL:HA	5	0.21
(2,4435)	1:94:A:VAL:HG21	1:94:A:VAL:HA	14	0.21
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	15	0.21
(2,4427)	1:8:A:PHE:HB2	1:7:A:GLU:HB3	7	0.21
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	4	0.21
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	1	0.21
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	7	0.21
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	9	0.21
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	12	0.21
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG12	11	0.21
(2,4332)	1:31:A:LEU:HD21	1:32:A:HIS:H	2	0.21
(2,4309)	1:182:A:LYS:HE2	1:183:A:LYS:H	4	0.21
(2,4309)	1:182:A:LYS:HE2	1:183:A:LYS:H	13	0.21
(2,4292)	1:48:A:GLU:HB3	1:49:A:ILE:HG21	6	0.21
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD11	3	0.21
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD11	7	0.21
(2,4232)	1:117:A:ILE:HG22	1:116:A:LEU:H	9	0.21
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	12	0.21
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	12	0.21
(2,4116)	1:79:A:LEU:HD13	1:78:A:GLU:H	11	0.21
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	6	0.21
(2,4110)	1:64:A:ILE:HG22	1:62:A:GLY:H	9	0.21
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	1	0.21
(2,4073)	1:131:A:ARG:HE	1:131:A:ARG:HG2	8	0.21
(2,4064)	1:17:A:MET:HE2	1:20:A:LEU:H	4	0.21
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD23	9	0.21
(2,4059)	1:83:A:GLU:HB3	1:85:A:LEU:H	5	0.21
(2,4043)	1:12:A:LYS:HB3	1:12:A:LYS:H	7	0.21
(2,4030)	1:118:A:LEU:HD22	1:118:A:LEU:H	8	0.21
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	10	0.21
(2,4018)	1:190:A:VAL:HG11	1:190:A:VAL:H	13	0.21
(2,4016)	1:64:A:ILE:HG21	1:61:A:PHE:H	14	0.21
(2,4015)	1:39:A:LEU:HD21	1:61:A:PHE:H	9	0.21
(2,3995)	1:17:A:MET:HE1	1:85:A:LEU:H	7	0.21
(2,3995)	1:17:A:MET:HE2	1:85:A:LEU:H	8	0.21
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	1	0.21
(2,3978)	1:23:A:THR:HG22	1:22:A:GLN:H	15	0.21
(2,3976)	1:37:A:THR:HG21	1:38:A:TYR:H	4	0.21
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD13	7	0.21
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	3	0.21
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	13	0.21
(2,3923)	1:49:A:ILE:HD11	1:42:A:MET:H	5	0.21
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD22	15	0.21
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG21	2	0.21
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	11	0.21
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	13	0.21
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	14	0.21
(2,3856)	1:135:A:ALA:HB3	1:136:A:ASN:HD21	2	0.21
(2,3856)	1:135:A:ALA:HB2	1:136:A:ASN:HD21	9	0.21
(2,3844)	1:184:A:ALA:HB1	1:185:A:ASN:H	13	0.21
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD21	9	0.21
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG22	2	0.21
(2,3713)	1:76:A:LEU:HD11	1:77:A:LYS:H	8	0.21
(2,3682)	1:54:A:LEU:HD23	1:55:A:ASN:HD21	1	0.21
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	11	0.21
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD23	7	0.21
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD21	11	0.21
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	6	0.21
(2,3640)	1:18:A:ALA:HB2	1:19:A:GLU:H	3	0.21
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	2	0.21
(2,3628)	1:3:A:LEU:HG	1:3:A:LEU:H	2	0.21
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	2	0.21
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	8	0.21
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG21	1	0.21
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD22	10	0.21
(2,3492)	1:100:A:PHE:HE1	1:71:A:HIS:HE1	13	0.21
(2,3482)	1:100:A:PHE:HD2	1:177:A:MET:HE3	11	0.21
(2,3464)	1:152:A:TYR:HE1	1:20:A:LEU:HD12	1	0.21
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG12	4	0.21
(2,3447)	1:40:A:TRP:HZ3	1:46:A:VAL:HG21	14	0.21
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD21	6	0.21
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD13	9	0.21
(2,2927)	1:156:A:LEU:HD21	1:173:A:GLY:H	4	0.21
(2,2907)	1:169:A:GLU:H	1:169:A:GLU:HA	6	0.21
(2,2896)	1:164:A:GLU:H	1:163:A:CYS:H	10	0.21
(2,2895)	1:164:A:GLU:H	1:163:A:CYS:HB2	10	0.21
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD23	1	0.21
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD21	8	0.21
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	8	0.21
(2,2675)	1:117:A:ILE:HD11	1:113:A:SER:H	14	0.21
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	7	0.21
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	15	0.21
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG21	4	0.21
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	2	0.21
(2,2342)	1:59:A:ILE:H	1:60:A:ILE:HG23	1	0.21
(2,2288)	1:21:A:LEU:HD13	1:22:A:GLN:H	5	0.21
(2,2288)	1:21:A:LEU:HD11	1:22:A:GLN:H	7	0.21
(2,2279)	1:153:A:GLN:HE21	1:178:A:LEU:HA	14	0.21
(2,2071)	1:91:A:HIS:H	1:82:A:TYR:HE2	8	0.21
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	10	0.21
(2,2068)	1:83:A:GLU:H	1:82:A:TYR:HE1	12	0.21
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD13	7	0.21
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	2	0.21
(2,1833)	1:13:A:LYS:H	1:13:A:LYS:HB2	7	0.21
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG13	6	0.21
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG13	8	0.21
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	8	0.21
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG23	12	0.21
(2,1526)	1:178:A:LEU:HD21	1:176:A:VAL:H	6	0.21
(2,1522)	1:76:A:LEU:HD13	1:68:A:TYR:HE1	12	0.21
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	3	0.21
(2,1476)	1:134:A:LEU:HD21	1:34:A:CYS:HA	11	0.21
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	12	0.21
(2,1394)	1:156:A:LEU:HD21	1:152:A:TYR:HA	12	0.21
(2,1371)	1:31:A:LEU:HD13	1:29:A:ARG:H	3	0.21
(2,1369)	1:156:A:LEU:HD12	1:170:A:LEU:HB3	4	0.21
(2,1369)	1:156:A:LEU:HD11	1:170:A:LEU:HB3	8	0.21
(2,1369)	1:156:A:LEU:HD11	1:170:A:LEU:HB3	11	0.21
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	12	0.21
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	1	0.21
(2,1350)	1:35:A:LEU:HD11	1:36:A:GLU:H	4	0.21
(2,1349)	1:20:A:LEU:HD12	1:23:A:THR:H	3	0.21
(2,1336)	1:46:A:VAL:HG13	1:46:A:VAL:HA	1	0.21
(2,1336)	1:46:A:VAL:HG13	1:46:A:VAL:HA	7	0.21
(2,1336)	1:46:A:VAL:HG13	1:46:A:VAL:HA	8	0.21
(2,1336)	1:46:A:VAL:HG12	1:46:A:VAL:HA	9	0.21
(2,1336)	1:46:A:VAL:HG11	1:46:A:VAL:HA	10	0.21
(2,1336)	1:46:A:VAL:HG12	1:46:A:VAL:HA	11	0.21
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	6	0.21
(2,1309)	1:134:A:LEU:HD21	1:132:A:HIS:HD2	5	0.21
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	12	0.21
(2,1279)	1:59:A:ILE:HG22	1:112:A:ASP:HB3	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1264)	1:60:A:ILE:HG23	1:42:A:MET:HE1	5	0.21
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	14	0.21
(2,1198)	1:188:A:MET:HA	1:187:A:ALA:HB3	11	0.21
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG21	10	0.21
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	1	0.21
(2,977)	1:104:A:VAL:HG13	1:104:A:VAL:HA	2	0.21
(2,918)	1:99:A:LYS:HD2	1:99:A:LYS:HE2	12	0.21
(2,886)	1:153:A:GLN:HB3	1:150:A:THR:HG23	4	0.21
(2,868)	1:18:A:ALA:HB1	1:22:A:GLN:HG3	7	0.21
(2,851)	1:134:A:LEU:HD23	1:129:A:GLN:HB3	4	0.21
(2,848)	1:143:A:ILE:HD12	1:146:A:VAL:HB	13	0.21
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	3	0.21
(2,727)	1:143:A:ILE:HD12	1:143:A:ILE:HG12	8	0.21
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	15	0.21
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	4	0.21
(2,696)	1:49:A:ILE:HD12	1:49:A:ILE:HG12	6	0.21
(2,696)	1:49:A:ILE:HD11	1:49:A:ILE:HG12	9	0.21
(2,696)	1:49:A:ILE:HD13	1:49:A:ILE:HG12	12	0.21
(2,695)	1:49:A:ILE:HG12	1:124:A:PHE:HD2	11	0.21
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	2	0.21
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	15	0.21
(2,643)	1:105:A:THR:HG23	1:106:A:TYR:HD2	4	0.21
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	2	0.21
(2,631)	1:64:A:ILE:HG21	1:35:A:LEU:HD23	3	0.21
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	6	0.21
(2,618)	1:43:A:THR:HG22	1:45:A:GLY:H	15	0.21
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	7	0.21
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	9	0.21
(2,602)	1:28:A:VAL:HG21	1:28:A:VAL:HB	13	0.21
(2,601)	1:28:A:VAL:HG22	1:71:A:HIS:HB2	9	0.21
(2,601)	1:28:A:VAL:HG22	1:71:A:HIS:HB2	14	0.21
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	4	0.21
(2,600)	1:28:A:VAL:HG21	1:28:A:VAL:HA	11	0.21
(2,600)	1:28:A:VAL:HG22	1:28:A:VAL:HA	13	0.21
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE1	4	0.21
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE3	6	0.21
(2,512)	1:170:A:LEU:HD22	1:170:A:LEU:HG	7	0.21
(2,512)	1:170:A:LEU:HD21	1:170:A:LEU:HG	9	0.21
(2,512)	1:170:A:LEU:HD23	1:170:A:LEU:HG	15	0.21
(2,492)	1:159:A:LEU:HD21	1:160:A:LEU:H	9	0.21
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	12	0.21
(2,492)	1:159:A:LEU:HD21	1:160:A:LEU:H	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG22	9	0.21
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	1	0.21
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	3	0.21
(2,383)	1:31:A:LEU:HD21	1:31:A:LEU:HA	5	0.21
(2,383)	1:31:A:LEU:HD21	1:31:A:LEU:HA	12	0.21
(2,377)	1:142:A:LEU:HD21	1:117:A:ILE:HD11	4	0.21
(2,332)	1:42:A:MET:HE2	1:60:A:ILE:HG13	8	0.21
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	12	0.21
(2,325)	1:17:A:MET:HE1	1:83:A:GLU:HA	2	0.21
(2,318)	1:20:A:LEU:HD23	1:152:A:TYR:HD1	5	0.21
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG22	4	0.21
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD11	3	0.21
(2,291)	1:172:A:ASP:HA	1:171:A:LYS:HG2	4	0.21
(2,285)	1:19:A:GLU:HA	1:22:A:GLN:HB3	5	0.21
(2,267)	1:183:A:LYS:HA	1:186:A:ASP:HB2	15	0.21
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG13	15	0.21
(2,231)	1:180:A:VAL:HA	1:184:A:ALA:HB2	11	0.21
(2,195)	1:41:A:GLU:HG2	1:40:A:TRP:HE3	6	0.21
(2,114)	1:177:A:MET:HE3	1:93:A:PHE:HE1	4	0.21
(2,74)	1:54:A:LEU:HD11	1:51:A:PRO:HB2	15	0.21
(2,39)	1:31:A:LEU:HD13	1:34:A:CYS:H	1	0.21
(2,39)	1:31:A:LEU:HD13	1:34:A:CYS:H	8	0.21
(2,39)	1:31:A:LEU:HD13	1:34:A:CYS:H	13	0.21
(2,19)	1:79:A:LEU:HD12	1:92:A:CYS:HG	14	0.21
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	5	0.21
(2,4841)	1:171:A:LYS:HG3	1:170:A:LEU:H	2	0.2
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	4	0.2
(2,4822)	1:51:A:PRO:HG2	1:54:A:LEU:H	7	0.2
(2,4816)	1:98:A:ASP:HB3	1:101:A:GLN:H	1	0.2
(2,4767)	1:8:A:PHE:HD2	1:9:A:PRO:HG3	8	0.2
(2,4756)	1:32:A:HIS:HD2	1:35:A:LEU:H	9	0.2
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	13	0.2
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	8	0.2
(2,4715)	1:7:A:GLU:H	1:6:A:PRO:HD2	11	0.2
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD22	15	0.2
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	5	0.2
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	11	0.2
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	12	0.2
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	1	0.2
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	2	0.2
(2,4624)	1:98:A:ASP:HB2	1:100:A:PHE:H	8	0.2
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4608)	1:28:A:VAL:H	1:29:A:ARG:HB3	12	0.2
(2,4603)	1:10:A:GLY:H	1:9:A:PRO:HG2	2	0.2
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	11	0.2
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD21	4	0.2
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	9	0.2
(2,4561)	1:23:A:THR:HG22	1:16:A:ILE:HA	2	0.2
(2,4529)	1:60:A:ILE:HG23	1:113:A:SER:HB2	1	0.2
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG12	13	0.2
(2,4489)	1:184:A:ALA:HB2	1:108:A:LYS:HE3	10	0.2
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD13	10	0.2
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD11	15	0.2
(2,4472)	1:20:A:LEU:HD23	1:155:A:LEU:HD13	4	0.2
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	14	0.2
(2,4451)	1:114:A:ASN:HA	1:115:A:GLN:HG2	4	0.2
(2,4435)	1:94:A:VAL:HG21	1:94:A:VAL:HA	10	0.2
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG22	13	0.2
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	14	0.2
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD3	8	0.2
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG21	14	0.2
(2,4423)	1:116:A:LEU:HD21	1:56:A:LYS:HE2	3	0.2
(2,4396)	1:48:A:GLU:HG2	1:49:A:ILE:HG22	5	0.2
(2,4393)	1:130:A:GLN:HB2	1:131:A:ARG:HG2	15	0.2
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	2	0.2
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	11	0.2
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	15	0.2
(2,4309)	1:182:A:LYS:HE2	1:183:A:LYS:H	5	0.2
(2,4292)	1:48:A:GLU:HB2	1:49:A:ILE:HG21	13	0.2
(2,4234)	1:54:A:LEU:HD22	1:53:A:ILE:H	2	0.2
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	7	0.2
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	8	0.2
(2,4229)	1:28:A:VAL:HG13	1:73:A:ASN:H	4	0.2
(2,4172)	1:18:A:ALA:HB2	1:22:A:GLN:HE22	5	0.2
(2,4112)	1:76:A:LEU:HD22	1:25:A:LYS:H	7	0.2
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	5	0.2
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD13	7	0.2
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD11	15	0.2
(2,4078)	1:28:A:VAL:HG23	1:30:A:ASP:H	2	0.2
(2,4064)	1:17:A:MET:HE2	1:20:A:LEU:H	10	0.2
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD21	7	0.2
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	14	0.2
(2,4046)	1:159:A:LEU:HD23	1:159:A:LEU:H	1	0.2
(2,4046)	1:159:A:LEU:HD21	1:159:A:LEU:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	11	0.2
(2,4043)	1:12:A:LYS:HB3	1:12:A:LYS:H	11	0.2
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	4	0.2
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	7	0.2
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	9	0.2
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	12	0.2
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	15	0.2
(2,4015)	1:39:A:LEU:HD23	1:61:A:PHE:H	6	0.2
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	6	0.2
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	14	0.2
(2,3998)	1:49:A:ILE:HD12	1:54:A:LEU:H	3	0.2
(2,3998)	1:49:A:ILE:HD12	1:54:A:LEU:H	5	0.2
(2,3995)	1:17:A:MET:HE1	1:85:A:LEU:H	2	0.2
(2,3995)	1:17:A:MET:HE1	1:85:A:LEU:H	15	0.2
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG21	8	0.2
(2,3982)	1:53:A:ILE:HD11	1:121:A:ALA:H	7	0.2
(2,3981)	1:53:A:ILE:HG22	1:121:A:ALA:H	15	0.2
(2,3978)	1:23:A:THR:HG23	1:22:A:GLN:H	4	0.2
(2,3978)	1:23:A:THR:HG23	1:22:A:GLN:H	7	0.2
(2,3978)	1:23:A:THR:HG23	1:22:A:GLN:H	9	0.2
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD13	13	0.2
(2,3956)	1:74:A:ILE:HG23	1:78:A:GLU:H	13	0.2
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG22	9	0.2
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	4	0.2
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG23	10	0.2
(2,3923)	1:49:A:ILE:HD13	1:42:A:MET:H	2	0.2
(2,3915)	1:121:A:ALA:HB2	1:119:A:GLU:H	10	0.2
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	13	0.2
(2,3875)	1:39:A:LEU:HD21	1:43:A:THR:H	4	0.2
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG23	1	0.2
(2,3856)	1:135:A:ALA:HB1	1:136:A:ASN:HD21	5	0.2
(2,3844)	1:184:A:ALA:HB1	1:185:A:ASN:H	2	0.2
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	3	0.2
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	10	0.2
(2,3830)	1:177:A:MET:HE1	1:178:A:LEU:H	1	0.2
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	11	0.2
(2,3713)	1:76:A:LEU:HD11	1:77:A:LYS:H	13	0.2
(2,3682)	1:54:A:LEU:HD23	1:55:A:ASN:HD21	6	0.2
(2,3682)	1:54:A:LEU:HD22	1:55:A:ASN:HD21	10	0.2
(2,3682)	1:54:A:LEU:HD23	1:55:A:ASN:HD21	14	0.2
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD22	14	0.2
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3622)	1:4:A:GLY:HA2	1:5:A:SER:H	9	0.2
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD13	15	0.2
(2,3569)	1:141:A:TYR:HE2	1:136:A:ASN:HB3	8	0.2
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	3	0.2
(2,3536)	1:32:A:HIS:HD2	1:32:A:HIS:HA	15	0.2
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD11	1	0.2
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG21	3	0.2
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG22	6	0.2
(2,3223)	1:117:A:ILE:HD12	1:139:A:SER:H	12	0.2
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	15	0.2
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD12	13	0.2
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD13	14	0.2
(2,3011)	1:12:A:LYS:HA	1:12:A:LYS:H	5	0.2
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	7	0.2
(2,2798)	1:141:A:TYR:HE2	1:137:A:SER:H	10	0.2
(2,2638)	1:180:A:VAL:HG22	1:104:A:VAL:H	7	0.2
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	4	0.2
(2,2585)	1:94:A:VAL:HG13	1:95:A:THR:H	5	0.2
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG22	15	0.2
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	3	0.2
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	10	0.2
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG13	15	0.2
(2,2527)	1:87:A:GLU:H	1:88:A:ASP:HB3	1	0.2
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD11	9	0.2
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	5	0.2
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	3	0.2
(2,2120)	1:153:A:GLN:HG2	1:153:A:GLN:H	12	0.2
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	6	0.2
(2,2028)	1:8:A:PHE:H	1:8:A:PHE:HB3	9	0.2
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	2	0.2
(2,1994)	1:67:A:ILE:HG22	1:71:A:HIS:H	6	0.2
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD13	4	0.2
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG21	15	0.2
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD12	3	0.2
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	4	0.2
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	14	0.2
(2,1783)	1:94:A:VAL:H	1:169:A:GLU:HB3	5	0.2
(2,1746)	1:77:A:LYS:H	1:75:A:PHE:HD2	7	0.2
(2,1744)	1:76:A:LEU:HD21	1:77:A:LYS:H	3	0.2
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	14	0.2
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG22	11	0.2
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG11	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1590)	1:18:A:ALA:HB1	1:20:A:LEU:HA	4	0.2
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG23	13	0.2
(2,1570)	1:156:A:LEU:HD21	1:178:A:LEU:H	14	0.2
(2,1543)	1:128:A:ILE:HD13	1:132:A:HIS:HD2	12	0.2
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	8	0.2
(2,1500)	1:49:A:ILE:HG21	1:53:A:ILE:HB	5	0.2
(2,1500)	1:49:A:ILE:HG22	1:53:A:ILE:HB	6	0.2
(2,1500)	1:49:A:ILE:HG22	1:53:A:ILE:HB	8	0.2
(2,1444)	1:43:A:THR:HG23	1:39:A:LEU:HB2	8	0.2
(2,1444)	1:43:A:THR:HG23	1:39:A:LEU:HB2	12	0.2
(2,1349)	1:20:A:LEU:HD11	1:23:A:THR:H	2	0.2
(2,1336)	1:46:A:VAL:HG12	1:46:A:VAL:HA	3	0.2
(2,1336)	1:46:A:VAL:HG11	1:46:A:VAL:HA	5	0.2
(2,1336)	1:46:A:VAL:HG11	1:46:A:VAL:HA	13	0.2
(2,1321)	1:23:A:THR:HG23	1:22:A:GLN:HB3	8	0.2
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	10	0.2
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB2	11	0.2
(2,1317)	1:43:A:THR:HG22	1:57:A:GLU:HB3	4	0.2
(2,1317)	1:43:A:THR:HG22	1:57:A:GLU:HB3	11	0.2
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD12	3	0.2
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD12	7	0.2
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG23	8	0.2
(2,1190)	1:19:A:GLU:HA	1:22:A:GLN:HG2	5	0.2
(2,1124)	1:48:A:GLU:HA	1:49:A:ILE:HD12	12	0.2
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	4	0.2
(2,977)	1:104:A:VAL:HG13	1:104:A:VAL:HA	8	0.2
(2,951)	1:15:A:PHE:HB2	1:18:A:ALA:HB1	12	0.2
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	13	0.2
(2,834)	1:51:A:PRO:HB2	1:52:A:GLY:HA2	5	0.2
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	3	0.2
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD21	9	0.2
(2,727)	1:143:A:ILE:HD12	1:143:A:ILE:HG12	12	0.2
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD21	10	0.2
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD22	11	0.2
(2,704)	1:18:A:ALA:HB3	1:21:A:LEU:HB3	10	0.2
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD23	15	0.2
(2,677)	1:146:A:VAL:HG12	1:146:A:VAL:HB	3	0.2
(2,677)	1:146:A:VAL:HG12	1:146:A:VAL:HB	7	0.2
(2,677)	1:146:A:VAL:HG12	1:146:A:VAL:HB	9	0.2
(2,677)	1:146:A:VAL:HG12	1:146:A:VAL:HB	10	0.2
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	15	0.2
(2,631)	1:64:A:ILE:HG21	1:35:A:LEU:HD21	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	12	0.2
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	14	0.2
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	5	0.2
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	14	0.2
(2,597)	1:28:A:VAL:HG22	1:72:A:ASN:HD22	12	0.2
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE3	3	0.2
(2,557)	1:60:A:ILE:HD12	1:42:A:MET:HE3	11	0.2
(2,553)	1:16:A:ILE:HG23	1:16:A:ILE:H	15	0.2
(2,530)	1:49:A:ILE:HD11	1:124:A:PHE:HZ	7	0.2
(2,529)	1:176:A:VAL:HG22	1:97:A:ALA:HB3	3	0.2
(2,512)	1:170:A:LEU:HD21	1:170:A:LEU:HG	6	0.2
(2,512)	1:170:A:LEU:HD23	1:170:A:LEU:HG	11	0.2
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	13	0.2
(2,477)	1:59:A:ILE:HG21	1:60:A:ILE:HD12	6	0.2
(2,468)	1:178:A:LEU:HD23	1:175:A:GLU:HA	10	0.2
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	7	0.2
(2,387)	1:31:A:LEU:HD22	1:67:A:ILE:HD12	5	0.2
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	8	0.2
(2,383)	1:31:A:LEU:HD21	1:31:A:LEU:HA	14	0.2
(2,383)	1:31:A:LEU:HD22	1:31:A:LEU:HA	15	0.2
(2,369)	1:138:A:ILE:HD12	1:60:A:ILE:HG22	5	0.2
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG22	11	0.2
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD13	10	0.2
(2,332)	1:42:A:MET:HE3	1:60:A:ILE:HG13	2	0.2
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	9	0.2
(2,332)	1:42:A:MET:HE3	1:60:A:ILE:HG13	11	0.2
(2,312)	1:3:A:LEU:HD22	1:3:A:LEU:HA	3	0.2
(2,195)	1:41:A:GLU:HG2	1:40:A:TRP:HE3	9	0.2
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD12	6	0.2
(2,171)	1:74:A:ILE:HG21	1:78:A:GLU:HG3	3	0.2
(2,157)	1:80:A:GLU:HG2	1:21:A:LEU:HD22	7	0.2
(2,134)	1:18:A:ALA:HB2	1:22:A:GLN:HB2	13	0.2
(2,134)	1:18:A:ALA:HB2	1:22:A:GLN:HB2	14	0.2
(2,61)	1:155:A:LEU:HD21	1:21:A:LEU:H	2	0.2
(2,46)	1:141:A:TYR:HE2	1:134:A:LEU:HD22	4	0.2
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	7	0.2
(2,36)	1:39:A:LEU:HD11	1:65:A:GLN:HG2	5	0.2
(2,19)	1:79:A:LEU:HD13	1:92:A:CYS:HG	12	0.2
(2,17)	1:39:A:LEU:HD22	1:42:A:MET:HG2	9	0.2
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	15	0.2
(1,3)	1:15:A:PHE:O	1:19:A:GLU:H	11	0.2
(2,4841)	1:171:A:LYS:HG2	1:170:A:LEU:H	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	13	0.19
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	1	0.19
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	11	0.19
(2,4800)	1:164:A:GLU:HG2	1:164:A:GLU:H	5	0.19
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	8	0.19
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	8	0.19
(2,4756)	1:32:A:HIS:HD2	1:35:A:LEU:H	4	0.19
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	14	0.19
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	6	0.19
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	12	0.19
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	6	0.19
(2,4715)	1:7:A:GLU:H	1:6:A:PRO:HD2	1	0.19
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	11	0.19
(2,4688)	1:18:A:ALA:H	1:19:A:GLU:HG2	15	0.19
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD21	1	0.19
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD21	4	0.19
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	2	0.19
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	4	0.19
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	13	0.19
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	11	0.19
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	5	0.19
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	10	0.19
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	4	0.19
(2,4601)	1:186:A:ASP:HB3	1:186:A:ASP:H	8	0.19
(2,4595)	1:152:A:TYR:H	1:154:A:LEU:HB2	2	0.19
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	1	0.19
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD23	9	0.19
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD11	5	0.19
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD12	7	0.19
(2,4529)	1:60:A:ILE:HG23	1:113:A:SER:HB2	6	0.19
(2,4521)	1:54:A:LEU:HD12	1:52:A:GLY:HA2	4	0.19
(2,4504)	1:190:A:VAL:HG23	1:190:A:VAL:HB	5	0.19
(2,4504)	1:190:A:VAL:HG23	1:190:A:VAL:HB	9	0.19
(2,4504)	1:190:A:VAL:HG22	1:190:A:VAL:HB	12	0.19
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	6	0.19
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD3	9	0.19
(2,4430)	1:11:A:ARG:HG2	1:11:A:ARG:HD2	2	0.19
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	9	0.19
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	11	0.19
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG23	13	0.19
(2,4385)	1:48:A:GLU:HB3	1:48:A:GLU:H	9	0.19
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	4	0.19
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	5	0.19
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	6	0.19
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	8	0.19
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	10	0.19
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	13	0.19
(2,4375)	1:6:A:PRO:HB3	1:6:A:PRO:HG3	14	0.19
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG11	12	0.19
(2,4353)	1:146:A:VAL:HG23	1:145:A:PRO:HG2	2	0.19
(2,4332)	1:31:A:LEU:HD21	1:32:A:HIS:H	5	0.19
(2,4329)	1:156:A:LEU:HD22	1:175:A:GLU:HG3	15	0.19
(2,4325)	1:188:A:MET:HE2	1:108:A:LYS:HE3	5	0.19
(2,4294)	1:164:A:GLU:HB2	1:164:A:GLU:HG2	2	0.19
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	8	0.19
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	14	0.19
(2,4267)	1:134:A:LEU:HD12	1:130:A:GLN:H	5	0.19
(2,4258)	1:95:A:THR:HG21	1:75:A:PHE:HD1	12	0.19
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	6	0.19
(2,4229)	1:28:A:VAL:HG12	1:73:A:ASN:H	14	0.19
(2,4200)	1:22:A:GLN:HE21	1:18:A:ALA:HB3	8	0.19
(2,4200)	1:22:A:GLN:HE21	1:18:A:ALA:HB3	15	0.19
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	6	0.19
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	3	0.19
(2,4197)	1:16:A:ILE:HG23	1:158:A:GLU:H	7	0.19
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	10	0.19
(2,4116)	1:79:A:LEU:HD12	1:78:A:GLU:H	7	0.19
(2,4116)	1:79:A:LEU:HD11	1:78:A:GLU:H	14	0.19
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	11	0.19
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	5	0.19
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD12	10	0.19
(2,4068)	1:26:A:ALA:HB1	1:24:A:GLU:H	7	0.19
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	2	0.19
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	12	0.19
(2,4049)	1:9:A:PRO:HG3	1:8:A:PHE:H	15	0.19
(2,4047)	1:156:A:LEU:HD13	1:159:A:LEU:H	1	0.19
(2,4047)	1:156:A:LEU:HD12	1:159:A:LEU:H	15	0.19
(2,4030)	1:118:A:LEU:HD22	1:118:A:LEU:H	5	0.19
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD2	2	0.19
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD2	10	0.19
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	10	0.19
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	13	0.19
(2,4003)	1:20:A:LEU:H	1:23:A:THR:HG22	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3998)	1:49:A:ILE:HD13	1:54:A:LEU:H	6	0.19
(2,3992)	1:35:A:LEU:HD23	1:65:A:GLN:H	7	0.19
(2,3992)	1:35:A:LEU:HD21	1:65:A:GLN:H	15	0.19
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG21	10	0.19
(2,3982)	1:53:A:ILE:HD12	1:121:A:ALA:H	10	0.19
(2,3978)	1:23:A:THR:HG21	1:22:A:GLN:H	5	0.19
(2,3978)	1:23:A:THR:HG21	1:22:A:GLN:H	6	0.19
(2,3978)	1:23:A:THR:HG21	1:22:A:GLN:H	12	0.19
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	10	0.19
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	8	0.19
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD13	15	0.19
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG22	5	0.19
(2,3942)	1:102:A:MET:HE2	1:102:A:MET:H	5	0.19
(2,3934)	1:42:A:MET:HE1	1:60:A:ILE:H	9	0.19
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG22	9	0.19
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG21	14	0.19
(2,3875)	1:39:A:LEU:HD23	1:43:A:THR:H	7	0.19
(2,3866)	1:35:A:LEU:HD23	1:65:A:GLN:HE21	10	0.19
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	14	0.19
(2,3844)	1:184:A:ALA:HB1	1:185:A:ASN:H	4	0.19
(2,3844)	1:184:A:ALA:HB1	1:185:A:ASN:H	7	0.19
(2,3844)	1:184:A:ALA:HB1	1:185:A:ASN:H	11	0.19
(2,3844)	1:184:A:ALA:HB2	1:185:A:ASN:H	15	0.19
(2,3837)	1:182:A:LYS:HD2	1:182:A:LYS:H	10	0.19
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD22	2	0.19
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD21	7	0.19
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG23	12	0.19
(2,3713)	1:76:A:LEU:HD13	1:77:A:LYS:H	6	0.19
(2,3713)	1:76:A:LEU:HD12	1:77:A:LYS:H	9	0.19
(2,3691)	1:64:A:ILE:HG22	1:65:A:GLN:H	3	0.19
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	10	0.19
(2,3691)	1:64:A:ILE:HG21	1:65:A:GLN:H	14	0.19
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	15	0.19
(2,3682)	1:54:A:LEU:HD22	1:55:A:ASN:HD21	5	0.19
(2,3680)	1:53:A:ILE:HG13	1:53:A:ILE:H	3	0.19
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD22	1	0.19
(2,3652)	1:161:A:THR:HG22	1:162:A:CYS:H	13	0.19
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	4	0.19
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	5	0.19
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	8	0.19
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	14	0.19
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3585)	1:100:A:PHE:HD1	1:97:A:ALA:HB1	4	0.19
(2,3563)	1:40:A:TRP:HD1	1:44:A:SER:HB2	15	0.19
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD13	5	0.19
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD12	15	0.19
(2,3376)	1:153:A:GLN:HE22	1:149:A:VAL:HG23	12	0.19
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD21	1	0.19
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD21	3	0.19
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD23	8	0.19
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG21	9	0.19
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG23	15	0.19
(2,3320)	1:143:A:ILE:HG21	1:142:A:LEU:H	8	0.19
(2,3100)	1:40:A:TRP:H	1:41:A:GLU:HB2	14	0.19
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD13	10	0.19
(2,3011)	1:12:A:LYS:HA	1:12:A:LYS:H	3	0.19
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	11	0.19
(2,2927)	1:156:A:LEU:HD23	1:173:A:GLY:H	8	0.19
(2,2927)	1:156:A:LEU:HD21	1:173:A:GLY:H	14	0.19
(2,2881)	1:158:A:GLU:H	1:156:A:LEU:HD22	13	0.19
(2,2721)	1:10:A:GLY:HA3	1:11:A:ARG:H	7	0.19
(2,2577)	1:89:A:VAL:HG12	1:92:A:CYS:H	12	0.19
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG13	13	0.19
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	4	0.19
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD12	2	0.19
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	1	0.19
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	15	0.19
(2,2287)	1:22:A:GLN:H	1:20:A:LEU:HB2	4	0.19
(2,2274)	1:189:A:HIS:H	1:188:A:MET:HB3	4	0.19
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	8	0.19
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	3	0.19
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG22	2	0.19
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD11	15	0.19
(2,1991)	1:35:A:LEU:HD22	1:68:A:TYR:H	3	0.19
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG23	10	0.19
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG22	13	0.19
(2,1887)	1:152:A:TYR:H	1:177:A:MET:HG2	9	0.19
(2,1855)	1:131:A:ARG:H	1:128:A:ILE:HG22	8	0.19
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD13	6	0.19
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	12	0.19
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG22	15	0.19
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG12	10	0.19
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG21	8	0.19
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1570)	1:156:A:LEU:HD21	1:178:A:LEU:H	2	0.19
(2,1555)	1:18:A:ALA:HB1	1:22:A:GLN:HB3	3	0.19
(2,1534)	1:53:A:ILE:HG23	1:60:A:ILE:HA	9	0.19
(2,1533)	1:53:A:ILE:HG22	1:117:A:ILE:H	10	0.19
(2,1520)	1:76:A:LEU:HD11	1:29:A:ARG:H	1	0.19
(2,1444)	1:43:A:THR:HG23	1:39:A:LEU:HB2	6	0.19
(2,1402)	1:35:A:LEU:HD12	1:65:A:GLN:HB2	11	0.19
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	8	0.19
(2,1350)	1:35:A:LEU:HD12	1:36:A:GLU:H	10	0.19
(2,1343)	1:17:A:MET:HE1	1:86:A:PRO:HA	5	0.19
(2,1343)	1:17:A:MET:HE2	1:86:A:PRO:HA	13	0.19
(2,1339)	1:47:A:GLU:HA	1:46:A:VAL:HG21	15	0.19
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	1	0.19
(2,1318)	1:177:A:MET:HE3	1:173:A:GLY:H	7	0.19
(2,1318)	1:177:A:MET:HE3	1:173:A:GLY:H	10	0.19
(2,1309)	1:134:A:LEU:HD21	1:132:A:HIS:HD2	8	0.19
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG23	8	0.19
(2,1255)	1:17:A:MET:HE3	1:82:A:TYR:HE2	13	0.19
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD13	10	0.19
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD12	11	0.19
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	9	0.19
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG21	5	0.19
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG23	7	0.19
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	4	0.19
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	10	0.19
(2,1152)	1:104:A:VAL:HG13	1:101:A:GLN:HA	5	0.19
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	2	0.19
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	4	0.19
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	9	0.19
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	10	0.19
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD13	11	0.19
(2,977)	1:104:A:VAL:HG13	1:104:A:VAL:HA	15	0.19
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	9	0.19
(2,868)	1:18:A:ALA:HB1	1:22:A:GLN:HG3	4	0.19
(2,859)	1:130:A:GLN:HG2	1:131:A:ARG:H	6	0.19
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD23	8	0.19
(2,761)	1:37:A:THR:HG21	1:36:A:GLU:HG2	11	0.19
(2,729)	1:97:A:ALA:HB2	1:100:A:PHE:HE1	7	0.19
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD22	6	0.19
(2,722)	1:118:A:LEU:HB2	1:118:A:LEU:HD22	8	0.19
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD23	1	0.19
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,677)	1:146:A:VAL:HG12	1:146:A:VAL:HB	5	0.19
(2,677)	1:146:A:VAL:HG12	1:146:A:VAL:HB	6	0.19
(2,677)	1:146:A:VAL:HG11	1:146:A:VAL:HB	8	0.19
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	11	0.19
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	12	0.19
(2,677)	1:146:A:VAL:HG11	1:146:A:VAL:HB	13	0.19
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	14	0.19
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	12	0.19
(2,642)	1:150:A:THR:HG21	1:154:A:LEU:HG	7	0.19
(2,638)	1:150:A:THR:HG22	1:153:A:GLN:HE21	9	0.19
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD22	15	0.19
(2,622)	1:43:A:THR:HG22	1:42:A:MET:HG3	11	0.19
(2,619)	1:40:A:TRP:HD1	1:43:A:THR:HG21	15	0.19
(2,609)	1:28:A:VAL:HG11	1:29:A:ARG:H	15	0.19
(2,602)	1:28:A:VAL:HG23	1:28:A:VAL:HB	3	0.19
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	8	0.19
(2,601)	1:28:A:VAL:HG23	1:71:A:HIS:HB2	10	0.19
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	6	0.19
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	8	0.19
(2,592)	1:64:A:ILE:HD13	1:31:A:LEU:HD23	1	0.19
(2,553)	1:16:A:ILE:HG22	1:16:A:ILE:H	8	0.19
(2,529)	1:176:A:VAL:HG23	1:97:A:ALA:HB2	9	0.19
(2,529)	1:176:A:VAL:HG21	1:97:A:ALA:HB1	10	0.19
(2,512)	1:170:A:LEU:HD22	1:170:A:LEU:HG	1	0.19
(2,505)	1:174:A:LEU:HD23	1:157:A:LYS:HE3	3	0.19
(2,475)	1:59:A:ILE:HG22	1:116:A:LEU:HB3	8	0.19
(2,444)	1:31:A:LEU:HD11	1:30:A:ASP:HB2	12	0.19
(2,392)	1:39:A:LEU:HD23	1:42:A:MET:HB2	3	0.19
(2,392)	1:39:A:LEU:HD21	1:42:A:MET:HB2	13	0.19
(2,383)	1:31:A:LEU:HD23	1:31:A:LEU:HA	6	0.19
(2,383)	1:31:A:LEU:HD23	1:31:A:LEU:HA	13	0.19
(2,379)	1:142:A:LEU:HD21	1:138:A:ILE:HD12	5	0.19
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	1	0.19
(2,364)	1:156:A:LEU:HD21	1:156:A:LEU:HG	4	0.19
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	8	0.19
(2,364)	1:156:A:LEU:HD21	1:156:A:LEU:HG	9	0.19
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	12	0.19
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	8	0.19
(2,338)	1:102:A:MET:HE3	1:70:A:PHE:HB3	7	0.19
(2,301)	1:186:A:ASP:HA	1:185:A:ASN:HB2	3	0.19
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG22	15	0.19
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG12	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG12	11	0.19
(2,199)	1:134:A:LEU:HD22	1:37:A:THR:HB	14	0.19
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	8	0.19
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG11	1	0.19
(2,134)	1:18:A:ALA:HB2	1:22:A:GLN:HB2	15	0.19
(2,133)	1:23:A:THR:HG22	1:22:A:GLN:HB2	14	0.19
(2,112)	1:177:A:MET:HE2	1:100:A:PHE:HE2	6	0.19
(2,108)	1:64:A:ILE:HG22	1:67:A:ILE:HB	6	0.19
(2,39)	1:31:A:LEU:HD13	1:34:A:CYS:H	10	0.19
(2,39)	1:31:A:LEU:HD11	1:34:A:CYS:H	14	0.19
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	1	0.19
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	13	0.19
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	8	0.18
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	9	0.18
(2,4800)	1:164:A:GLU:HG3	1:164:A:GLU:H	4	0.18
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	15	0.18
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	2	0.18
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	9	0.18
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG22	13	0.18
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	4	0.18
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	3	0.18
(2,4658)	1:87:A:GLU:HG3	1:88:A:ASP:H	14	0.18
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	14	0.18
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	15	0.18
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE3	7	0.18
(2,4599)	1:173:A:GLY:H	1:94:A:VAL:HB	1	0.18
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG22	15	0.18
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	5	0.18
(2,4586)	1:93:A:PHE:H	1:176:A:VAL:HG13	6	0.18
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD23	11	0.18
(2,4577)	1:64:A:ILE:H	1:66:A:GLU:HB3	2	0.18
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	5	0.18
(2,4561)	1:23:A:THR:HG23	1:16:A:ILE:HA	7	0.18
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	10	0.18
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD12	4	0.18
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD13	12	0.18
(2,4492)	1:79:A:LEU:HD21	1:25:A:LYS:HG3	5	0.18
(2,4486)	1:104:A:VAL:HG12	1:108:A:LYS:HD2	4	0.18
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD12	7	0.18
(2,4457)	1:164:A:GLU:HG2	1:164:A:GLU:HA	7	0.18
(2,4435)	1:94:A:VAL:HG22	1:94:A:VAL:HA	1	0.18
(2,4435)	1:176:A:VAL:HA	1:176:A:VAL:HG23	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4435)	1:94:A:VAL:HG21	1:94:A:VAL:HA	15	0.18
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	1	0.18
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG21	4	0.18
(2,4419)	1:103:A:TYR:HB2	1:104:A:VAL:HG13	5	0.18
(2,4393)	1:130:A:GLN:HB2	1:131:A:ARG:HG2	12	0.18
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD21	3	0.18
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	1	0.18
(2,4382)	1:85:A:LEU:HB3	1:82:A:TYR:HE1	13	0.18
(2,4353)	1:146:A:VAL:HG22	1:145:A:PRO:HG2	1	0.18
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	4	0.18
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	11	0.18
(2,4214)	1:156:A:LEU:HD13	1:173:A:GLY:H	4	0.18
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	15	0.18
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	2	0.18
(2,4143)	1:101:A:GLN:HA	1:104:A:VAL:H	2	0.18
(2,4116)	1:79:A:LEU:HD11	1:78:A:GLU:H	6	0.18
(2,4112)	1:76:A:LEU:HD21	1:25:A:LYS:H	14	0.18
(2,4110)	1:64:A:ILE:HG21	1:62:A:GLY:H	4	0.18
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD13	12	0.18
(2,4068)	1:26:A:ALA:HB3	1:24:A:GLU:H	2	0.18
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD21	10	0.18
(2,4057)	1:163:A:CYS:HB2	1:163:A:CYS:H	1	0.18
(2,4056)	1:163:A:CYS:H	1:163:A:CYS:HB3	1	0.18
(2,4056)	1:163:A:CYS:H	1:163:A:CYS:HB3	10	0.18
(2,4046)	1:159:A:LEU:HD21	1:159:A:LEU:H	15	0.18
(2,4038)	1:29:A:ARG:HG2	1:29:A:ARG:H	13	0.18
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	1	0.18
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	13	0.18
(2,4022)	1:143:A:ILE:HD11	1:147:A:GLN:HE22	4	0.18
(2,4022)	1:143:A:ILE:HD11	1:147:A:GLN:HE22	5	0.18
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	15	0.18
(2,4015)	1:39:A:LEU:HD21	1:61:A:PHE:H	1	0.18
(2,4015)	1:39:A:LEU:HD22	1:61:A:PHE:H	8	0.18
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	8	0.18
(2,3998)	1:49:A:ILE:HD12	1:54:A:LEU:H	4	0.18
(2,3988)	1:21:A:LEU:HD11	1:83:A:GLU:H	2	0.18
(2,3986)	1:47:A:GLU:H	1:46:A:VAL:HG21	1	0.18
(2,3983)	1:177:A:MET:HB2	1:178:A:LEU:H	1	0.18
(2,3983)	1:177:A:MET:HB2	1:178:A:LEU:H	14	0.18
(2,3979)	1:18:A:ALA:HB1	1:22:A:GLN:H	7	0.18
(2,3978)	1:23:A:THR:HG21	1:22:A:GLN:H	1	0.18
(2,3974)	1:161:A:THR:HG21	1:160:A:LEU:H	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3969)	1:184:A:ALA:HB2	1:108:A:LYS:H	9	0.18
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	7	0.18
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	11	0.18
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	13	0.18
(2,3924)	1:185:A:ASN:H	1:104:A:VAL:HG23	8	0.18
(2,3915)	1:121:A:ALA:HB2	1:119:A:GLU:H	9	0.18
(2,3910)	1:156:A:LEU:HD23	1:153:A:GLN:H	1	0.18
(2,3905)	1:28:A:VAL:HG12	1:72:A:ASN:H	3	0.18
(2,3871)	1:62:A:GLY:H	1:60:A:ILE:HG21	8	0.18
(2,3866)	1:35:A:LEU:HD21	1:65:A:GLN:HE21	3	0.18
(2,3808)	1:143:A:ILE:HG21	1:144:A:LYS:H	9	0.18
(2,3796)	1:135:A:ALA:HB3	1:136:A:ASN:HD22	6	0.18
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD21	4	0.18
(2,3792)	1:135:A:ALA:H	1:134:A:LEU:HD23	6	0.18
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	14	0.18
(2,3682)	1:54:A:LEU:HD21	1:55:A:ASN:HD21	12	0.18
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD23	3	0.18
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD23	5	0.18
(2,3657)	1:33:A:GLU:HB3	1:33:A:GLU:H	3	0.18
(2,3654)	1:31:A:LEU:HD21	1:31:A:LEU:H	2	0.18
(2,3647)	1:26:A:ALA:HB2	1:26:A:ALA:H	7	0.18
(2,3640)	1:18:A:ALA:HB1	1:19:A:GLU:H	10	0.18
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	5	0.18
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	7	0.18
(2,3585)	1:100:A:PHE:HD1	1:97:A:ALA:HB3	2	0.18
(2,3581)	1:96:A:TRP:HH2	1:74:A:ILE:HD11	8	0.18
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD12	10	0.18
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	10	0.18
(2,3555)	1:96:A:TRP:HD1	1:95:A:THR:HG21	2	0.18
(2,3513)	1:125:A:PHE:HZ	1:60:A:ILE:HD11	9	0.18
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG22	11	0.18
(2,3481)	1:100:A:PHE:HD2	1:176:A:VAL:HG22	14	0.18
(2,3455)	1:71:A:HIS:HE1	1:28:A:VAL:HG13	11	0.18
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD22	2	0.18
(2,3344)	1:170:A:LEU:HD12	1:171:A:LYS:H	9	0.18
(2,3326)	1:46:A:VAL:HB	1:46:A:VAL:H	15	0.18
(2,3233)	1:166:A:GLY:H	1:165:A:GLU:HB3	5	0.18
(2,3223)	1:117:A:ILE:HD13	1:139:A:SER:H	6	0.18
(2,3200)	1:5:A:SER:H	1:6:A:PRO:HA	2	0.18
(2,3100)	1:40:A:TRP:H	1:41:A:GLU:HB2	13	0.18
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD11	1	0.18
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD11	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD12	8	0.18
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD11	12	0.18
(2,3052)	1:28:A:VAL:H	1:76:A:LEU:HD12	15	0.18
(2,3011)	1:12:A:LYS:HA	1:12:A:LYS:H	6	0.18
(2,2870)	1:156:A:LEU:H	1:155:A:LEU:HG	13	0.18
(2,2866)	1:155:A:LEU:H	1:155:A:LEU:HD22	5	0.18
(2,2675)	1:117:A:ILE:HD12	1:113:A:SER:H	7	0.18
(2,2630)	1:150:A:THR:HG23	1:154:A:LEU:H	14	0.18
(2,2585)	1:94:A:VAL:HG13	1:95:A:THR:H	3	0.18
(2,2585)	1:94:A:VAL:HG13	1:95:A:THR:H	4	0.18
(2,2585)	1:94:A:VAL:HG11	1:95:A:THR:H	10	0.18
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	12	0.18
(2,2536)	1:87:A:GLU:H	1:89:A:VAL:H	12	0.18
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	14	0.18
(2,2273)	1:189:A:HIS:H	1:189:A:HIS:HB2	4	0.18
(2,2230)	1:124:A:PHE:H	1:122:A:GLY:HA2	8	0.18
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	12	0.18
(2,2004)	1:162:A:CYS:H	1:163:A:CYS:HA	6	0.18
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB2	13	0.18
(2,1994)	1:67:A:ILE:HG22	1:71:A:HIS:H	10	0.18
(2,1991)	1:35:A:LEU:HD22	1:68:A:TYR:H	15	0.18
(2,1939)	1:20:A:LEU:H	1:16:A:ILE:HA	1	0.18
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	12	0.18
(2,1909)	1:177:A:MET:H	1:153:A:GLN:HG2	15	0.18
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG21	1	0.18
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD11	6	0.18
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	4	0.18
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	8	0.18
(2,1828)	1:131:A:ARG:HE	1:47:A:GLU:HG3	13	0.18
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG22	11	0.18
(2,1744)	1:76:A:LEU:HD23	1:77:A:LYS:H	5	0.18
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG21	5	0.18
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	11	0.18
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	2	0.18
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	15	0.18
(2,1590)	1:18:A:ALA:HB2	1:20:A:LEU:HA	5	0.18
(2,1586)	1:154:A:LEU:HD12	1:150:A:THR:HA	6	0.18
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	2	0.18
(2,1510)	1:116:A:LEU:HD21	1:54:A:LEU:H	6	0.18
(2,1510)	1:116:A:LEU:HD21	1:54:A:LEU:H	9	0.18
(2,1500)	1:49:A:ILE:HG21	1:53:A:ILE:HB	15	0.18
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	8	0.18
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	14	0.18
(2,1444)	1:43:A:THR:HG22	1:39:A:LEU:HB2	11	0.18
(2,1444)	1:43:A:THR:HG21	1:39:A:LEU:HB2	14	0.18
(2,1403)	1:80:A:GLU:HA	1:21:A:LEU:HD13	8	0.18
(2,1399)	1:7:A:GLU:HG3	1:8:A:PHE:HD2	7	0.18
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	6	0.18
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	9	0.18
(2,1369)	1:156:A:LEU:HD12	1:170:A:LEU:HB3	15	0.18
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	2	0.18
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	6	0.18
(2,1343)	1:17:A:MET:HE3	1:86:A:PRO:HA	4	0.18
(2,1336)	1:46:A:VAL:HG12	1:46:A:VAL:HA	14	0.18
(2,1331)	1:89:A:VAL:HG22	1:89:A:VAL:HA	12	0.18
(2,1323)	1:147:A:GLN:HG3	1:143:A:ILE:HG21	12	0.18
(2,1318)	1:177:A:MET:HE2	1:173:A:GLY:H	8	0.18
(2,1317)	1:43:A:THR:HG22	1:57:A:GLU:HB3	5	0.18
(2,1282)	1:64:A:ILE:HG23	1:35:A:LEU:H	4	0.18
(2,1282)	1:64:A:ILE:HG21	1:35:A:LEU:H	9	0.18
(2,1245)	1:20:A:LEU:HD11	1:24:A:GLU:H	2	0.18
(2,1237)	1:88:A:ASP:HA	1:85:A:LEU:HB2	12	0.18
(2,1221)	1:17:A:MET:HA	1:20:A:LEU:HD21	15	0.18
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	11	0.18
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	9	0.18
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	4	0.18
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	5	0.18
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	6	0.18
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	12	0.18
(2,1097)	1:78:A:GLU:HA	1:81:A:LYS:HG3	7	0.18
(2,1094)	1:150:A:THR:HG21	1:151:A:LYS:HA	4	0.18
(2,1092)	1:59:A:ILE:HG23	1:59:A:ILE:HA	7	0.18
(2,1092)	1:59:A:ILE:HG22	1:59:A:ILE:HA	9	0.18
(2,1092)	1:59:A:ILE:HG21	1:59:A:ILE:HA	12	0.18
(2,1028)	1:105:A:THR:HA	1:104:A:VAL:HG21	1	0.18
(2,1028)	1:105:A:THR:HA	1:104:A:VAL:HG23	5	0.18
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	6	0.18
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	7	0.18
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	11	0.18
(2,974)	1:153:A:GLN:HA	1:174:A:LEU:HD23	11	0.18
(2,951)	1:15:A:PHE:HB2	1:18:A:ALA:HB1	1	0.18
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	14	0.18
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG23	10	0.18
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD21	6	0.18
(2,706)	1:18:A:ALA:HB3	1:21:A:LEU:HD12	3	0.18
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	2	0.18
(2,643)	1:105:A:THR:HG22	1:106:A:TYR:HD2	15	0.18
(2,642)	1:150:A:THR:HG21	1:154:A:LEU:HG	6	0.18
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	10	0.18
(2,622)	1:43:A:THR:HG21	1:42:A:MET:HG3	14	0.18
(2,619)	1:40:A:TRP:HD1	1:43:A:THR:HG22	1	0.18
(2,618)	1:43:A:THR:HG21	1:45:A:GLY:H	13	0.18
(2,609)	1:28:A:VAL:HG12	1:29:A:ARG:H	5	0.18
(2,603)	1:28:A:VAL:HG22	1:72:A:ASN:HB3	9	0.18
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	1	0.18
(2,600)	1:28:A:VAL:HG22	1:28:A:VAL:HA	15	0.18
(2,530)	1:49:A:ILE:HD13	1:124:A:PHE:HZ	2	0.18
(2,512)	1:170:A:LEU:HD23	1:170:A:LEU:HG	5	0.18
(2,512)	1:170:A:LEU:HD22	1:170:A:LEU:HG	8	0.18
(2,512)	1:170:A:LEU:HD21	1:170:A:LEU:HG	10	0.18
(2,512)	1:170:A:LEU:HD23	1:170:A:LEU:HG	12	0.18
(2,492)	1:159:A:LEU:HD23	1:160:A:LEU:H	1	0.18
(2,477)	1:59:A:ILE:HG22	1:60:A:ILE:HD12	15	0.18
(2,473)	1:59:A:ILE:HG21	1:112:A:ASP:HB2	12	0.18
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG23	2	0.18
(2,423)	1:42:A:MET:HE3	1:49:A:ILE:HG23	8	0.18
(2,422)	1:49:A:ILE:HG21	1:124:A:PHE:HB3	7	0.18
(2,401)	1:35:A:LEU:HD23	1:31:A:LEU:HB3	2	0.18
(2,392)	1:39:A:LEU:HD21	1:42:A:MET:HB2	2	0.18
(2,392)	1:39:A:LEU:HD23	1:42:A:MET:HB2	7	0.18
(2,392)	1:39:A:LEU:HD21	1:42:A:MET:HB2	11	0.18
(2,392)	1:39:A:LEU:HD23	1:42:A:MET:HB2	12	0.18
(2,392)	1:39:A:LEU:HD22	1:42:A:MET:HB2	14	0.18
(2,389)	1:39:A:LEU:HD21	1:41:A:GLU:H	2	0.18
(2,386)	1:31:A:LEU:HD23	1:31:A:LEU:HG	2	0.18
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG21	2	0.18
(2,369)	1:138:A:ILE:HD12	1:60:A:ILE:HG23	15	0.18
(2,364)	1:156:A:LEU:HD21	1:156:A:LEU:HG	2	0.18
(2,364)	1:156:A:LEU:HD21	1:156:A:LEU:HG	14	0.18
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	7	0.18
(2,332)	1:42:A:MET:HE2	1:60:A:ILE:HG13	14	0.18
(2,329)	1:89:A:VAL:HG11	1:17:A:MET:HE2	5	0.18
(2,312)	1:3:A:LEU:HD22	1:3:A:LEU:HA	11	0.18
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG22	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,183)	1:92:A:CYS:HB3	1:79:A:LEU:HD12	1	0.18
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	3	0.18
(2,171)	1:74:A:ILE:HG21	1:78:A:GLU:HG3	8	0.18
(2,170)	1:37:A:THR:HG23	1:33:A:GLU:HG3	14	0.18
(2,168)	1:33:A:GLU:HG3	1:37:A:THR:H	12	0.18
(2,133)	1:23:A:THR:HG23	1:22:A:GLN:HB2	9	0.18
(2,133)	1:23:A:THR:HG21	1:22:A:GLN:HB2	12	0.18
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	4	0.18
(2,92)	1:116:A:LEU:HD11	1:115:A:GLN:HB2	9	0.18
(2,86)	1:67:A:ILE:HG23	1:106:A:TYR:HD2	2	0.18
(2,82)	1:76:A:LEU:HD12	1:77:A:LYS:HE2	10	0.18
(2,74)	1:54:A:LEU:HD12	1:51:A:PRO:HB2	1	0.18
(2,25)	1:37:A:THR:HG23	1:33:A:GLU:HG2	4	0.18
(2,18)	1:79:A:LEU:HD12	1:92:A:CYS:HB2	1	0.18
(1,20)	1:23:A:THR:O	1:27:A:TYR:N	4	0.18
(2,4812)	1:162:A:CYS:H	1:160:A:LEU:HB2	14	0.17
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	6	0.17
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	4	0.17
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	13	0.17
(2,4803)	1:167:A:LYS:H	1:167:A:LYS:HE2	8	0.17
(2,4800)	1:164:A:GLU:HG2	1:164:A:GLU:H	9	0.17
(2,4781)	1:48:A:GLU:HG2	1:49:A:ILE:H	4	0.17
(2,4778)	1:11:A:ARG:HD3	1:12:A:LYS:H	10	0.17
(2,4772)	1:32:A:HIS:HE1	1:36:A:GLU:HA	4	0.17
(2,4767)	1:8:A:PHE:HD2	1:9:A:PRO:HG3	15	0.17
(2,4756)	1:32:A:HIS:HD2	1:35:A:LEU:H	1	0.17
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	14	0.17
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	12	0.17
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	15	0.17
(2,4659)	1:87:A:GLU:HA	1:88:A:ASP:H	12	0.17
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	9	0.17
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	13	0.17
(2,4629)	1:126:A:ASP:H	1:129:A:GLN:HB3	11	0.17
(2,4624)	1:98:A:ASP:HB2	1:100:A:PHE:H	6	0.17
(2,4617)	1:54:A:LEU:H	1:56:A:LYS:HE2	12	0.17
(2,4601)	1:186:A:ASP:HB3	1:186:A:ASP:H	3	0.17
(2,4601)	1:186:A:ASP:HB3	1:186:A:ASP:H	9	0.17
(2,4597)	1:169:A:GLU:H	1:94:A:VAL:HG23	2	0.17
(2,4587)	1:94:A:VAL:H	1:169:A:GLU:HG2	12	0.17
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD23	13	0.17
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD13	9	0.17
(2,4504)	1:190:A:VAL:HG23	1:190:A:VAL:HB	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4504)	1:190:A:VAL:HG23	1:190:A:VAL:HB	11	0.17
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD11	4	0.17
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD12	14	0.17
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	11	0.17
(2,4435)	1:94:A:VAL:HG23	1:94:A:VAL:HA	12	0.17
(2,4347)	1:76:A:LEU:HD21	1:77:A:LYS:HE3	3	0.17
(2,4332)	1:31:A:LEU:HD21	1:32:A:HIS:H	11	0.17
(2,4331)	1:95:A:THR:HG23	1:92:A:CYS:HG	13	0.17
(2,4329)	1:156:A:LEU:HD23	1:175:A:GLU:HG3	7	0.17
(2,4300)	1:92:A:CYS:HB2	1:75:A:PHE:HE2	9	0.17
(2,4267)	1:134:A:LEU:HD13	1:132:A:HIS:H	4	0.17
(2,4264)	1:16:A:ILE:HD11	1:19:A:GLU:HB3	1	0.17
(2,4264)	1:16:A:ILE:HD12	1:19:A:GLU:HB3	2	0.17
(2,4243)	1:94:A:VAL:HG23	1:92:A:CYS:H	5	0.17
(2,4243)	1:94:A:VAL:HG23	1:92:A:CYS:H	15	0.17
(2,4232)	1:117:A:ILE:HG23	1:116:A:LEU:H	10	0.17
(2,4214)	1:156:A:LEU:HD11	1:173:A:GLY:H	12	0.17
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	3	0.17
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	14	0.17
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD12	9	0.17
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD12	11	0.17
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	15	0.17
(2,4120)	1:7:A:GLU:HG3	1:7:A:GLU:H	4	0.17
(2,4119)	1:7:A:GLU:HG2	1:7:A:GLU:H	4	0.17
(2,4116)	1:79:A:LEU:HD11	1:78:A:GLU:H	3	0.17
(2,4116)	1:79:A:LEU:HD12	1:78:A:GLU:H	12	0.17
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	1	0.17
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	8	0.17
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD23	5	0.17
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD21	12	0.17
(2,4056)	1:163:A:CYS:H	1:163:A:CYS:HB3	7	0.17
(2,4056)	1:163:A:CYS:H	1:163:A:CYS:HB3	14	0.17
(2,4046)	1:159:A:LEU:HD22	1:159:A:LEU:H	13	0.17
(2,4015)	1:39:A:LEU:HD22	1:61:A:PHE:H	5	0.17
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	2	0.17
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	9	0.17
(2,3998)	1:49:A:ILE:HD12	1:54:A:LEU:H	7	0.17
(2,3998)	1:49:A:ILE:HD12	1:54:A:LEU:H	9	0.17
(2,3998)	1:49:A:ILE:HD13	1:54:A:LEU:H	10	0.17
(2,3995)	1:17:A:MET:HE1	1:85:A:LEU:H	12	0.17
(2,3981)	1:53:A:ILE:HG22	1:121:A:ALA:H	1	0.17
(2,3981)	1:53:A:ILE:HG23	1:121:A:ALA:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3979)	1:18:A:ALA:HB3	1:22:A:GLN:H	2	0.17
(2,3978)	1:23:A:THR:HG22	1:22:A:GLN:H	13	0.17
(2,3978)	1:23:A:THR:HG22	1:22:A:GLN:H	14	0.17
(2,3975)	1:7:A:GLU:H	1:8:A:PHE:HA	1	0.17
(2,3974)	1:161:A:THR:HG21	1:160:A:LEU:H	15	0.17
(2,3923)	1:49:A:ILE:HD11	1:42:A:MET:H	3	0.17
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD22	8	0.17
(2,3877)	1:43:A:THR:H	1:49:A:ILE:HD11	9	0.17
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	1	0.17
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	6	0.17
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	8	0.17
(2,3814)	1:155:A:LEU:HB3	1:156:A:LEU:H	13	0.17
(2,3812)	1:154:A:LEU:HB3	1:154:A:LEU:H	13	0.17
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG21	6	0.17
(2,3743)	1:97:A:ALA:HB1	1:97:A:ALA:H	3	0.17
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	6	0.17
(2,3743)	1:97:A:ALA:HB3	1:97:A:ALA:H	9	0.17
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	13	0.17
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	12	0.17
(2,3682)	1:54:A:LEU:HD22	1:55:A:ASN:HD21	3	0.17
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	6	0.17
(2,3640)	1:18:A:ALA:HB1	1:19:A:GLU:H	12	0.17
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	13	0.17
(2,3640)	1:18:A:ALA:HB3	1:19:A:GLU:H	15	0.17
(2,3639)	1:18:A:ALA:HB2	1:18:A:ALA:H	4	0.17
(2,3639)	1:18:A:ALA:HB1	1:18:A:ALA:H	12	0.17
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	8	0.17
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	4	0.17
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	10	0.17
(2,3595)	1:132:A:HIS:HE1	1:37:A:THR:HG21	9	0.17
(2,3557)	1:141:A:TYR:HD2	1:136:A:ASN:HB2	2	0.17
(2,3436)	1:82:A:TYR:HD1	1:85:A:LEU:HD22	3	0.17
(2,3344)	1:170:A:LEU:HD13	1:171:A:LYS:H	4	0.17
(2,3320)	1:143:A:ILE:HG22	1:142:A:LEU:H	15	0.17
(2,3260)	1:161:A:THR:HG23	1:158:A:GLU:H	6	0.17
(2,3012)	1:12:A:LYS:H	1:12:A:LYS:HB2	2	0.17
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	10	0.17
(2,3002)	1:186:A:ASP:H	1:187:A:ALA:HB3	8	0.17
(2,2927)	1:156:A:LEU:HD23	1:173:A:GLY:H	6	0.17
(2,2908)	1:169:A:GLU:H	1:168:A:GLY:HA2	8	0.17
(2,2901)	1:166:A:GLY:HA2	1:167:A:LYS:H	9	0.17
(2,2869)	1:156:A:LEU:H	1:153:A:GLN:HA	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2766)	1:131:A:ARG:HG2	1:131:A:ARG:H	8	0.17
(2,2718)	1:11:A:ARG:H	1:11:A:ARG:HB3	2	0.17
(2,2582)	1:94:A:VAL:H	1:95:A:THR:HG22	14	0.17
(2,2577)	1:89:A:VAL:HG12	1:92:A:CYS:H	2	0.17
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD11	5	0.17
(2,2287)	1:22:A:GLN:H	1:20:A:LEU:HB2	5	0.17
(2,2272)	1:189:A:HIS:H	1:189:A:HIS:HB3	9	0.17
(2,2186)	1:107:A:CYS:H	1:105:A:THR:HG21	8	0.17
(2,2128)	1:163:A:CYS:H	1:163:A:CYS:HA	11	0.17
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	1	0.17
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	7	0.17
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	1	0.17
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	3	0.17
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB2	11	0.17
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	12	0.17
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	4	0.17
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	15	0.17
(2,1897)	1:159:A:LEU:H	1:161:A:THR:HG21	2	0.17
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD12	8	0.17
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	1	0.17
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	9	0.17
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	14	0.17
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	3	0.17
(2,1770)	1:88:A:ASP:H	1:87:A:GLU:HB2	12	0.17
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	2	0.17
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	8	0.17
(2,1630)	1:178:A:LEU:HD23	1:153:A:GLN:H	4	0.17
(2,1629)	1:100:A:PHE:H	1:101:A:GLN:HB3	2	0.17
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	1	0.17
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	6	0.17
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	13	0.17
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG21	4	0.17
(2,1570)	1:156:A:LEU:HD22	1:178:A:LEU:H	1	0.17
(2,1547)	1:95:A:THR:HG22	1:78:A:GLU:HB2	11	0.17
(2,1534)	1:53:A:ILE:HG21	1:60:A:ILE:HA	10	0.17
(2,1534)	1:53:A:ILE:HG23	1:60:A:ILE:HA	12	0.17
(2,1520)	1:76:A:LEU:HD13	1:29:A:ARG:H	10	0.17
(2,1512)	1:142:A:LEU:HD13	1:117:A:ILE:H	3	0.17
(2,1510)	1:116:A:LEU:HD22	1:54:A:LEU:H	2	0.17
(2,1510)	1:116:A:LEU:HD22	1:54:A:LEU:H	3	0.17
(2,1500)	1:49:A:ILE:HG23	1:53:A:ILE:HB	11	0.17
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	9	0.17
(2,1397)	1:188:A:MET:HE2	1:190:A:VAL:HG12	8	0.17
(2,1384)	1:33:A:GLU:HG2	1:141:A:TYR:HE2	15	0.17
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	5	0.17
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	11	0.17
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	13	0.17
(2,1369)	1:156:A:LEU:HD12	1:170:A:LEU:HB3	6	0.17
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	3	0.17
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	8	0.17
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	10	0.17
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	11	0.17
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	14	0.17
(2,1355)	1:131:A:ARG:HG2	1:131:A:ARG:HD3	1	0.17
(2,1349)	1:20:A:LEU:HD13	1:23:A:THR:H	5	0.17
(2,1331)	1:89:A:VAL:HG21	1:89:A:VAL:HA	7	0.17
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG23	7	0.17
(2,1300)	1:117:A:ILE:HG22	1:60:A:ILE:HG21	9	0.17
(2,1288)	1:89:A:VAL:HG12	1:88:A:ASP:H	14	0.17
(2,1255)	1:17:A:MET:HE3	1:82:A:TYR:HE2	3	0.17
(2,1245)	1:20:A:LEU:HD13	1:24:A:GLU:H	9	0.17
(2,1245)	1:20:A:LEU:HD13	1:24:A:GLU:H	14	0.17
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD11	1	0.17
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG21	15	0.17
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	1	0.17
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	12	0.17
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	6	0.17
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	11	0.17
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	13	0.17
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	14	0.17
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG22	5	0.17
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	7	0.17
(2,1092)	1:59:A:ILE:HG21	1:59:A:ILE:HA	8	0.17
(2,1092)	1:59:A:ILE:HG21	1:59:A:ILE:HA	15	0.17
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG21	14	0.17
(2,977)	1:104:A:VAL:HG11	1:104:A:VAL:HA	14	0.17
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	15	0.17
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	4	0.17
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	14	0.17
(2,858)	1:92:A:CYS:HB3	1:89:A:VAL:HG21	12	0.17
(2,851)	1:134:A:LEU:HD23	1:129:A:GLN:HB3	1	0.17
(2,851)	1:134:A:LEU:HD21	1:129:A:GLN:HB3	8	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG22	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG22	5	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG21	7	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG22	9	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG21	11	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG21	12	0.17
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG22	14	0.17
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	4	0.17
(2,788)	1:143:A:ILE:HG23	1:143:A:ILE:HB	15	0.17
(2,704)	1:18:A:ALA:HB2	1:21:A:LEU:HB3	15	0.17
(2,690)	1:184:A:ALA:HB1	1:185:A:ASN:HB3	5	0.17
(2,677)	1:146:A:VAL:HG13	1:146:A:VAL:HB	4	0.17
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	2	0.17
(2,638)	1:150:A:THR:HG22	1:153:A:GLN:HE21	8	0.17
(2,618)	1:43:A:THR:HG22	1:45:A:GLY:H	4	0.17
(2,609)	1:28:A:VAL:HG13	1:29:A:ARG:H	7	0.17
(2,603)	1:28:A:VAL:HG21	1:72:A:ASN:HB3	13	0.17
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	12	0.17
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	1	0.17
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	4	0.17
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	9	0.17
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	11	0.17
(2,512)	1:170:A:LEU:HD21	1:170:A:LEU:HG	4	0.17
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	5	0.17
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG21	10	0.17
(2,475)	1:59:A:ILE:HG22	1:116:A:LEU:HB3	12	0.17
(2,468)	1:178:A:LEU:HD23	1:175:A:GLU:HA	1	0.17
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	2	0.17
(2,422)	1:49:A:ILE:HG23	1:124:A:PHE:HB3	3	0.17
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	2	0.17
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	11	0.17
(2,401)	1:35:A:LEU:HD22	1:31:A:LEU:HB3	15	0.17
(2,392)	1:39:A:LEU:HD22	1:42:A:MET:HB2	1	0.17
(2,392)	1:39:A:LEU:HD23	1:42:A:MET:HB2	8	0.17
(2,379)	1:142:A:LEU:HD23	1:138:A:ILE:HD11	8	0.17
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	5	0.17
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	6	0.17
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	7	0.17
(2,364)	1:156:A:LEU:HD22	1:156:A:LEU:HG	15	0.17
(2,362)	1:156:A:LEU:HD22	1:152:A:TYR:HB2	11	0.17
(2,332)	1:42:A:MET:HE3	1:60:A:ILE:HG13	3	0.17
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	13	0.17
(2,332)	1:42:A:MET:HE3	1:60:A:ILE:HG13	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,325)	1:17:A:MET:HE3	1:83:A:GLU:HA	6	0.17
(2,316)	1:20:A:LEU:HD12	1:152:A:TYR:HB3	7	0.17
(2,316)	1:20:A:LEU:HD11	1:152:A:TYR:HB3	15	0.17
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD13	2	0.17
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD12	4	0.17
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD11	7	0.17
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG22	11	0.17
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG23	12	0.17
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG11	1	0.17
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	2	0.17
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	13	0.17
(2,157)	1:80:A:GLU:HG2	1:21:A:LEU:HD23	3	0.17
(2,134)	1:18:A:ALA:HB1	1:22:A:GLN:HB2	3	0.17
(2,73)	1:76:A:LEU:HD22	1:80:A:GLU:H	14	0.17
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	3	0.17
(2,39)	1:31:A:LEU:HD12	1:34:A:CYS:H	9	0.17
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	4	0.17
(1,20)	1:23:A:THR:O	1:27:A:TYR:N	5	0.17
(1,3)	1:15:A:PHE:O	1:19:A:GLU:H	5	0.17
(2,4829)	1:77:A:LYS:HE3	1:78:A:GLU:H	5	0.16
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	10	0.16
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	9	0.16
(2,4808)	1:133:A:GLY:H	1:130:A:GLN:HB3	7	0.16
(2,4800)	1:164:A:GLU:HG3	1:164:A:GLU:H	10	0.16
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	1	0.16
(2,4687)	1:11:A:ARG:HG3	1:12:A:LYS:H	13	0.16
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD22	6	0.16
(2,4654)	1:83:A:GLU:HG2	1:84:A:GLN:HE21	7	0.16
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	8	0.16
(2,4642)	1:62:A:GLY:H	1:64:A:ILE:HB	9	0.16
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	8	0.16
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	5	0.16
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	7	0.16
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	10	0.16
(2,4599)	1:173:A:GLY:H	1:169:A:GLU:HB2	13	0.16
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	14	0.16
(2,4513)	1:5:A:SER:HB3	1:6:A:PRO:HB3	11	0.16
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG13	2	0.16
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG12	7	0.16
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG12	8	0.16
(2,4504)	1:190:A:VAL:HG23	1:190:A:VAL:HB	14	0.16
(2,4504)	1:190:A:VAL:HG22	1:190:A:VAL:HB	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	9	0.16
(2,4457)	1:164:A:GLU:HG2	1:164:A:GLU:HA	12	0.16
(2,4430)	1:11:A:ARG:HG3	1:11:A:ARG:HD2	14	0.16
(2,4422)	1:56:A:LYS:HE2	1:56:A:LYS:HG2	7	0.16
(2,4422)	1:56:A:LYS:HE2	1:56:A:LYS:HG2	15	0.16
(2,4409)	1:172:A:ASP:HB2	1:94:A:VAL:HB	14	0.16
(2,4409)	1:172:A:ASP:HB2	1:94:A:VAL:HB	15	0.16
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD22	8	0.16
(2,4385)	1:48:A:GLU:HB3	1:48:A:GLU:H	11	0.16
(2,4309)	1:182:A:LYS:HE2	1:183:A:LYS:H	14	0.16
(2,4284)	1:171:A:LYS:HG2	1:172:A:ASP:H	1	0.16
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	3	0.16
(2,4267)	1:134:A:LEU:HD12	1:132:A:HIS:H	15	0.16
(2,4264)	1:16:A:ILE:HD11	1:19:A:GLU:HB3	12	0.16
(2,4229)	1:28:A:VAL:HG12	1:73:A:ASN:H	13	0.16
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	10	0.16
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	6	0.16
(2,4073)	1:131:A:ARG:HE	1:131:A:ARG:HG2	14	0.16
(2,4072)	1:131:A:ARG:HE	1:131:A:ARG:HB2	9	0.16
(2,4022)	1:143:A:ILE:HD11	1:147:A:GLN:HE22	11	0.16
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD1	7	0.16
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	3	0.16
(2,3992)	1:35:A:LEU:HD21	1:65:A:GLN:H	1	0.16
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	8	0.16
(2,3974)	1:161:A:THR:HG23	1:160:A:LEU:H	9	0.16
(2,3974)	1:161:A:THR:HG23	1:160:A:LEU:H	12	0.16
(2,3953)	1:183:A:LYS:HB2	1:183:A:LYS:H	15	0.16
(2,3915)	1:121:A:ALA:HB3	1:119:A:GLU:H	11	0.16
(2,3895)	1:143:A:ILE:HD12	1:146:A:VAL:H	10	0.16
(2,3895)	1:143:A:ILE:HD12	1:146:A:VAL:H	13	0.16
(2,3875)	1:39:A:LEU:HD22	1:43:A:THR:H	1	0.16
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	1	0.16
(2,3844)	1:184:A:ALA:HB3	1:185:A:ASN:H	9	0.16
(2,3837)	1:182:A:LYS:HD2	1:182:A:LYS:H	13	0.16
(2,3817)	1:157:A:LYS:H	1:156:A:LEU:HD23	3	0.16
(2,3808)	1:143:A:ILE:HG23	1:144:A:LYS:H	6	0.16
(2,3796)	1:135:A:ALA:HB1	1:136:A:ASN:HD22	3	0.16
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG22	10	0.16
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG21	15	0.16
(2,3728)	1:87:A:GLU:HG3	1:87:A:GLU:H	14	0.16
(2,3710)	1:73:A:ASN:HD21	1:69:A:ASP:HA	7	0.16
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3682)	1:54:A:LEU:HD23	1:55:A:ASN:HD21	8	0.16
(2,3682)	1:54:A:LEU:HD21	1:55:A:ASN:HD21	11	0.16
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD21	2	0.16
(2,3639)	1:18:A:ALA:HB1	1:18:A:ALA:H	1	0.16
(2,3639)	1:18:A:ALA:HB2	1:18:A:ALA:H	11	0.16
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	9	0.16
(2,3584)	1:40:A:TRP:HZ2	1:41:A:GLU:HA	2	0.16
(2,3581)	1:96:A:TRP:HH2	1:74:A:ILE:HD11	11	0.16
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD12	1	0.16
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD11	2	0.16
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD13	14	0.16
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD13	8	0.16
(2,3536)	1:32:A:HIS:HD2	1:32:A:HIS:HA	5	0.16
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD12	3	0.16
(2,3344)	1:170:A:LEU:HD12	1:171:A:LYS:H	3	0.16
(2,3320)	1:143:A:ILE:HG23	1:142:A:LEU:H	2	0.16
(2,3009)	1:10:A:GLY:H	1:8:A:PHE:HB2	12	0.16
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	1	0.16
(2,2922)	1:170:A:LEU:H	1:159:A:LEU:HD13	15	0.16
(2,2882)	1:158:A:GLU:H	1:157:A:LYS:HG3	11	0.16
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD21	6	0.16
(2,2630)	1:150:A:THR:HG21	1:154:A:LEU:H	3	0.16
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	10	0.16
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	11	0.16
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	7	0.16
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	9	0.16
(2,2468)	1:71:A:HIS:HA	1:76:A:LEU:H	2	0.16
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD12	3	0.16
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD13	11	0.16
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD13	13	0.16
(2,2313)	1:54:A:LEU:HD23	1:55:A:ASN:HD22	7	0.16
(2,2264)	1:142:A:LEU:H	1:141:A:TYR:HB3	7	0.16
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	14	0.16
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	14	0.16
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB2	5	0.16
(2,1991)	1:35:A:LEU:HD23	1:68:A:TYR:H	5	0.16
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	7	0.16
(2,1932)	1:10:A:GLY:H	1:11:A:ARG:HB3	2	0.16
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD11	10	0.16
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	2	0.16
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	3	0.16
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	7	0.16
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	10	0.16
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	11	0.16
(2,1861)	1:141:A:TYR:HE2	1:136:A:ASN:H	9	0.16
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD13	8	0.16
(2,1841)	1:158:A:GLU:H	1:158:A:GLU:HB3	5	0.16
(2,1836)	1:63:A:ASN:HD22	1:105:A:THR:HG21	5	0.16
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	11	0.16
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG12	1	0.16
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG11	3	0.16
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG13	9	0.16
(2,1744)	1:76:A:LEU:HD22	1:77:A:LYS:H	2	0.16
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG23	12	0.16
(2,1630)	1:178:A:LEU:HD22	1:153:A:GLN:H	5	0.16
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	6	0.16
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG22	6	0.16
(2,1543)	1:128:A:ILE:HD11	1:132:A:HIS:HD2	3	0.16
(2,1543)	1:128:A:ILE:HD13	1:132:A:HIS:HD2	5	0.16
(2,1533)	1:53:A:ILE:HG21	1:117:A:ILE:H	13	0.16
(2,1526)	1:178:A:LEU:HD21	1:176:A:VAL:H	10	0.16
(2,1512)	1:142:A:LEU:HD12	1:117:A:ILE:H	15	0.16
(2,1510)	1:116:A:LEU:HD23	1:54:A:LEU:H	11	0.16
(2,1500)	1:49:A:ILE:HG23	1:53:A:ILE:HB	1	0.16
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	4	0.16
(2,1444)	1:43:A:THR:HG23	1:39:A:LEU:HB2	10	0.16
(2,1422)	1:116:A:LEU:HD23	1:60:A:ILE:HA	1	0.16
(2,1404)	1:148:A:ARG:HG3	1:148:A:ARG:HD3	11	0.16
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	15	0.16
(2,1384)	1:33:A:GLU:HG2	1:141:A:TYR:HE2	3	0.16
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	3	0.16
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	7	0.16
(2,1371)	1:31:A:LEU:HD11	1:29:A:ARG:H	9	0.16
(2,1371)	1:31:A:LEU:HD12	1:29:A:ARG:H	11	0.16
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	9	0.16
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	13	0.16
(2,1341)	1:140:A:SER:HB3	1:140:A:SER:H	10	0.16
(2,1318)	1:177:A:MET:HE3	1:173:A:GLY:H	3	0.16
(2,1309)	1:134:A:LEU:HD21	1:132:A:HIS:HD2	15	0.16
(2,1279)	1:59:A:ILE:HG23	1:112:A:ASP:HB3	6	0.16
(2,1255)	1:17:A:MET:HE2	1:82:A:TYR:HE2	12	0.16
(2,1254)	1:17:A:MET:HE1	1:82:A:TYR:H	5	0.16
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD11	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG23	3	0.16
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG21	14	0.16
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	2	0.16
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	9	0.16
(2,1152)	1:104:A:VAL:HG13	1:101:A:GLN:HA	9	0.16
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	3	0.16
(2,1144)	1:164:A:GLU:HA	1:163:A:CYS:HB3	7	0.16
(2,1094)	1:150:A:THR:HG21	1:151:A:LYS:HA	7	0.16
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	2	0.16
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	12	0.16
(2,995)	1:117:A:ILE:HG23	1:117:A:ILE:HA	1	0.16
(2,995)	1:117:A:ILE:HG22	1:117:A:ILE:HA	15	0.16
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	3	0.16
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	9	0.16
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	13	0.16
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	10	0.16
(2,868)	1:18:A:ALA:HB3	1:22:A:GLN:HG3	1	0.16
(2,868)	1:18:A:ALA:HB2	1:22:A:GLN:HG3	5	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG22	1	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG21	2	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG21	4	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG23	6	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG22	8	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG23	13	0.16
(2,806)	1:149:A:VAL:HB	1:149:A:VAL:HG21	15	0.16
(2,788)	1:143:A:ILE:HG21	1:143:A:ILE:HB	2	0.16
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD21	4	0.16
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	4	0.16
(2,690)	1:184:A:ALA:HB1	1:185:A:ASN:HB3	7	0.16
(2,652)	1:177:A:MET:HE2	1:179:A:SER:H	14	0.16
(2,642)	1:150:A:THR:HG21	1:154:A:LEU:HG	1	0.16
(2,642)	1:150:A:THR:HG23	1:154:A:LEU:HG	2	0.16
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	15	0.16
(2,622)	1:43:A:THR:HG22	1:42:A:MET:HG3	4	0.16
(2,618)	1:43:A:THR:HG23	1:45:A:GLY:H	7	0.16
(2,616)	1:28:A:VAL:HG13	1:72:A:ASN:HB2	12	0.16
(2,609)	1:28:A:VAL:HG13	1:29:A:ARG:H	3	0.16
(2,602)	1:28:A:VAL:HG22	1:28:A:VAL:HB	6	0.16
(2,601)	1:28:A:VAL:HG23	1:71:A:HIS:HB2	3	0.16
(2,600)	1:28:A:VAL:HG23	1:28:A:VAL:HA	7	0.16
(2,557)	1:60:A:ILE:HD11	1:42:A:MET:HE1	13	0.16
(2,553)	1:16:A:ILE:HG23	1:16:A:ILE:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,475)	1:59:A:ILE:HG21	1:116:A:LEU:HB3	3	0.16
(2,473)	1:59:A:ILE:HG21	1:112:A:ASP:HB2	13	0.16
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	5	0.16
(2,423)	1:42:A:MET:HE1	1:49:A:ILE:HG22	3	0.16
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	1	0.16
(2,403)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	3	0.16
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	4	0.16
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	5	0.16
(2,403)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	6	0.16
(2,403)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	8	0.16
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	14	0.16
(2,403)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	15	0.16
(2,401)	1:35:A:LEU:HD22	1:31:A:LEU:HB3	3	0.16
(2,392)	1:39:A:LEU:HD21	1:42:A:MET:HB2	4	0.16
(2,392)	1:39:A:LEU:HD23	1:42:A:MET:HB2	5	0.16
(2,379)	1:142:A:LEU:HD22	1:138:A:ILE:HD11	6	0.16
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD13	11	0.16
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG22	10	0.16
(2,364)	1:156:A:LEU:HD22	1:156:A:LEU:HG	3	0.16
(2,364)	1:156:A:LEU:HD23	1:156:A:LEU:HG	10	0.16
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	9	0.16
(2,332)	1:42:A:MET:HE3	1:60:A:ILE:HG13	6	0.16
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE2	7	0.16
(2,325)	1:17:A:MET:HE3	1:83:A:GLU:HA	1	0.16
(2,325)	1:17:A:MET:HE1	1:83:A:GLU:HA	12	0.16
(2,312)	1:3:A:LEU:HD23	1:3:A:LEU:HA	8	0.16
(2,242)	1:181:A:PRO:HD3	1:149:A:VAL:HG12	2	0.16
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	14	0.16
(2,199)	1:134:A:LEU:HD22	1:37:A:THR:HB	6	0.16
(2,199)	1:134:A:LEU:HD22	1:37:A:THR:HB	9	0.16
(2,194)	1:153:A:GLN:HG2	1:178:A:LEU:HD21	7	0.16
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	11	0.16
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	12	0.16
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	14	0.16
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG22	12	0.16
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG13	5	0.16
(2,155)	1:181:A:PRO:HG3	1:149:A:VAL:HG13	15	0.16
(2,139)	1:36:A:GLU:HG3	1:32:A:HIS:HE1	7	0.16
(2,61)	1:155:A:LEU:HD21	1:21:A:LEU:H	4	0.16
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	5	0.16
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	9	0.16
(2,39)	1:31:A:LEU:HD12	1:34:A:CYS:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,14)	1:75:A:PHE:HD2	1:79:A:LEU:HD13	9	0.16
(1,123)	1:154:A:LEU:O	1:158:A:GLU:H	4	0.16
(1,3)	1:15:A:PHE:O	1:19:A:GLU:H	12	0.16
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	3	0.16
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	10	0.16
(2,4840)	1:167:A:LYS:HG3	1:166:A:GLY:H	9	0.15
(2,4829)	1:77:A:LYS:HE3	1:78:A:GLU:H	6	0.15
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	14	0.15
(2,4813)	1:188:A:MET:H	1:186:A:ASP:HB3	3	0.15
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	7	0.15
(2,4804)	1:167:A:LYS:HE2	1:168:A:GLY:H	2	0.15
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	5	0.15
(2,4771)	1:124:A:PHE:HE2	1:43:A:THR:H	11	0.15
(2,4756)	1:32:A:HIS:HD2	1:35:A:LEU:H	14	0.15
(2,4755)	1:124:A:PHE:HE1	1:48:A:GLU:HB2	9	0.15
(2,4732)	1:121:A:ALA:H	1:119:A:GLU:HA	4	0.15
(2,4732)	1:121:A:ALA:H	1:119:A:GLU:HA	15	0.15
(2,4678)	1:168:A:GLY:H	1:169:A:GLU:HG2	9	0.15
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	4	0.15
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	6	0.15
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	2	0.15
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	8	0.15
(2,4601)	1:186:A:ASP:HB2	1:186:A:ASP:H	13	0.15
(2,4599)	1:173:A:GLY:H	1:169:A:GLU:HB2	14	0.15
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD23	15	0.15
(2,4581)	1:69:A:ASP:H	1:66:A:GLU:HG3	12	0.15
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	13	0.15
(2,4561)	1:23:A:THR:HG23	1:16:A:ILE:HA	9	0.15
(2,4561)	1:23:A:THR:HG22	1:16:A:ILE:HA	13	0.15
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG13	3	0.15
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG12	6	0.15
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD13	5	0.15
(2,4435)	1:94:A:VAL:HG23	1:94:A:VAL:HA	8	0.15
(2,4428)	1:42:A:MET:HG2	1:128:A:ILE:HD11	10	0.15
(2,4427)	1:8:A:PHE:HB2	1:7:A:GLU:HB2	13	0.15
(2,4385)	1:48:A:GLU:HB2	1:48:A:GLU:H	10	0.15
(2,4378)	1:11:A:ARG:HB2	1:11:A:ARG:HG2	12	0.15
(2,4358)	1:177:A:MET:HE1	1:173:A:GLY:HA3	14	0.15
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG11	13	0.15
(2,4339)	1:134:A:LEU:HD21	1:129:A:GLN:HG3	7	0.15
(2,4329)	1:156:A:LEU:HD21	1:175:A:GLU:HG3	14	0.15
(2,4300)	1:92:A:CYS:HB2	1:75:A:PHE:HE1	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4271)	1:116:A:LEU:HD23	1:56:A:LYS:HE2	10	0.15
(2,4267)	1:134:A:LEU:HD11	1:130:A:GLN:H	9	0.15
(2,4265)	1:142:A:LEU:HD11	1:110:A:LYS:HB2	3	0.15
(2,4264)	1:16:A:ILE:HD13	1:19:A:GLU:HB3	7	0.15
(2,4198)	1:189:A:HIS:HD2	1:189:A:HIS:H	7	0.15
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD11	5	0.15
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD13	6	0.15
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	5	0.15
(2,4116)	1:79:A:LEU:HD12	1:78:A:GLU:H	13	0.15
(2,4110)	1:64:A:ILE:HG21	1:62:A:GLY:H	14	0.15
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	4	0.15
(2,4022)	1:143:A:ILE:HD13	1:147:A:GLN:HE22	2	0.15
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD1	14	0.15
(2,4016)	1:64:A:ILE:HG23	1:61:A:PHE:H	8	0.15
(2,3998)	1:49:A:ILE:HD11	1:54:A:LEU:H	1	0.15
(2,3998)	1:49:A:ILE:HD13	1:54:A:LEU:H	8	0.15
(2,3956)	1:74:A:ILE:HG22	1:78:A:GLU:H	6	0.15
(2,3956)	1:74:A:ILE:HG23	1:78:A:GLU:H	10	0.15
(2,3956)	1:74:A:ILE:HG21	1:78:A:GLU:H	15	0.15
(2,3953)	1:183:A:LYS:HB2	1:183:A:LYS:H	5	0.15
(2,3898)	1:46:A:VAL:HG22	1:46:A:VAL:H	15	0.15
(2,3892)	1:133:A:GLY:H	1:134:A:LEU:HD21	2	0.15
(2,3875)	1:39:A:LEU:HD22	1:43:A:THR:H	9	0.15
(2,3808)	1:143:A:ILE:HG22	1:144:A:LYS:H	12	0.15
(2,3779)	1:121:A:ALA:HB3	1:121:A:ALA:H	12	0.15
(2,3745)	1:97:A:ALA:HB1	1:98:A:ASP:H	3	0.15
(2,3745)	1:97:A:ALA:HB2	1:98:A:ASP:H	10	0.15
(2,3745)	1:97:A:ALA:HB2	1:98:A:ASP:H	13	0.15
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	8	0.15
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	10	0.15
(2,3713)	1:76:A:LEU:HD13	1:77:A:LYS:H	5	0.15
(2,3691)	1:64:A:ILE:HG21	1:65:A:GLN:H	4	0.15
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	8	0.15
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	11	0.15
(2,3671)	1:43:A:THR:HG22	1:43:A:THR:H	4	0.15
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD21	4	0.15
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD21	6	0.15
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD23	8	0.15
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD22	10	0.15
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD21	13	0.15
(2,3657)	1:33:A:GLU:HB3	1:33:A:GLU:H	5	0.15
(2,3640)	1:18:A:ALA:HB2	1:19:A:GLU:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3635)	1:12:A:LYS:HA	1:13:A:LYS:H	7	0.15
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	6	0.15
(2,3581)	1:96:A:TRP:HH2	1:74:A:ILE:HD13	9	0.15
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD12	7	0.15
(2,3580)	1:82:A:TYR:HE1	1:85:A:LEU:HD12	11	0.15
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD11	6	0.15
(2,3391)	1:153:A:GLN:H	1:153:A:GLN:HB3	7	0.15
(2,3379)	1:173:A:GLY:H	1:169:A:GLU:HB3	2	0.15
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD22	10	0.15
(2,3326)	1:46:A:VAL:HB	1:46:A:VAL:H	13	0.15
(2,3257)	1:170:A:LEU:HD21	1:160:A:LEU:H	15	0.15
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	11	0.15
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	6	0.15
(2,3041)	1:22:A:GLN:HG2	1:23:A:THR:H	5	0.15
(2,3006)	1:10:A:GLY:H	1:8:A:PHE:HA	7	0.15
(2,3006)	1:10:A:GLY:H	1:8:A:PHE:HA	10	0.15
(2,2764)	1:162:A:CYS:H	1:163:A:CYS:H	1	0.15
(2,2695)	1:111:A:PRO:HA	1:114:A:ASN:HD22	1	0.15
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD23	9	0.15
(2,2583)	1:94:A:VAL:H	1:177:A:MET:HE2	5	0.15
(2,2583)	1:94:A:VAL:H	1:177:A:MET:HE1	11	0.15
(2,2579)	1:140:A:SER:H	1:143:A:ILE:HG23	3	0.15
(2,2468)	1:71:A:HIS:HA	1:76:A:LEU:H	11	0.15
(2,2313)	1:54:A:LEU:HD22	1:55:A:ASN:HD22	3	0.15
(2,2313)	1:54:A:LEU:HD21	1:55:A:ASN:HD22	13	0.15
(2,2279)	1:153:A:GLN:HE21	1:178:A:LEU:HA	2	0.15
(2,2264)	1:142:A:LEU:H	1:141:A:TYR:HB3	11	0.15
(2,2264)	1:142:A:LEU:H	1:141:A:TYR:HB3	14	0.15
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	7	0.15
(2,2120)	1:153:A:GLN:HG2	1:153:A:GLN:H	10	0.15
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	13	0.15
(2,2069)	1:91:A:HIS:HB3	1:91:A:HIS:H	15	0.15
(2,2027)	1:8:A:PHE:HB2	1:8:A:PHE:H	7	0.15
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	12	0.15
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB1	9	0.15
(2,1994)	1:67:A:ILE:HG21	1:71:A:HIS:H	8	0.15
(2,1994)	1:67:A:ILE:HG21	1:71:A:HIS:H	15	0.15
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG22	10	0.15
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG23	12	0.15
(2,1991)	1:35:A:LEU:HD23	1:68:A:TYR:H	2	0.15
(2,1991)	1:35:A:LEU:HD21	1:68:A:TYR:H	7	0.15
(2,1991)	1:35:A:LEU:HD21	1:68:A:TYR:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1921)	1:184:A:ALA:H	1:104:A:VAL:HA	4	0.15
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD13	2	0.15
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	6	0.15
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	1	0.15
(2,1841)	1:158:A:GLU:H	1:158:A:GLU:HB3	13	0.15
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG23	9	0.15
(2,1783)	1:94:A:VAL:H	1:169:A:GLU:HB3	8	0.15
(2,1783)	1:94:A:VAL:H	1:169:A:GLU:HB3	11	0.15
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	14	0.15
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	1	0.15
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	11	0.15
(2,1592)	1:135:A:ALA:HB1	1:129:A:GLN:HE22	9	0.15
(2,1588)	1:153:A:GLN:HG2	1:174:A:LEU:HB2	3	0.15
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG23	2	0.15
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG21	9	0.15
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG21	15	0.15
(2,1536)	1:60:A:ILE:HD12	1:53:A:ILE:HG23	8	0.15
(2,1525)	1:143:A:ILE:HG21	1:144:A:LYS:HE3	13	0.15
(2,1510)	1:116:A:LEU:HD22	1:54:A:LEU:H	12	0.15
(2,1426)	1:168:A:GLY:HA3	1:170:A:LEU:HD11	7	0.15
(2,1384)	1:33:A:GLU:HG2	1:141:A:TYR:HE2	1	0.15
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	10	0.15
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	14	0.15
(2,1349)	1:20:A:LEU:HD13	1:23:A:THR:H	9	0.15
(2,1349)	1:20:A:LEU:HD11	1:23:A:THR:H	11	0.15
(2,1331)	1:89:A:VAL:HG23	1:89:A:VAL:HA	2	0.15
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	8	0.15
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	9	0.15
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	12	0.15
(2,1300)	1:117:A:ILE:HG23	1:60:A:ILE:HG21	10	0.15
(2,1255)	1:17:A:MET:HE2	1:82:A:TYR:HE2	14	0.15
(2,1254)	1:17:A:MET:HE3	1:82:A:TYR:H	10	0.15
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG22	4	0.15
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG21	10	0.15
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	10	0.15
(2,1203)	1:47:A:GLU:HA	1:47:A:GLU:HG2	11	0.15
(2,1165)	1:161:A:THR:HG23	1:161:A:THR:HA	5	0.15
(2,1152)	1:104:A:VAL:HG13	1:101:A:GLN:HA	3	0.15
(2,1145)	1:164:A:GLU:HB2	1:164:A:GLU:HA	7	0.15
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	15	0.15
(2,1092)	1:59:A:ILE:HG22	1:59:A:ILE:HA	4	0.15
(2,1092)	1:59:A:ILE:HG23	1:59:A:ILE:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1092)	1:59:A:ILE:HG22	1:59:A:ILE:HA	11	0.15
(2,1092)	1:59:A:ILE:HG21	1:59:A:ILE:HA	13	0.15
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	7	0.15
(2,1038)	1:49:A:ILE:HD13	1:54:A:LEU:HA	6	0.15
(2,1038)	1:49:A:ILE:HD13	1:54:A:LEU:HA	10	0.15
(2,1037)	1:143:A:ILE:HG23	1:140:A:SER:HB2	1	0.15
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	6	0.15
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	10	0.15
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	11	0.15
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	12	0.15
(2,977)	1:104:A:VAL:HG11	1:104:A:VAL:HA	10	0.15
(2,977)	1:104:A:VAL:HG13	1:104:A:VAL:HA	12	0.15
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	11	0.15
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	7	0.15
(2,729)	1:97:A:ALA:HB3	1:100:A:PHE:HE1	12	0.15
(2,704)	1:18:A:ALA:HB2	1:21:A:LEU:HB3	6	0.15
(2,704)	1:18:A:ALA:HB2	1:21:A:LEU:HB3	8	0.15
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	5	0.15
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	9	0.15
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	11	0.15
(2,657)	1:104:A:VAL:HG11	1:101:A:GLN:HE22	9	0.15
(2,652)	1:177:A:MET:HE1	1:179:A:SER:H	1	0.15
(2,642)	1:150:A:THR:HG23	1:154:A:LEU:HG	9	0.15
(2,638)	1:150:A:THR:HG23	1:153:A:GLN:HE21	6	0.15
(2,636)	1:176:A:VAL:HG12	1:175:A:GLU:HB2	13	0.15
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD21	5	0.15
(2,592)	1:64:A:ILE:HD11	1:31:A:LEU:HD22	5	0.15
(2,553)	1:16:A:ILE:HG23	1:16:A:ILE:H	5	0.15
(2,553)	1:16:A:ILE:HG23	1:16:A:ILE:H	13	0.15
(2,541)	1:116:A:LEU:HD21	1:116:A:LEU:HB3	9	0.15
(2,541)	1:116:A:LEU:HD23	1:116:A:LEU:HB3	11	0.15
(2,530)	1:49:A:ILE:HD11	1:124:A:PHE:HZ	9	0.15
(2,529)	1:176:A:VAL:HG21	1:97:A:ALA:HB1	6	0.15
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	6	0.15
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	8	0.15
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG21	14	0.15
(2,461)	1:134:A:LEU:HD21	1:33:A:GLU:HG2	13	0.15
(2,422)	1:49:A:ILE:HG22	1:124:A:PHE:HB3	15	0.15
(2,418)	1:53:A:ILE:HD13	1:124:A:PHE:HB3	12	0.15
(2,406)	1:156:A:LEU:HD13	1:93:A:PHE:HZ	11	0.15
(2,403)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	1	0.15
(2,403)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	12	0.15
(2,403)	1:35:A:LEU:HD21	1:35:A:LEU:HB2	13	0.15
(2,401)	1:35:A:LEU:HD23	1:31:A:LEU:HB3	5	0.15
(2,401)	1:35:A:LEU:HD21	1:31:A:LEU:HB3	7	0.15
(2,392)	1:39:A:LEU:HD22	1:42:A:MET:HB2	10	0.15
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	4	0.15
(2,379)	1:142:A:LEU:HD22	1:138:A:ILE:HD11	2	0.15
(2,379)	1:142:A:LEU:HD23	1:138:A:ILE:HD11	13	0.15
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG22	12	0.15
(2,364)	1:156:A:LEU:HD21	1:156:A:LEU:HG	11	0.15
(2,351)	1:188:A:MET:HE2	1:108:A:LYS:HA	15	0.15
(2,337)	1:102:A:MET:HE2	1:66:A:GLU:HA	11	0.15
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD12	9	0.15
(2,332)	1:42:A:MET:HE1	1:60:A:ILE:HG13	5	0.15
(2,328)	1:42:A:MET:HE3	1:60:A:ILE:HB	10	0.15
(2,312)	1:3:A:LEU:HD23	1:3:A:LEU:HA	9	0.15
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG22	1	0.15
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG21	6	0.15
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	6	0.15
(2,206)	1:60:A:ILE:HA	1:113:A:SER:HG	3	0.15
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	7	0.15
(2,133)	1:23:A:THR:HG21	1:22:A:GLN:HB2	1	0.15
(2,133)	1:23:A:THR:HG21	1:22:A:GLN:HB2	6	0.15
(2,124)	1:187:A:ALA:HB2	1:183:A:LYS:HE2	4	0.15
(2,116)	1:177:A:MET:HE2	1:100:A:PHE:HB2	15	0.15
(2,106)	1:43:A:THR:HG23	1:42:A:MET:HG2	12	0.15
(2,106)	1:43:A:THR:HG22	1:42:A:MET:HG2	15	0.15
(2,92)	1:116:A:LEU:HD11	1:115:A:GLN:HB2	7	0.15
(2,92)	1:116:A:LEU:HD11	1:115:A:GLN:HB2	12	0.15
(2,92)	1:116:A:LEU:HD12	1:115:A:GLN:HB2	15	0.15
(2,73)	1:76:A:LEU:HD22	1:80:A:GLU:H	2	0.15
(2,63)	1:174:A:LEU:HD23	1:175:A:GLU:HA	1	0.15
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	1	0.15
(2,57)	1:142:A:LEU:HD12	1:61:A:PHE:HE1	3	0.15
(2,39)	1:31:A:LEU:HD11	1:34:A:CYS:H	7	0.15
(2,36)	1:39:A:LEU:HD12	1:65:A:GLN:HG2	15	0.15
(1,113)	1:149:A:VAL:O	1:153:A:GLN:H	4	0.15
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	9	0.15
(1,12)	1:19:A:GLU:O	1:23:A:THR:N	5	0.15
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	15	0.15
(2,4841)	1:171:A:LYS:HG2	1:170:A:LEU:H	14	0.14
(2,4829)	1:77:A:LYS:HE2	1:78:A:GLU:H	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4824)	1:12:A:LYS:H	1:12:A:LYS:HD2	14	0.14
(2,4813)	1:188:A:MET:H	1:186:A:ASP:HB2	7	0.14
(2,4812)	1:162:A:CYS:H	1:160:A:LEU:HB2	12	0.14
(2,4771)	1:124:A:PHE:HE2	1:43:A:THR:H	2	0.14
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	5	0.14
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	10	0.14
(2,4735)	1:159:A:LEU:H	1:157:A:LYS:H	13	0.14
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	5	0.14
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	7	0.14
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD22	3	0.14
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD23	7	0.14
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD21	13	0.14
(2,4640)	1:57:A:GLU:H	1:42:A:MET:HB3	13	0.14
(2,4624)	1:98:A:ASP:HB2	1:100:A:PHE:H	10	0.14
(2,4603)	1:10:A:GLY:H	1:9:A:PRO:HG2	15	0.14
(2,4599)	1:173:A:GLY:H	1:169:A:GLU:HB2	7	0.14
(2,4599)	1:173:A:GLY:H	1:94:A:VAL:HB	8	0.14
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD21	3	0.14
(2,4579)	1:69:A:ASP:H	1:67:A:ILE:HG12	1	0.14
(2,4579)	1:69:A:ASP:H	1:67:A:ILE:HG12	7	0.14
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	1	0.14
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	8	0.14
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	12	0.14
(2,4561)	1:23:A:THR:HG21	1:16:A:ILE:HA	6	0.14
(2,4553)	1:64:A:ILE:HG23	1:65:A:GLN:HE21	14	0.14
(2,4543)	1:157:A:LYS:HB2	1:156:A:LEU:HD21	5	0.14
(2,4519)	1:59:A:ILE:HG22	1:56:A:LYS:HE2	7	0.14
(2,4457)	1:164:A:GLU:HG2	1:164:A:GLU:HA	9	0.14
(2,4447)	1:179:A:SER:HB3	1:182:A:LYS:HD3	3	0.14
(2,4385)	1:48:A:GLU:HB3	1:48:A:GLU:H	6	0.14
(2,4374)	1:11:A:ARG:HB3	1:11:A:ARG:HG2	14	0.14
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG13	5	0.14
(2,4309)	1:182:A:LYS:HE2	1:183:A:LYS:H	6	0.14
(2,4309)	1:182:A:LYS:HE2	1:183:A:LYS:H	15	0.14
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	6	0.14
(2,4299)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	13	0.14
(2,4284)	1:171:A:LYS:HG3	1:172:A:ASP:H	2	0.14
(2,4277)	1:16:A:ILE:HG22	1:158:A:GLU:HB2	2	0.14
(2,4268)	1:99:A:LYS:HG3	1:101:A:GLN:H	13	0.14
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD12	12	0.14
(2,4258)	1:95:A:THR:HG21	1:75:A:PHE:HD2	4	0.14
(2,4245)	1:167:A:LYS:HB2	1:166:A:GLY:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	8	0.14
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	6	0.14
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD11	4	0.14
(2,4116)	1:79:A:LEU:HD12	1:78:A:GLU:H	5	0.14
(2,4104)	1:45:A:GLY:HA2	1:46:A:VAL:H	8	0.14
(2,4103)	1:41:A:GLU:HA	1:46:A:VAL:H	15	0.14
(2,4091)	1:36:A:GLU:H	1:36:A:GLU:HG3	15	0.14
(2,4079)	1:79:A:LEU:HD22	1:78:A:GLU:H	2	0.14
(2,4057)	1:163:A:CYS:HB2	1:163:A:CYS:H	14	0.14
(2,4050)	1:8:A:PHE:H	1:9:A:PRO:HD3	7	0.14
(2,4031)	1:54:A:LEU:HD23	1:55:A:ASN:H	1	0.14
(2,4030)	1:118:A:LEU:HD21	1:118:A:LEU:H	3	0.14
(2,4017)	1:170:A:LEU:HD11	1:170:A:LEU:H	15	0.14
(2,4015)	1:39:A:LEU:HD21	1:61:A:PHE:H	15	0.14
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	4	0.14
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	6	0.14
(2,3974)	1:161:A:THR:HG21	1:160:A:LEU:H	11	0.14
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD13	6	0.14
(2,3956)	1:74:A:ILE:HG22	1:78:A:GLU:H	14	0.14
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG23	10	0.14
(2,3920)	1:42:A:MET:HE3	1:42:A:MET:H	1	0.14
(2,3920)	1:42:A:MET:HE2	1:42:A:MET:H	10	0.14
(2,3920)	1:42:A:MET:HE3	1:42:A:MET:H	13	0.14
(2,3910)	1:156:A:LEU:HD22	1:153:A:GLN:H	14	0.14
(2,3898)	1:46:A:VAL:HG23	1:46:A:VAL:H	14	0.14
(2,3895)	1:143:A:ILE:HD12	1:146:A:VAL:H	1	0.14
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD13	10	0.14
(2,3887)	1:94:A:VAL:HG21	1:173:A:GLY:H	14	0.14
(2,3853)	1:190:A:VAL:HB	1:190:A:VAL:H	15	0.14
(2,3796)	1:135:A:ALA:HB1	1:136:A:ASN:HD22	8	0.14
(2,3796)	1:135:A:ALA:HB2	1:136:A:ASN:HD22	12	0.14
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG22	14	0.14
(2,3779)	1:121:A:ALA:HB1	1:121:A:ALA:H	4	0.14
(2,3779)	1:121:A:ALA:HB1	1:121:A:ALA:H	5	0.14
(2,3779)	1:121:A:ALA:HB1	1:121:A:ALA:H	6	0.14
(2,3779)	1:121:A:ALA:HB3	1:121:A:ALA:H	7	0.14
(2,3779)	1:121:A:ALA:HB2	1:121:A:ALA:H	10	0.14
(2,3779)	1:121:A:ALA:HB2	1:121:A:ALA:H	14	0.14
(2,3745)	1:97:A:ALA:HB3	1:98:A:ASP:H	9	0.14
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	10	0.14
(2,3714)	1:77:A:LYS:HG3	1:77:A:LYS:H	3	0.14
(2,3682)	1:54:A:LEU:HD23	1:55:A:ASN:HD21	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3671)	1:43:A:THR:HG22	1:43:A:THR:H	5	0.14
(2,3665)	1:40:A:TRP:H	1:39:A:LEU:HD23	12	0.14
(2,3581)	1:96:A:TRP:HH2	1:74:A:ILE:HD11	14	0.14
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	6	0.14
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	8	0.14
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	11	0.14
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	14	0.14
(2,3543)	1:68:A:TYR:HD1	1:28:A:VAL:HG23	14	0.14
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD23	4	0.14
(2,3492)	1:100:A:PHE:HE1	1:71:A:HIS:HE1	1	0.14
(2,3465)	1:68:A:TYR:HE1	1:28:A:VAL:HG23	7	0.14
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	12	0.14
(2,3391)	1:153:A:GLN:H	1:153:A:GLN:HB3	3	0.14
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	6	0.14
(2,3326)	1:46:A:VAL:HB	1:46:A:VAL:H	14	0.14
(2,3223)	1:117:A:ILE:HD11	1:139:A:SER:H	7	0.14
(2,3188)	1:72:A:ASN:H	1:68:A:TYR:H	5	0.14
(2,3058)	1:30:A:ASP:H	1:32:A:HIS:H	7	0.14
(2,3014)	1:16:A:ILE:H	1:14:A:GLU:HB3	3	0.14
(2,2943)	1:138:A:ILE:H	1:137:A:SER:HA	9	0.14
(2,2922)	1:170:A:LEU:H	1:159:A:LEU:HD13	3	0.14
(2,2922)	1:170:A:LEU:H	1:159:A:LEU:HD13	13	0.14
(2,2903)	1:167:A:LYS:HA	1:167:A:LYS:H	8	0.14
(2,2899)	1:165:A:GLU:H	1:164:A:GLU:H	6	0.14
(2,2848)	1:150:A:THR:H	1:153:A:GLN:HG2	4	0.14
(2,2735)	1:127:A:GLU:HG3	1:127:A:GLU:H	7	0.14
(2,2686)	1:114:A:ASN:H	1:112:A:ASP:HB2	3	0.14
(2,2675)	1:117:A:ILE:HD11	1:113:A:SER:H	6	0.14
(2,2577)	1:89:A:VAL:HG11	1:92:A:CYS:H	8	0.14
(2,2577)	1:89:A:VAL:HG11	1:92:A:CYS:H	9	0.14
(2,2560)	1:89:A:VAL:H	1:82:A:TYR:HE2	7	0.14
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG13	6	0.14
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG13	8	0.14
(2,2521)	1:87:A:GLU:H	1:88:A:ASP:HA	12	0.14
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	7	0.14
(2,2484)	1:17:A:MET:H	1:15:A:PHE:HB3	1	0.14
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD12	7	0.14
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD11	1	0.14
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	7	0.14
(2,2313)	1:54:A:LEU:HD21	1:55:A:ASN:HD22	11	0.14
(2,2313)	1:54:A:LEU:HD21	1:55:A:ASN:HD22	12	0.14
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	12	0.14
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	15	0.14
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	8	0.14
(2,2120)	1:153:A:GLN:HG2	1:153:A:GLN:H	14	0.14
(2,2049)	1:72:A:ASN:H	1:73:A:ASN:HD21	7	0.14
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	14	0.14
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB2	2	0.14
(2,1997)	1:104:A:VAL:H	1:184:A:ALA:HB3	15	0.14
(2,1994)	1:67:A:ILE:HG21	1:71:A:HIS:H	11	0.14
(2,1992)	1:70:A:PHE:H	1:74:A:ILE:HD11	6	0.14
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	4	0.14
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	13	0.14
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD12	12	0.14
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	8	0.14
(2,1842)	1:158:A:GLU:H	1:158:A:GLU:HG3	15	0.14
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	2	0.14
(2,1829)	1:131:A:ARG:HE	1:131:A:ARG:HD2	1	0.14
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG21	8	0.14
(2,1805)	1:185:A:ASN:HD21	1:182:A:LYS:HA	10	0.14
(2,1732)	1:69:A:ASP:H	1:72:A:ASN:HB3	12	0.14
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG23	13	0.14
(2,1718)	1:65:A:GLN:H	1:61:A:PHE:HD1	10	0.14
(2,1672)	1:133:A:GLY:H	1:130:A:GLN:HG3	6	0.14
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	1	0.14
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	15	0.14
(2,1647)	1:40:A:TRP:HE1	1:46:A:VAL:HG12	6	0.14
(2,1645)	1:174:A:LEU:H	1:178:A:LEU:HG	1	0.14
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	7	0.14
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	9	0.14
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	12	0.14
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	14	0.14
(2,1594)	1:135:A:ALA:HA	1:129:A:GLN:HE22	13	0.14
(2,1593)	1:135:A:ALA:HB3	1:129:A:GLN:HE21	1	0.14
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG22	1	0.14
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG21	10	0.14
(2,1543)	1:128:A:ILE:HD12	1:132:A:HIS:HD2	2	0.14
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG22	15	0.14
(2,1534)	1:53:A:ILE:HG23	1:60:A:ILE:HA	13	0.14
(2,1512)	1:142:A:LEU:HD12	1:117:A:ILE:H	1	0.14
(2,1500)	1:49:A:ILE:HG23	1:53:A:ILE:HB	2	0.14
(2,1444)	1:43:A:THR:HG23	1:39:A:LEU:HB2	3	0.14
(2,1444)	1:43:A:THR:HG22	1:39:A:LEU:HB2	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1437)	1:97:A:ALA:HB2	1:94:A:VAL:HA	2	0.14
(2,1424)	1:145:A:PRO:HA	1:31:A:LEU:HD11	8	0.14
(2,1422)	1:116:A:LEU:HD23	1:60:A:ILE:HA	12	0.14
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	2	0.14
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	6	0.14
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	10	0.14
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	1	0.14
(2,1369)	1:156:A:LEU:HD13	1:170:A:LEU:HB3	9	0.14
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	15	0.14
(2,1350)	1:35:A:LEU:HD13	1:36:A:GLU:H	8	0.14
(2,1343)	1:17:A:MET:HE2	1:86:A:PRO:HA	3	0.14
(2,1331)	1:89:A:VAL:HG22	1:89:A:VAL:HA	4	0.14
(2,1331)	1:89:A:VAL:HG23	1:89:A:VAL:HA	5	0.14
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB2	13	0.14
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	14	0.14
(2,1318)	1:177:A:MET:HE1	1:173:A:GLY:H	2	0.14
(2,1317)	1:43:A:THR:HG23	1:57:A:GLU:HB3	12	0.14
(2,1255)	1:17:A:MET:HE2	1:82:A:TYR:HE2	2	0.14
(2,1245)	1:20:A:LEU:HD13	1:24:A:GLU:H	7	0.14
(2,1238)	1:145:A:PRO:HA	1:148:A:ARG:HB3	4	0.14
(2,1152)	1:104:A:VAL:HG13	1:101:A:GLN:HA	1	0.14
(2,1152)	1:104:A:VAL:HG11	1:101:A:GLN:HA	12	0.14
(2,1151)	1:43:A:THR:HA	1:39:A:LEU:HD22	9	0.14
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	1	0.14
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	12	0.14
(2,1110)	1:184:A:ALA:HA	1:104:A:VAL:HG23	2	0.14
(2,1094)	1:150:A:THR:HG23	1:151:A:LYS:HA	2	0.14
(2,1092)	1:59:A:ILE:HG22	1:59:A:ILE:HA	1	0.14
(2,1092)	1:59:A:ILE:HG22	1:59:A:ILE:HA	2	0.14
(2,1092)	1:59:A:ILE:HG23	1:59:A:ILE:HA	10	0.14
(2,1092)	1:59:A:ILE:HG23	1:59:A:ILE:HA	14	0.14
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	8	0.14
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	9	0.14
(2,1028)	1:105:A:THR:HA	1:104:A:VAL:HG22	12	0.14
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	2	0.14
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	7	0.14
(2,995)	1:117:A:ILE:HG23	1:117:A:ILE:HA	14	0.14
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	1	0.14
(2,977)	1:104:A:VAL:HG12	1:104:A:VAL:HA	5	0.14
(2,886)	1:153:A:GLN:HB3	1:150:A:THR:HG23	13	0.14
(2,874)	1:188:A:MET:HG3	1:108:A:LYS:HG2	2	0.14
(2,874)	1:188:A:MET:HG3	1:108:A:LYS:HG2	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE1	9	0.14
(2,830)	1:174:A:LEU:HD21	1:175:A:GLU:HG3	13	0.14
(2,788)	1:143:A:ILE:HG23	1:143:A:ILE:HB	11	0.14
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	12	0.14
(2,704)	1:18:A:ALA:HB2	1:21:A:LEU:HB3	9	0.14
(2,704)	1:18:A:ALA:HB2	1:21:A:LEU:HB3	13	0.14
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	1	0.14
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	3	0.14
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	10	0.14
(2,644)	1:105:A:THR:HG22	1:108:A:LYS:HD3	1	0.14
(2,643)	1:105:A:THR:HG22	1:106:A:TYR:HD2	3	0.14
(2,642)	1:150:A:THR:HG21	1:154:A:LEU:HG	3	0.14
(2,642)	1:150:A:THR:HG21	1:154:A:LEU:HG	12	0.14
(2,642)	1:150:A:THR:HG23	1:154:A:LEU:HG	14	0.14
(2,642)	1:150:A:THR:HG22	1:154:A:LEU:HG	15	0.14
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD21	2	0.14
(2,631)	1:64:A:ILE:HG23	1:35:A:LEU:HD23	14	0.14
(2,622)	1:43:A:THR:HG22	1:42:A:MET:HG3	9	0.14
(2,601)	1:28:A:VAL:HG21	1:71:A:HIS:HB2	13	0.14
(2,600)	1:28:A:VAL:HG21	1:28:A:VAL:HA	3	0.14
(2,597)	1:28:A:VAL:HG22	1:72:A:ASN:HD22	9	0.14
(2,554)	1:67:A:ILE:HG22	1:31:A:LEU:HD21	1	0.14
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	3	0.14
(2,541)	1:116:A:LEU:HD21	1:116:A:LEU:HB3	6	0.14
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	7	0.14
(2,530)	1:49:A:ILE:HD11	1:124:A:PHE:HZ	5	0.14
(2,512)	1:170:A:LEU:HD23	1:170:A:LEU:HG	3	0.14
(2,512)	1:170:A:LEU:HD22	1:170:A:LEU:HG	13	0.14
(2,492)	1:159:A:LEU:HD21	1:160:A:LEU:H	4	0.14
(2,478)	1:59:A:ILE:HG21	1:60:A:ILE:HG23	7	0.14
(2,473)	1:59:A:ILE:HG23	1:112:A:ASP:HB2	14	0.14
(2,465)	1:134:A:LEU:HD23	1:37:A:THR:HG23	10	0.14
(2,449)	1:53:A:ILE:HG21	1:125:A:PHE:HZ	8	0.14
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG21	5	0.14
(2,423)	1:42:A:MET:HE2	1:49:A:ILE:HG23	7	0.14
(2,420)	1:53:A:ILE:HD12	1:60:A:ILE:HG13	1	0.14
(2,420)	1:53:A:ILE:HD12	1:60:A:ILE:HG13	2	0.14
(2,420)	1:53:A:ILE:HD12	1:60:A:ILE:HG13	15	0.14
(2,403)	1:35:A:LEU:HD22	1:35:A:LEU:HB2	9	0.14
(2,403)	1:35:A:LEU:HD23	1:35:A:LEU:HB2	10	0.14
(2,392)	1:39:A:LEU:HD21	1:42:A:MET:HB2	6	0.14
(2,392)	1:39:A:LEU:HD22	1:42:A:MET:HB2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	1	0.14
(2,386)	1:31:A:LEU:HD22	1:31:A:LEU:HG	6	0.14
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	8	0.14
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	10	0.14
(2,386)	1:31:A:LEU:HD23	1:31:A:LEU:HG	12	0.14
(2,386)	1:31:A:LEU:HD22	1:31:A:LEU:HG	13	0.14
(2,379)	1:142:A:LEU:HD21	1:138:A:ILE:HD13	1	0.14
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD13	1	0.14
(2,377)	1:142:A:LEU:HD23	1:117:A:ILE:HD12	9	0.14
(2,377)	1:142:A:LEU:HD22	1:117:A:ILE:HD12	15	0.14
(2,335)	1:102:A:MET:HE1	1:71:A:HIS:HE1	4	0.14
(2,334)	1:42:A:MET:HE3	1:53:A:ILE:HD11	6	0.14
(2,329)	1:89:A:VAL:HG11	1:17:A:MET:HE1	11	0.14
(2,325)	1:17:A:MET:HE3	1:83:A:GLU:HA	11	0.14
(2,288)	1:102:A:MET:HA	1:105:A:THR:HG23	10	0.14
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG21	12	0.14
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	9	0.14
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	13	0.14
(2,133)	1:23:A:THR:HG22	1:22:A:GLN:HB2	2	0.14
(2,133)	1:23:A:THR:HG22	1:22:A:GLN:HB2	15	0.14
(2,114)	1:177:A:MET:HE3	1:93:A:PHE:HE1	15	0.14
(2,106)	1:43:A:THR:HG23	1:42:A:MET:HG2	3	0.14
(2,106)	1:43:A:THR:HG21	1:42:A:MET:HG2	13	0.14
(2,102)	1:28:A:VAL:HG13	1:72:A:ASN:HB3	15	0.14
(2,82)	1:76:A:LEU:HD12	1:77:A:LYS:HE2	9	0.14
(2,82)	1:76:A:LEU:HD13	1:77:A:LYS:HE2	11	0.14
(2,57)	1:142:A:LEU:HD12	1:61:A:PHE:HE1	6	0.14
(2,42)	1:53:A:ILE:HG22	1:120:A:HIS:HD2	5	0.14
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	5	0.14
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	6	0.14
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	7	0.14
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	8	0.14
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	8	0.14
(2,4813)	1:188:A:MET:H	1:186:A:ASP:HB2	12	0.13
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	11	0.13
(2,4802)	1:167:A:LYS:HD2	1:167:A:LYS:H	5	0.13
(2,4759)	1:141:A:TYR:HD1	1:34:A:CYS:HB3	6	0.13
(2,4750)	1:120:A:HIS:HD2	1:116:A:LEU:HA	8	0.13
(2,4745)	1:106:A:TYR:HE1	1:110:A:LYS:HG2	7	0.13
(2,4743)	1:103:A:TYR:HD1	1:149:A:VAL:HG21	9	0.13
(2,4732)	1:121:A:ALA:H	1:118:A:LEU:HA	2	0.13
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4715)	1:7:A:GLU:H	1:6:A:PRO:HD2	10	0.13
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	12	0.13
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD23	5	0.13
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD22	9	0.13
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD21	10	0.13
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD21	11	0.13
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD21	12	0.13
(2,4675)	1:157:A:LYS:H	1:160:A:LEU:HD23	14	0.13
(2,4662)	1:104:A:VAL:H	1:183:A:LYS:HB3	14	0.13
(2,4642)	1:62:A:GLY:H	1:64:A:ILE:HB	12	0.13
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	3	0.13
(2,4608)	1:28:A:VAL:H	1:29:A:ARG:HB3	10	0.13
(2,4599)	1:173:A:GLY:H	1:94:A:VAL:HB	10	0.13
(2,4599)	1:173:A:GLY:H	1:94:A:VAL:HB	11	0.13
(2,4586)	1:93:A:PHE:H	1:20:A:LEU:HD23	14	0.13
(2,4584)	1:170:A:LEU:HD23	1:90:A:GLY:H	3	0.13
(2,4562)	1:115:A:GLN:HG2	1:120:A:HIS:HD2	2	0.13
(2,4521)	1:54:A:LEU:HD11	1:52:A:GLY:HA2	7	0.13
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG11	1	0.13
(2,4492)	1:79:A:LEU:HD22	1:25:A:LYS:HG3	10	0.13
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD12	8	0.13
(2,4478)	1:121:A:ALA:HA	1:60:A:ILE:HD12	11	0.13
(2,4460)	1:19:A:GLU:HA	1:23:A:THR:HG22	14	0.13
(2,4435)	1:94:A:VAL:HG21	1:94:A:VAL:HA	4	0.13
(2,4428)	1:42:A:MET:HG2	1:128:A:ILE:HD11	2	0.13
(2,4428)	1:42:A:MET:HG2	1:128:A:ILE:HD12	7	0.13
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG21	11	0.13
(2,4421)	1:56:A:LYS:HE3	1:56:A:LYS:HD2	1	0.13
(2,4421)	1:56:A:LYS:HE3	1:56:A:LYS:HD2	3	0.13
(2,4395)	1:48:A:GLU:HB3	1:48:A:GLU:HG3	5	0.13
(2,4389)	1:80:A:GLU:HG2	1:25:A:LYS:HG3	11	0.13
(2,4342)	1:174:A:LEU:HD23	1:172:A:ASP:H	2	0.13
(2,4332)	1:31:A:LEU:HD22	1:32:A:HIS:H	4	0.13
(2,4294)	1:164:A:GLU:HB2	1:164:A:GLU:HG2	8	0.13
(2,4229)	1:28:A:VAL:HG11	1:73:A:ASN:H	5	0.13
(2,4188)	1:101:A:GLN:HG3	1:100:A:PHE:H	12	0.13
(2,4116)	1:79:A:LEU:HD12	1:78:A:GLU:H	10	0.13
(2,4112)	1:76:A:LEU:HD21	1:25:A:LYS:H	5	0.13
(2,4101)	1:41:A:GLU:H	1:128:A:ILE:HD13	8	0.13
(2,4057)	1:163:A:CYS:HB2	1:163:A:CYS:H	7	0.13
(2,4043)	1:12:A:LYS:HB3	1:12:A:LYS:H	4	0.13
(2,4015)	1:39:A:LEU:HD22	1:61:A:PHE:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4013)	1:98:A:ASP:H	1:94:A:VAL:HA	1	0.13
(2,3992)	1:35:A:LEU:HD23	1:65:A:GLN:H	10	0.13
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	12	0.13
(2,3975)	1:7:A:GLU:H	1:8:A:PHE:HA	11	0.13
(2,3942)	1:102:A:MET:HE3	1:102:A:MET:H	13	0.13
(2,3923)	1:49:A:ILE:HD13	1:42:A:MET:H	11	0.13
(2,3910)	1:156:A:LEU:HD23	1:153:A:GLN:H	3	0.13
(2,3905)	1:28:A:VAL:HG13	1:72:A:ASN:H	12	0.13
(2,3895)	1:143:A:ILE:HD12	1:146:A:VAL:H	14	0.13
(2,3887)	1:94:A:VAL:HG23	1:173:A:GLY:H	1	0.13
(2,3830)	1:177:A:MET:HE3	1:178:A:LEU:H	10	0.13
(2,3822)	1:160:A:LEU:HD11	1:161:A:THR:H	8	0.13
(2,3806)	1:143:A:ILE:H	1:143:A:ILE:HG21	8	0.13
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG22	5	0.13
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG21	9	0.13
(2,3779)	1:121:A:ALA:HB2	1:121:A:ALA:H	1	0.13
(2,3779)	1:121:A:ALA:HB1	1:121:A:ALA:H	2	0.13
(2,3779)	1:121:A:ALA:HB2	1:121:A:ALA:H	3	0.13
(2,3779)	1:121:A:ALA:HB3	1:121:A:ALA:H	11	0.13
(2,3779)	1:121:A:ALA:HB1	1:121:A:ALA:H	13	0.13
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	9	0.13
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	1	0.13
(2,3682)	1:54:A:LEU:HD21	1:55:A:ASN:HD21	13	0.13
(2,3671)	1:43:A:THR:HG23	1:43:A:THR:H	1	0.13
(2,3671)	1:43:A:THR:HG22	1:43:A:THR:H	11	0.13
(2,3671)	1:43:A:THR:HG21	1:43:A:THR:H	13	0.13
(2,3640)	1:18:A:ALA:HB1	1:19:A:GLU:H	1	0.13
(2,3640)	1:18:A:ALA:HB2	1:19:A:GLU:H	11	0.13
(2,3636)	1:13:A:LYS:HA	1:14:A:GLU:H	1	0.13
(2,3555)	1:96:A:TRP:HD1	1:95:A:THR:HG23	9	0.13
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD13	9	0.13
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	3	0.13
(2,3546)	1:68:A:TYR:HE1	1:29:A:ARG:HA	6	0.13
(2,3538)	1:32:A:HIS:HD2	1:36:A:GLU:H	13	0.13
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD13	13	0.13
(2,3481)	1:100:A:PHE:HD1	1:176:A:VAL:HG23	15	0.13
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG23	8	0.13
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD13	10	0.13
(2,3374)	1:152:A:TYR:H	1:155:A:LEU:HD22	7	0.13
(2,3341)	1:188:A:MET:H	1:185:A:ASN:HB2	3	0.13
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	9	0.13
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	14	0.13
(2,3276)	1:163:A:CYS:H	1:161:A:THR:HG21	13	0.13
(2,3229)	1:160:A:LEU:H	1:159:A:LEU:HD11	6	0.13
(2,3188)	1:72:A:ASN:H	1:68:A:TYR:H	10	0.13
(2,3188)	1:72:A:ASN:H	1:68:A:TYR:H	13	0.13
(2,3181)	1:65:A:GLN:HB3	1:65:A:GLN:H	9	0.13
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	3	0.13
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	12	0.13
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	14	0.13
(2,3094)	1:39:A:LEU:H	1:38:A:TYR:HB3	2	0.13
(2,3089)	1:36:A:GLU:HG2	1:37:A:THR:H	7	0.13
(2,3041)	1:22:A:GLN:HG2	1:23:A:THR:H	4	0.13
(2,3014)	1:16:A:ILE:H	1:14:A:GLU:HB3	4	0.13
(2,2943)	1:138:A:ILE:H	1:137:A:SER:HA	2	0.13
(2,2927)	1:156:A:LEU:HD23	1:173:A:GLY:H	5	0.13
(2,2899)	1:165:A:GLU:H	1:164:A:GLU:H	8	0.13
(2,2879)	1:157:A:LYS:HG3	1:157:A:LYS:H	10	0.13
(2,2736)	1:127:A:GLU:HB2	1:127:A:GLU:H	6	0.13
(2,2704)	1:131:A:ARG:HE	1:131:A:ARG:HD3	1	0.13
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD23	1	0.13
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD23	2	0.13
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD21	3	0.13
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD22	14	0.13
(2,2585)	1:94:A:VAL:HG12	1:95:A:THR:H	2	0.13
(2,2577)	1:89:A:VAL:HG11	1:92:A:CYS:H	4	0.13
(2,2577)	1:89:A:VAL:HG13	1:92:A:CYS:H	5	0.13
(2,2577)	1:89:A:VAL:HG11	1:92:A:CYS:H	6	0.13
(2,2556)	1:89:A:VAL:H	1:88:A:ASP:HB3	14	0.13
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	15	0.13
(2,2484)	1:17:A:MET:H	1:15:A:PHE:HB3	5	0.13
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD12	1	0.13
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD13	7	0.13
(2,2325)	1:56:A:LYS:H	1:54:A:LEU:HD13	15	0.13
(2,2313)	1:54:A:LEU:HD21	1:55:A:ASN:HD22	2	0.13
(2,2313)	1:54:A:LEU:HD23	1:55:A:ASN:HD22	8	0.13
(2,2276)	1:190:A:VAL:H	1:188:A:MET:HA	7	0.13
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	2	0.13
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	10	0.13
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	14	0.13
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	15	0.13
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	7	0.13
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG22	6	0.13
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG21	15	0.13
(2,1939)	1:20:A:LEU:H	1:16:A:ILE:HA	12	0.13
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	1	0.13
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	6	0.13
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	11	0.13
(2,1895)	1:159:A:LEU:H	1:158:A:GLU:HB2	13	0.13
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD13	13	0.13
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD11	14	0.13
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	15	0.13
(2,1861)	1:141:A:TYR:HE2	1:136:A:ASN:H	10	0.13
(2,1838)	1:16:A:ILE:HD12	1:158:A:GLU:H	5	0.13
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	4	0.13
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	15	0.13
(2,1810)	1:108:A:LYS:H	1:104:A:VAL:HG22	7	0.13
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	2	0.13
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG23	5	0.13
(2,1700)	1:56:A:LYS:H	1:53:A:ILE:HG21	15	0.13
(2,1638)	1:42:A:MET:H	1:124:A:PHE:HZ	13	0.13
(2,1637)	1:105:A:THR:H	1:103:A:TYR:HD1	9	0.13
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	3	0.13
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG21	14	0.13
(2,1570)	1:156:A:LEU:HD23	1:178:A:LEU:H	8	0.13
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG23	4	0.13
(2,1520)	1:76:A:LEU:HD11	1:29:A:ARG:H	2	0.13
(2,1510)	1:116:A:LEU:HD22	1:54:A:LEU:H	7	0.13
(2,1486)	1:41:A:GLU:HG3	1:40:A:TRP:HZ3	6	0.13
(2,1427)	1:19:A:GLU:HA	1:22:A:GLN:HG3	5	0.13
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	14	0.13
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	15	0.13
(2,1402)	1:35:A:LEU:HD13	1:65:A:GLN:HB2	2	0.13
(2,1394)	1:156:A:LEU:HD21	1:152:A:TYR:HA	7	0.13
(2,1349)	1:20:A:LEU:HD13	1:23:A:THR:H	4	0.13
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB2	5	0.13
(2,1318)	1:177:A:MET:HE1	1:173:A:GLY:H	12	0.13
(2,1282)	1:64:A:ILE:HG22	1:35:A:LEU:H	11	0.13
(2,1278)	1:54:A:LEU:HA	1:42:A:MET:HE1	15	0.13
(2,1261)	1:17:A:MET:HE3	1:21:A:LEU:HD23	7	0.13
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG23	6	0.13
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	6	0.13
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	11	0.13
(2,1185)	1:97:A:ALA:HA	1:97:A:ALA:HB2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1156)	1:57:A:GLU:HA	1:60:A:ILE:HG23	4	0.13
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG22	7	0.13
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD12	9	0.13
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	2	0.13
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	4	0.13
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	13	0.13
(2,1094)	1:150:A:THR:HG23	1:151:A:LYS:HA	9	0.13
(2,1092)	1:59:A:ILE:HG23	1:59:A:ILE:HA	5	0.13
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG23	1	0.13
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	1	0.13
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	3	0.13
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	5	0.13
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	6	0.13
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	11	0.13
(2,1038)	1:49:A:ILE:HD11	1:54:A:LEU:HA	1	0.13
(2,1038)	1:49:A:ILE:HD12	1:54:A:LEU:HA	3	0.13
(2,1038)	1:49:A:ILE:HD12	1:54:A:LEU:HA	9	0.13
(2,1038)	1:49:A:ILE:HD12	1:54:A:LEU:HA	15	0.13
(2,1028)	1:105:A:THR:HA	1:104:A:VAL:HG22	7	0.13
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	3	0.13
(2,995)	1:117:A:ILE:HG22	1:117:A:ILE:HA	5	0.13
(2,995)	1:117:A:ILE:HG23	1:117:A:ILE:HA	9	0.13
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	13	0.13
(2,951)	1:15:A:PHE:HB2	1:18:A:ALA:HB2	11	0.13
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	4	0.13
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE3	7	0.13
(2,788)	1:143:A:ILE:HG22	1:143:A:ILE:HB	8	0.13
(2,726)	1:81:A:LYS:HD2	1:81:A:LYS:HG3	2	0.13
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD23	3	0.13
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD21	8	0.13
(2,666)	1:77:A:LYS:HG3	1:77:A:LYS:HE2	12	0.13
(2,635)	1:176:A:VAL:HG13	1:176:A:VAL:HB	2	0.13
(2,635)	1:176:A:VAL:HG11	1:176:A:VAL:HB	5	0.13
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	7	0.13
(2,622)	1:43:A:THR:HG23	1:42:A:MET:HG3	1	0.13
(2,618)	1:43:A:THR:HG21	1:45:A:GLY:H	14	0.13
(2,554)	1:67:A:ILE:HG21	1:31:A:LEU:HD22	11	0.13
(2,553)	1:16:A:ILE:HG23	1:16:A:ILE:H	10	0.13
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	8	0.13
(2,541)	1:116:A:LEU:HD21	1:116:A:LEU:HB3	10	0.13
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	13	0.13
(2,541)	1:116:A:LEU:HD23	1:116:A:LEU:HB3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,541)	1:116:A:LEU:HD21	1:116:A:LEU:HB3	15	0.13
(2,492)	1:159:A:LEU:HD22	1:160:A:LEU:H	2	0.13
(2,478)	1:59:A:ILE:HG23	1:60:A:ILE:HG21	11	0.13
(2,475)	1:59:A:ILE:HG23	1:116:A:LEU:HB3	4	0.13
(2,468)	1:178:A:LEU:HD21	1:175:A:GLU:HA	12	0.13
(2,447)	1:31:A:LEU:HD12	1:31:A:LEU:HB3	2	0.13
(2,420)	1:53:A:ILE:HD12	1:60:A:ILE:HG13	12	0.13
(2,389)	1:39:A:LEU:HD22	1:41:A:GLU:H	1	0.13
(2,389)	1:39:A:LEU:HD23	1:41:A:GLU:H	7	0.13
(2,389)	1:39:A:LEU:HD22	1:41:A:GLU:H	15	0.13
(2,386)	1:31:A:LEU:HD23	1:31:A:LEU:HG	11	0.13
(2,377)	1:142:A:LEU:HD22	1:117:A:ILE:HD11	13	0.13
(2,369)	1:138:A:ILE:HD12	1:60:A:ILE:HG21	7	0.13
(2,337)	1:102:A:MET:HE1	1:66:A:GLU:HA	9	0.13
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD11	13	0.13
(2,334)	1:42:A:MET:HE2	1:53:A:ILE:HD12	14	0.13
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE1	4	0.13
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE1	6	0.13
(2,329)	1:89:A:VAL:HG11	1:17:A:MET:HE1	10	0.13
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE2	15	0.13
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD11	5	0.13
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG23	9	0.13
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG22	10	0.13
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG22	14	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	1	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	2	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	5	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	6	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	7	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	8	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	10	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	11	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	12	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	14	0.13
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	15	0.13
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	8	0.13
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	4	0.13
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG21	3	0.13
(2,139)	1:36:A:GLU:HG3	1:32:A:HIS:HE1	4	0.13
(2,132)	1:23:A:THR:HG22	1:148:A:ARG:HD2	9	0.13
(2,73)	1:76:A:LEU:HD23	1:80:A:GLU:H	3	0.13
(2,63)	1:174:A:LEU:HD22	1:175:A:GLU:HA	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,57)	1:142:A:LEU:HD13	1:61:A:PHE:HE1	9	0.13
(2,39)	1:31:A:LEU:HD11	1:34:A:CYS:H	4	0.13
(2,25)	1:37:A:THR:HG22	1:33:A:GLU:HG2	9	0.13
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	13	0.13
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	10	0.13
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	11	0.13
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	14	0.13
(1,3)	1:15:A:PHE:O	1:19:A:GLU:H	1	0.13
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	2	0.13
(1,1)	1:14:A:GLU:O	1:18:A:ALA:H	4	0.13
(2,4816)	1:98:A:ASP:HB3	1:101:A:GLN:H	13	0.12
(2,4810)	1:185:A:ASN:H	1:183:A:LYS:HB3	2	0.12
(2,4788)	1:99:A:LYS:H	1:98:A:ASP:HB3	15	0.12
(2,4780)	1:47:A:GLU:HG2	1:47:A:GLU:H	1	0.12
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	2	0.12
(2,4748)	1:106:A:TYR:HD1	1:110:A:LYS:HB2	11	0.12
(2,4730)	1:114:A:ASN:H	1:110:A:LYS:HG2	15	0.12
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	10	0.12
(2,4645)	1:85:A:LEU:H	1:84:A:GLN:HG3	6	0.12
(2,4636)	1:77:A:LYS:HB2	1:78:A:GLU:H	1	0.12
(2,4634)	1:138:A:ILE:HG12	1:141:A:TYR:H	7	0.12
(2,4624)	1:98:A:ASP:HB2	1:100:A:PHE:H	11	0.12
(2,4603)	1:10:A:GLY:H	1:9:A:PRO:HG3	5	0.12
(2,4595)	1:152:A:TYR:H	1:154:A:LEU:HB2	5	0.12
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	13	0.12
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	6	0.12
(2,4553)	1:64:A:ILE:HG22	1:65:A:GLN:HE21	15	0.12
(2,4546)	1:67:A:ILE:HG23	1:67:A:ILE:HB	1	0.12
(2,4546)	1:67:A:ILE:HG22	1:67:A:ILE:HB	2	0.12
(2,4546)	1:16:A:ILE:HG21	1:16:A:ILE:HB	4	0.12
(2,4546)	1:16:A:ILE:HG23	1:16:A:ILE:HB	10	0.12
(2,4546)	1:16:A:ILE:HG23	1:16:A:ILE:HB	13	0.12
(2,4546)	1:67:A:ILE:HG21	1:67:A:ILE:HB	15	0.12
(2,4504)	1:190:A:VAL:HB	1:190:A:VAL:HG11	4	0.12
(2,4472)	1:20:A:LEU:HD23	1:155:A:LEU:HD13	3	0.12
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD2	2	0.12
(2,4433)	1:104:A:VAL:HA	1:108:A:LYS:HD2	3	0.12
(2,4432)	1:104:A:VAL:HA	1:108:A:LYS:HB2	6	0.12
(2,4421)	1:56:A:LYS:HE2	1:56:A:LYS:HD3	12	0.12
(2,4410)	1:101:A:GLN:HG2	1:176:A:VAL:HG22	12	0.12
(2,4409)	1:172:A:ASP:HB3	1:94:A:VAL:HB	8	0.12
(2,4344)	1:21:A:LEU:HD12	1:83:A:GLU:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4339)	1:134:A:LEU:HD21	1:129:A:GLN:HG3	9	0.12
(2,4338)	1:39:A:LEU:HD13	1:43:A:THR:HG22	7	0.12
(2,4329)	1:156:A:LEU:HD23	1:175:A:GLU:HG3	10	0.12
(2,4304)	1:186:A:ASP:HB3	1:183:A:LYS:HG3	8	0.12
(2,4276)	1:103:A:TYR:HE2	1:67:A:ILE:HG23	15	0.12
(2,4267)	1:134:A:LEU:HD11	1:132:A:HIS:H	7	0.12
(2,4214)	1:156:A:LEU:HD11	1:173:A:GLY:H	8	0.12
(2,4200)	1:22:A:GLN:HE21	1:18:A:ALA:HB1	2	0.12
(2,4197)	1:16:A:ILE:HG22	1:158:A:GLU:H	4	0.12
(2,4179)	1:183:A:LYS:HA	1:187:A:ALA:H	4	0.12
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD11	8	0.12
(2,4138)	1:100:A:PHE:HD1	1:97:A:ALA:H	5	0.12
(2,4112)	1:76:A:LEU:HD23	1:25:A:LYS:H	10	0.12
(2,4084)	1:162:A:CYS:H	1:162:A:CYS:HB2	3	0.12
(2,4084)	1:162:A:CYS:H	1:162:A:CYS:HB2	11	0.12
(2,4052)	1:185:A:ASN:HB2	1:186:A:ASP:H	8	0.12
(2,4019)	1:18:A:ALA:H	1:15:A:PHE:HD1	13	0.12
(2,4015)	1:39:A:LEU:HD23	1:61:A:PHE:H	4	0.12
(2,3992)	1:35:A:LEU:HD21	1:65:A:GLN:H	14	0.12
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	9	0.12
(2,3981)	1:53:A:ILE:HG21	1:121:A:ALA:H	13	0.12
(2,3961)	1:155:A:LEU:HD11	1:155:A:LEU:H	3	0.12
(2,3953)	1:183:A:LYS:HB2	1:183:A:LYS:H	14	0.12
(2,3920)	1:42:A:MET:HE2	1:42:A:MET:H	6	0.12
(2,3920)	1:42:A:MET:HE2	1:42:A:MET:H	11	0.12
(2,3910)	1:156:A:LEU:HD22	1:153:A:GLN:H	13	0.12
(2,3895)	1:143:A:ILE:HD13	1:146:A:VAL:H	5	0.12
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD12	11	0.12
(2,3837)	1:182:A:LYS:HD2	1:182:A:LYS:H	14	0.12
(2,3806)	1:143:A:ILE:H	1:143:A:ILE:HG22	5	0.12
(2,3796)	1:135:A:ALA:HB3	1:136:A:ASN:HD22	1	0.12
(2,3722)	1:84:A:GLN:HG3	1:84:A:GLN:H	2	0.12
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	11	0.12
(2,3691)	1:64:A:ILE:HG23	1:65:A:GLN:H	2	0.12
(2,3691)	1:64:A:ILE:HG22	1:65:A:GLN:H	7	0.12
(2,3671)	1:43:A:THR:HG23	1:43:A:THR:H	3	0.12
(2,3671)	1:43:A:THR:HG23	1:43:A:THR:H	12	0.12
(2,3671)	1:43:A:THR:HG21	1:43:A:THR:H	14	0.12
(2,3657)	1:33:A:GLU:HB3	1:33:A:GLU:H	8	0.12
(2,3639)	1:18:A:ALA:HB3	1:18:A:ALA:H	5	0.12
(2,3636)	1:13:A:LYS:HA	1:14:A:GLU:H	9	0.12
(2,3631)	1:6:A:PRO:HB2	1:7:A:GLU:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3630)	1:7:A:GLU:HA	1:8:A:PHE:H	4	0.12
(2,3615)	1:132:A:HIS:HE1	1:40:A:TRP:HH2	12	0.12
(2,3596)	1:132:A:HIS:HE1	1:131:A:ARG:HB2	10	0.12
(2,3585)	1:100:A:PHE:HD1	1:97:A:ALA:HB3	1	0.12
(2,3573)	1:32:A:HIS:HD2	1:36:A:GLU:HG3	3	0.12
(2,3562)	1:152:A:TYR:HD2	1:156:A:LEU:HD23	13	0.12
(2,3541)	1:68:A:TYR:HD1	1:32:A:HIS:HB2	12	0.12
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD13	4	0.12
(2,3489)	1:120:A:HIS:HD2	1:119:A:GLU:HB2	7	0.12
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	7	0.12
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	15	0.12
(2,3337)	1:73:A:ASN:H	1:70:A:PHE:HA	7	0.12
(2,3320)	1:143:A:ILE:HG23	1:142:A:LEU:H	3	0.12
(2,3218)	1:125:A:PHE:H	1:123:A:THR:H	11	0.12
(2,3188)	1:72:A:ASN:H	1:68:A:TYR:H	4	0.12
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	8	0.12
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	9	0.12
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	10	0.12
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	11	0.12
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	13	0.12
(2,3094)	1:39:A:LEU:H	1:38:A:TYR:HB3	6	0.12
(2,3094)	1:39:A:LEU:H	1:38:A:TYR:HB3	7	0.12
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	6	0.12
(2,2943)	1:138:A:ILE:H	1:137:A:SER:HA	6	0.12
(2,2943)	1:138:A:ILE:H	1:137:A:SER:HA	8	0.12
(2,2927)	1:156:A:LEU:HD23	1:173:A:GLY:H	7	0.12
(2,2903)	1:167:A:LYS:HA	1:167:A:LYS:H	11	0.12
(2,2896)	1:164:A:GLU:H	1:163:A:CYS:H	6	0.12
(2,2887)	1:7:A:GLU:HA	1:7:A:GLU:H	1	0.12
(2,2718)	1:11:A:ARG:H	1:11:A:ARG:HB3	12	0.12
(2,2635)	1:175:A:GLU:H	1:174:A:LEU:HD22	11	0.12
(2,2556)	1:89:A:VAL:H	1:88:A:ASP:HB3	10	0.12
(2,2541)	1:84:A:GLN:HE21	1:84:A:GLN:HB2	13	0.12
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG13	9	0.12
(2,2532)	1:87:A:GLU:H	1:89:A:VAL:HG12	10	0.12
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	8	0.12
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	12	0.12
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	13	0.12
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	3	0.12
(2,2500)	1:81:A:LYS:H	1:79:A:LEU:HB3	15	0.12
(2,2313)	1:54:A:LEU:HD23	1:55:A:ASN:HD22	1	0.12
(2,2313)	1:54:A:LEU:HD22	1:55:A:ASN:HD22	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2287)	1:22:A:GLN:H	1:20:A:LEU:HB2	2	0.12
(2,2280)	1:101:A:GLN:HE21	1:183:A:LYS:HG3	2	0.12
(2,2264)	1:142:A:LEU:H	1:141:A:TYR:HB3	2	0.12
(2,2264)	1:142:A:LEU:H	1:141:A:TYR:HB3	5	0.12
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	4	0.12
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	5	0.12
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	11	0.12
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	5	0.12
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	10	0.12
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	12	0.12
(2,2168)	1:174:A:LEU:H	1:171:A:LYS:HB2	5	0.12
(2,2120)	1:153:A:GLN:HG2	1:153:A:GLN:H	2	0.12
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	5	0.12
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	13	0.12
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	15	0.12
(2,1994)	1:67:A:ILE:HG22	1:71:A:HIS:H	4	0.12
(2,1994)	1:67:A:ILE:HG22	1:71:A:HIS:H	7	0.12
(2,1991)	1:35:A:LEU:HD22	1:68:A:TYR:H	11	0.12
(2,1930)	1:11:A:ARG:H	1:11:A:ARG:HB2	8	0.12
(2,1913)	1:178:A:LEU:H	1:153:A:GLN:HE22	10	0.12
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD13	3	0.12
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD12	5	0.12
(2,1889)	1:155:A:LEU:H	1:155:A:LEU:HB2	12	0.12
(2,1887)	1:152:A:TYR:H	1:177:A:MET:HG2	8	0.12
(2,1842)	1:158:A:GLU:H	1:158:A:GLU:HG3	9	0.12
(2,1830)	1:131:A:ARG:HE	1:128:A:ILE:HA	6	0.12
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG12	5	0.12
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	4	0.12
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	5	0.12
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	7	0.12
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	9	0.12
(2,1732)	1:69:A:ASP:H	1:72:A:ASN:HB3	3	0.12
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	2	0.12
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	3	0.12
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	4	0.12
(2,1693)	1:38:A:TYR:H	1:38:A:TYR:HB2	4	0.12
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	2	0.12
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	4	0.12
(2,1658)	1:128:A:ILE:H	1:38:A:TYR:HD1	13	0.12
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	10	0.12
(2,1592)	1:135:A:ALA:HB2	1:129:A:GLN:HE22	6	0.12
(2,1536)	1:60:A:ILE:HD13	1:53:A:ILE:HG21	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1510)	1:116:A:LEU:HD22	1:54:A:LEU:H	13	0.12
(2,1486)	1:41:A:GLU:HG3	1:40:A:TRP:HZ3	9	0.12
(2,1481)	1:99:A:LYS:HD3	1:100:A:PHE:H	13	0.12
(2,1422)	1:116:A:LEU:HD23	1:60:A:ILE:HA	8	0.12
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	8	0.12
(2,1331)	1:89:A:VAL:HG22	1:89:A:VAL:HA	3	0.12
(2,1331)	1:89:A:VAL:HG22	1:89:A:VAL:HA	6	0.12
(2,1331)	1:89:A:VAL:HG21	1:89:A:VAL:HA	8	0.12
(2,1331)	1:89:A:VAL:HG21	1:89:A:VAL:HA	9	0.12
(2,1321)	1:23:A:THR:HG23	1:22:A:GLN:HB3	9	0.12
(2,1318)	1:177:A:MET:HE1	1:173:A:GLY:H	9	0.12
(2,1308)	1:142:A:LEU:HD21	1:61:A:PHE:HD2	5	0.12
(2,1279)	1:59:A:ILE:HG21	1:112:A:ASP:HB3	12	0.12
(2,1279)	1:59:A:ILE:HG21	1:112:A:ASP:HB3	13	0.12
(2,1261)	1:17:A:MET:HE2	1:21:A:LEU:HD22	9	0.12
(2,1261)	1:17:A:MET:HE2	1:21:A:LEU:HD23	10	0.12
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG21	11	0.12
(2,1141)	1:43:A:THR:HG23	1:43:A:THR:HB	5	0.12
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	6	0.12
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	10	0.12
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	12	0.12
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD13	12	0.12
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	3	0.12
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	8	0.12
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	11	0.12
(2,1110)	1:184:A:ALA:HA	1:104:A:VAL:HG21	4	0.12
(2,1094)	1:150:A:THR:HG21	1:151:A:LYS:HA	12	0.12
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG21	13	0.12
(2,1083)	1:40:A:TRP:HA	1:43:A:THR:HG22	15	0.12
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	10	0.12
(2,1037)	1:143:A:ILE:HG23	1:140:A:SER:HB2	3	0.12
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	4	0.12
(2,995)	1:117:A:ILE:HG21	1:117:A:ILE:HA	8	0.12
(2,928)	1:29:A:ARG:HD2	1:29:A:ARG:H	13	0.12
(2,914)	1:77:A:LYS:HE2	1:77:A:LYS:H	1	0.12
(2,894)	1:99:A:LYS:HE3	1:75:A:PHE:H	12	0.12
(2,891)	1:42:A:MET:HG3	1:49:A:ILE:HD12	5	0.12
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	3	0.12
(2,830)	1:174:A:LEU:HD23	1:175:A:GLU:HG3	1	0.12
(2,809)	1:9:A:PRO:HB3	1:9:A:PRO:HD3	15	0.12
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD22	15	0.12
(2,715)	1:182:A:LYS:HG2	1:182:A:LYS:HE3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD23	4	0.12
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	4	0.12
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	13	0.12
(2,642)	1:150:A:THR:HG21	1:154:A:LEU:HG	10	0.12
(2,642)	1:150:A:THR:HG22	1:154:A:LEU:HG	11	0.12
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	4	0.12
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	8	0.12
(2,635)	1:176:A:VAL:HG13	1:176:A:VAL:HB	9	0.12
(2,635)	1:176:A:VAL:HG13	1:176:A:VAL:HB	13	0.12
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	15	0.12
(2,632)	1:64:A:ILE:HG23	1:39:A:LEU:HB2	3	0.12
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD22	8	0.12
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD22	10	0.12
(2,631)	1:64:A:ILE:HG22	1:35:A:LEU:HD23	11	0.12
(2,616)	1:28:A:VAL:HG11	1:72:A:ASN:HB2	8	0.12
(2,554)	1:67:A:ILE:HG22	1:31:A:LEU:HD23	4	0.12
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	1	0.12
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	12	0.12
(2,529)	1:176:A:VAL:HG22	1:97:A:ALA:HB1	11	0.12
(2,523)	1:99:A:LYS:HG3	1:99:A:LYS:HE3	10	0.12
(2,478)	1:59:A:ILE:HG22	1:60:A:ILE:HG23	8	0.12
(2,473)	1:59:A:ILE:HG22	1:112:A:ASP:HB2	10	0.12
(2,465)	1:134:A:LEU:HD22	1:37:A:THR:HG22	6	0.12
(2,447)	1:31:A:LEU:HD11	1:31:A:LEU:HB3	5	0.12
(2,447)	1:31:A:LEU:HD13	1:31:A:LEU:HB3	11	0.12
(2,420)	1:53:A:ILE:HD13	1:60:A:ILE:HG13	3	0.12
(2,420)	1:53:A:ILE:HD11	1:60:A:ILE:HG13	6	0.12
(2,420)	1:53:A:ILE:HD12	1:60:A:ILE:HG13	9	0.12
(2,420)	1:53:A:ILE:HD13	1:60:A:ILE:HG13	11	0.12
(2,401)	1:35:A:LEU:HD22	1:31:A:LEU:HB3	1	0.12
(2,401)	1:35:A:LEU:HD22	1:31:A:LEU:HB3	6	0.12
(2,401)	1:35:A:LEU:HD21	1:31:A:LEU:HB3	8	0.12
(2,401)	1:35:A:LEU:HD22	1:31:A:LEU:HB3	11	0.12
(2,389)	1:39:A:LEU:HD23	1:41:A:GLU:H	5	0.12
(2,389)	1:39:A:LEU:HD22	1:41:A:GLU:H	10	0.12
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	3	0.12
(2,386)	1:31:A:LEU:HD23	1:31:A:LEU:HG	5	0.12
(2,386)	1:31:A:LEU:HD23	1:31:A:LEU:HG	7	0.12
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	9	0.12
(2,386)	1:31:A:LEU:HD21	1:31:A:LEU:HG	15	0.12
(2,379)	1:142:A:LEU:HD21	1:138:A:ILE:HD11	9	0.12
(2,364)	1:156:A:LEU:HD22	1:156:A:LEU:HG	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,362)	1:156:A:LEU:HD21	1:152:A:TYR:HB2	5	0.12
(2,334)	1:42:A:MET:HE3	1:53:A:ILE:HD13	3	0.12
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD11	5	0.12
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE3	8	0.12
(2,325)	1:17:A:MET:HE2	1:83:A:GLU:HA	8	0.12
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG21	1	0.12
(2,298)	1:132:A:HIS:HA	1:37:A:THR:HG21	14	0.12
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG22	11	0.12
(2,236)	1:25:A:LYS:HA	1:76:A:LEU:HD12	3	0.12
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	3	0.12
(2,227)	1:171:A:LYS:HA	1:171:A:LYS:HB3	4	0.12
(2,223)	1:129:A:GLN:HA	1:134:A:LEU:HB2	6	0.12
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	1	0.12
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	3	0.12
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	9	0.12
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	5	0.12
(2,174)	1:41:A:GLU:HG3	1:40:A:TRP:HE3	10	0.12
(2,171)	1:74:A:ILE:HG23	1:78:A:GLU:HG3	2	0.12
(2,171)	1:74:A:ILE:HG21	1:78:A:GLU:HG3	4	0.12
(2,154)	1:181:A:PRO:HG3	1:153:A:GLN:HE21	4	0.12
(2,134)	1:18:A:ALA:HB2	1:22:A:GLN:HB2	8	0.12
(2,133)	1:23:A:THR:HG22	1:22:A:GLN:HB2	13	0.12
(2,106)	1:43:A:THR:HG22	1:42:A:MET:HG2	5	0.12
(2,106)	1:43:A:THR:HG23	1:42:A:MET:HG2	8	0.12
(2,73)	1:76:A:LEU:HD21	1:80:A:GLU:H	1	0.12
(2,63)	1:174:A:LEU:HD21	1:175:A:GLU:HA	3	0.12
(2,57)	1:142:A:LEU:HD12	1:61:A:PHE:HE1	12	0.12
(2,14)	1:75:A:PHE:HD2	1:79:A:LEU:HD12	12	0.12
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	11	0.12
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	15	0.12
(1,123)	1:154:A:LEU:O	1:158:A:GLU:H	5	0.12
(1,12)	1:19:A:GLU:O	1:23:A:THR:N	4	0.12
(2,4788)	1:98:A:ASP:HB2	1:99:A:LYS:H	4	0.11
(2,4767)	1:8:A:PHE:HD2	1:9:A:PRO:HG3	2	0.11
(2,4763)	1:141:A:TYR:HE2	1:134:A:LEU:HG	13	0.11
(2,4732)	1:121:A:ALA:H	1:119:A:GLU:HA	9	0.11
(2,4732)	1:121:A:ALA:H	1:119:A:GLU:HA	13	0.11
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	7	0.11
(2,4716)	1:163:A:CYS:H	1:163:A:CYS:HB3	14	0.11
(2,4687)	1:11:A:ARG:HG3	1:12:A:LYS:H	11	0.11
(2,4658)	1:87:A:GLU:HG3	1:88:A:ASP:H	3	0.11
(2,4658)	1:87:A:GLU:HG3	1:88:A:ASP:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4629)	1:126:A:ASP:H	1:124:A:PHE:HB3	1	0.11
(2,4624)	1:98:A:ASP:HB2	1:100:A:PHE:H	14	0.11
(2,4601)	1:186:A:ASP:HB3	1:186:A:ASP:H	2	0.11
(2,4596)	1:166:A:GLY:H	1:167:A:LYS:HD2	5	0.11
(2,4574)	1:59:A:ILE:H	1:56:A:LYS:HD2	3	0.11
(2,4553)	1:64:A:ILE:HG21	1:65:A:GLN:HE21	3	0.11
(2,4546)	1:16:A:ILE:HG21	1:16:A:ILE:HB	3	0.11
(2,4546)	1:67:A:ILE:HG21	1:67:A:ILE:HB	5	0.11
(2,4546)	1:67:A:ILE:HG22	1:67:A:ILE:HB	7	0.11
(2,4546)	1:67:A:ILE:HG21	1:67:A:ILE:HB	8	0.11
(2,4546)	1:16:A:ILE:HG21	1:16:A:ILE:HB	9	0.11
(2,4546)	1:67:A:ILE:HG21	1:67:A:ILE:HB	11	0.11
(2,4546)	1:16:A:ILE:HG23	1:16:A:ILE:HB	14	0.11
(2,4542)	1:157:A:LYS:HB2	1:156:A:LEU:HD13	1	0.11
(2,4529)	1:60:A:ILE:HG22	1:113:A:SER:HB2	9	0.11
(2,4472)	1:20:A:LEU:HD22	1:155:A:LEU:HD11	9	0.11
(2,4466)	1:98:A:ASP:HA	1:101:A:GLN:HB2	3	0.11
(2,4428)	1:42:A:MET:HG2	1:49:A:ILE:HG23	6	0.11
(2,4423)	1:174:A:LEU:HD12	1:157:A:LYS:HE2	6	0.11
(2,4421)	1:56:A:LYS:HE3	1:56:A:LYS:HD2	14	0.11
(2,4390)	1:83:A:GLU:HG2	1:21:A:LEU:HD22	12	0.11
(2,4356)	1:103:A:TYR:HD2	1:180:A:VAL:HG13	15	0.11
(2,4344)	1:21:A:LEU:HD11	1:83:A:GLU:H	5	0.11
(2,4332)	1:31:A:LEU:HD22	1:32:A:HIS:H	1	0.11
(2,4332)	1:31:A:LEU:HD23	1:32:A:HIS:H	6	0.11
(2,4313)	1:171:A:LYS:HG3	1:171:A:LYS:HA	11	0.11
(2,4300)	1:92:A:CYS:HB2	1:75:A:PHE:HE2	8	0.11
(2,4272)	1:174:A:LEU:HD23	1:175:A:GLU:HB2	5	0.11
(2,4267)	1:134:A:LEU:HD11	1:132:A:HIS:H	8	0.11
(2,4262)	1:141:A:TYR:HD1	1:31:A:LEU:HD13	1	0.11
(2,4258)	1:95:A:THR:HG22	1:75:A:PHE:HD2	13	0.11
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	4	0.11
(2,4199)	1:188:A:MET:HB2	1:189:A:HIS:H	9	0.11
(2,4198)	1:189:A:HIS:HD2	1:189:A:HIS:H	6	0.11
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD12	1	0.11
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD13	10	0.11
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD11	14	0.11
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	3	0.11
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	8	0.11
(2,4138)	1:100:A:PHE:HD1	1:97:A:ALA:H	3	0.11
(2,4119)	1:7:A:GLU:HG2	1:7:A:GLU:H	2	0.11
(2,4112)	1:76:A:LEU:HD23	1:25:A:LYS:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4110)	1:64:A:ILE:HG22	1:62:A:GLY:H	3	0.11
(2,4110)	1:64:A:ILE:HG23	1:62:A:GLY:H	10	0.11
(2,4091)	1:36:A:GLU:H	1:36:A:GLU:HG3	7	0.11
(2,4056)	1:163:A:CYS:H	1:163:A:CYS:HB3	3	0.11
(2,4056)	1:163:A:CYS:H	1:163:A:CYS:HB3	11	0.11
(2,4043)	1:12:A:LYS:HB3	1:12:A:LYS:H	15	0.11
(2,4022)	1:143:A:ILE:HD12	1:147:A:GLN:HE22	3	0.11
(2,3981)	1:53:A:ILE:HG22	1:121:A:ALA:H	3	0.11
(2,3981)	1:53:A:ILE:HG23	1:121:A:ALA:H	11	0.11
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD11	4	0.11
(2,3966)	1:66:A:GLU:H	1:67:A:ILE:HD12	9	0.11
(2,3956)	1:74:A:ILE:HG21	1:78:A:GLU:H	1	0.11
(2,3956)	1:74:A:ILE:HG21	1:78:A:GLU:H	4	0.11
(2,3956)	1:74:A:ILE:HG21	1:78:A:GLU:H	8	0.11
(2,3954)	1:183:A:LYS:H	1:104:A:VAL:HG21	6	0.11
(2,3920)	1:42:A:MET:HE2	1:42:A:MET:H	3	0.11
(2,3920)	1:42:A:MET:HE1	1:42:A:MET:H	8	0.11
(2,3898)	1:46:A:VAL:HG21	1:46:A:VAL:H	13	0.11
(2,3895)	1:143:A:ILE:HD11	1:146:A:VAL:H	3	0.11
(2,3889)	1:85:A:LEU:HD21	1:84:A:GLN:H	6	0.11
(2,3887)	1:94:A:VAL:HG23	1:173:A:GLY:H	13	0.11
(2,3837)	1:182:A:LYS:HD2	1:182:A:LYS:H	15	0.11
(2,3808)	1:143:A:ILE:HG21	1:144:A:LYS:H	14	0.11
(2,3806)	1:143:A:ILE:H	1:143:A:ILE:HG23	3	0.11
(2,3796)	1:135:A:ALA:HB3	1:136:A:ASN:HD22	14	0.11
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG22	3	0.11
(2,3779)	1:121:A:ALA:HB1	1:121:A:ALA:H	8	0.11
(2,3779)	1:121:A:ALA:HB3	1:121:A:ALA:H	15	0.11
(2,3745)	1:97:A:ALA:HB2	1:98:A:ASP:H	14	0.11
(2,3743)	1:97:A:ALA:HB2	1:97:A:ALA:H	5	0.11
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	15	0.11
(2,3713)	1:76:A:LEU:HD13	1:77:A:LYS:H	12	0.11
(2,3682)	1:54:A:LEU:HD21	1:55:A:ASN:HD21	2	0.11
(2,3672)	1:44:A:SER:HB3	1:44:A:SER:H	15	0.11
(2,3671)	1:43:A:THR:HG22	1:43:A:THR:H	9	0.11
(2,3671)	1:43:A:THR:HG23	1:43:A:THR:H	10	0.11
(2,3671)	1:43:A:THR:HG22	1:43:A:THR:H	15	0.11
(2,3657)	1:33:A:GLU:HB3	1:33:A:GLU:H	12	0.11
(2,3635)	1:12:A:LYS:HA	1:13:A:LYS:H	10	0.11
(2,3625)	1:3:A:LEU:H	1:2:A:PRO:HA	9	0.11
(2,3598)	1:103:A:TYR:HE2	1:100:A:PHE:HE2	13	0.11
(2,3584)	1:40:A:TRP:HZ2	1:41:A:GLU:HA	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3577)	1:152:A:TYR:HD1	1:155:A:LEU:HG	4	0.11
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD13	10	0.11
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	4	0.11
(2,3549)	1:82:A:TYR:HE1	1:88:A:ASP:HB2	15	0.11
(2,3546)	1:68:A:TYR:HE1	1:29:A:ARG:HA	8	0.11
(2,3543)	1:68:A:TYR:HD1	1:28:A:VAL:HG23	6	0.11
(2,3543)	1:68:A:TYR:HD1	1:28:A:VAL:HG23	8	0.11
(2,3543)	1:68:A:TYR:HD1	1:28:A:VAL:HG22	13	0.11
(2,3538)	1:32:A:HIS:HD2	1:36:A:GLU:H	10	0.11
(2,3538)	1:32:A:HIS:HD2	1:36:A:GLU:H	12	0.11
(2,3510)	1:32:A:HIS:HD2	1:35:A:LEU:HD21	9	0.11
(2,3504)	1:58:A:HIS:HD2	1:59:A:ILE:HD11	15	0.11
(2,3494)	1:132:A:HIS:HD2	1:134:A:LEU:HD11	8	0.11
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG22	4	0.11
(2,3471)	1:152:A:TYR:HD1	1:20:A:LEU:HD11	3	0.11
(2,3446)	1:40:A:TRP:HZ3	1:41:A:GLU:HA	2	0.11
(2,3446)	1:40:A:TRP:HZ3	1:41:A:GLU:HA	8	0.11
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	6	0.11
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	8	0.11
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	9	0.11
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	10	0.11
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	11	0.11
(2,3373)	1:146:A:VAL:H	1:145:A:PRO:HB2	13	0.11
(2,3355)	1:103:A:TYR:H	1:180:A:VAL:HG21	12	0.11
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	4	0.11
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	8	0.11
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	11	0.11
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	12	0.11
(2,3320)	1:143:A:ILE:HG23	1:142:A:LEU:H	4	0.11
(2,3320)	1:143:A:ILE:HG22	1:142:A:LEU:H	5	0.11
(2,3320)	1:143:A:ILE:HG21	1:142:A:LEU:H	14	0.11
(2,3240)	1:190:A:VAL:H	1:189:A:HIS:H	6	0.11
(2,3218)	1:125:A:PHE:H	1:123:A:THR:H	2	0.11
(2,3218)	1:125:A:PHE:H	1:123:A:THR:H	7	0.11
(2,3198)	1:5:A:SER:H	1:6:A:PRO:HD3	12	0.11
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	1	0.11
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	2	0.11
(2,3114)	1:44:A:SER:H	1:45:A:GLY:HA3	4	0.11
(2,3094)	1:39:A:LEU:H	1:38:A:TYR:HB3	3	0.11
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	2	0.11
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	4	0.11
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3089)	1:36:A:GLU:HG2	1:37:A:THR:H	2	0.11
(2,3058)	1:30:A:ASP:H	1:32:A:HIS:H	2	0.11
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	8	0.11
(2,3007)	1:10:A:GLY:H	1:9:A:PRO:HA	14	0.11
(2,2943)	1:138:A:ILE:H	1:137:A:SER:HA	7	0.11
(2,2922)	1:170:A:LEU:H	1:159:A:LEU:HD12	5	0.11
(2,2906)	1:168:A:GLY:HA3	1:168:A:GLY:H	3	0.11
(2,2906)	1:168:A:GLY:HA3	1:168:A:GLY:H	4	0.11
(2,2906)	1:168:A:GLY:HA3	1:168:A:GLY:H	6	0.11
(2,2906)	1:168:A:GLY:HA3	1:168:A:GLY:H	7	0.11
(2,2903)	1:167:A:LYS:HA	1:167:A:LYS:H	14	0.11
(2,2894)	1:164:A:GLU:HA	1:164:A:GLU:H	9	0.11
(2,2879)	1:157:A:LYS:HG3	1:157:A:LYS:H	11	0.11
(2,2826)	1:144:A:LYS:H	1:144:A:LYS:HB2	13	0.11
(2,2789)	1:136:A:ASN:HD21	1:136:A:ASN:H	6	0.11
(2,2766)	1:131:A:ARG:HG2	1:131:A:ARG:H	14	0.11
(2,2761)	1:147:A:GLN:H	1:147:A:GLN:HB2	13	0.11
(2,2686)	1:114:A:ASN:H	1:112:A:ASP:HB2	9	0.11
(2,2545)	1:89:A:VAL:HG22	1:88:A:ASP:H	6	0.11
(2,2545)	1:89:A:VAL:HG21	1:88:A:ASP:H	11	0.11
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	4	0.11
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	10	0.11
(2,2484)	1:17:A:MET:H	1:15:A:PHE:HB3	11	0.11
(2,2484)	1:17:A:MET:H	1:15:A:PHE:HB3	12	0.11
(2,2440)	1:73:A:ASN:H	1:75:A:PHE:H	5	0.11
(2,2391)	1:65:A:GLN:H	1:67:A:ILE:HD13	4	0.11
(2,2366)	1:63:A:ASN:HA	1:64:A:ILE:H	14	0.11
(2,2273)	1:189:A:HIS:H	1:189:A:HIS:HB2	13	0.11
(2,2270)	1:141:A:TYR:H	1:138:A:ILE:HG13	2	0.11
(2,2270)	1:141:A:TYR:H	1:138:A:ILE:HG13	11	0.11
(2,2270)	1:141:A:TYR:H	1:138:A:ILE:HG13	14	0.11
(2,2264)	1:142:A:LEU:H	1:141:A:TYR:HB3	3	0.11
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	3	0.11
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	9	0.11
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	13	0.11
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	1	0.11
(2,2190)	1:120:A:HIS:H	1:122:A:GLY:H	2	0.11
(2,2128)	1:163:A:CYS:H	1:163:A:CYS:HA	15	0.11
(2,2097)	1:101:A:GLN:H	1:102:A:MET:H	2	0.11
(2,2056)	1:72:A:ASN:H	1:73:A:ASN:HB3	3	0.11
(2,2003)	1:157:A:LYS:HB2	1:158:A:GLU:H	6	0.11
(2,1994)	1:67:A:ILE:HG22	1:71:A:HIS:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1991)	1:35:A:LEU:HD23	1:68:A:TYR:H	4	0.11
(2,1939)	1:20:A:LEU:H	1:16:A:ILE:HA	11	0.11
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	8	0.11
(2,1936)	1:34:A:CYS:H	1:37:A:THR:H	10	0.11
(2,1930)	1:11:A:ARG:H	1:11:A:ARG:HB2	9	0.11
(2,1894)	1:159:A:LEU:H	1:159:A:LEU:HD11	11	0.11
(2,1844)	1:122:A:GLY:H	1:53:A:ILE:HD11	7	0.11
(2,1835)	1:63:A:ASN:HD22	1:102:A:MET:HA	2	0.11
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	7	0.11
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	12	0.11
(2,1830)	1:131:A:ARG:HE	1:128:A:ILE:HA	5	0.11
(2,1829)	1:131:A:ARG:HE	1:131:A:ARG:HD2	15	0.11
(2,1815)	1:139:A:SER:H	1:140:A:SER:HA	1	0.11
(2,1815)	1:139:A:SER:H	1:140:A:SER:HA	10	0.11
(2,1766)	1:83:A:GLU:H	1:89:A:VAL:HG11	2	0.11
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	10	0.11
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	15	0.11
(2,1730)	1:69:A:ASP:H	1:67:A:ILE:HG22	9	0.11
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	12	0.11
(2,1693)	1:38:A:TYR:H	1:38:A:TYR:HB2	8	0.11
(2,1678)	1:190:A:VAL:H	1:189:A:HIS:HA	7	0.11
(2,1659)	1:128:A:ILE:H	1:124:A:PHE:HD1	5	0.11
(2,1645)	1:174:A:LEU:H	1:178:A:LEU:HG	13	0.11
(2,1645)	1:174:A:LEU:H	1:178:A:LEU:HG	14	0.11
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	4	0.11
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	8	0.11
(2,1623)	1:93:A:PHE:H	1:89:A:VAL:HA	10	0.11
(2,1608)	1:68:A:TYR:H	1:65:A:GLN:HG2	5	0.11
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	3	0.11
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	5	0.11
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG23	8	0.11
(2,1587)	1:117:A:ILE:HA	1:60:A:ILE:HG21	11	0.11
(2,1586)	1:154:A:LEU:HD12	1:150:A:THR:HA	14	0.11
(2,1579)	1:124:A:PHE:HB2	1:50:A:PRO:HG2	2	0.11
(2,1579)	1:124:A:PHE:HB2	1:50:A:PRO:HG2	11	0.11
(2,1575)	1:53:A:ILE:HD13	1:53:A:ILE:HG13	14	0.11
(2,1570)	1:156:A:LEU:HD23	1:178:A:LEU:H	9	0.11
(2,1536)	1:60:A:ILE:HD11	1:53:A:ILE:HG22	1	0.11
(2,1534)	1:53:A:ILE:HG21	1:60:A:ILE:HA	3	0.11
(2,1534)	1:53:A:ILE:HG22	1:60:A:ILE:HA	11	0.11
(2,1522)	1:76:A:LEU:HD13	1:68:A:TYR:HE1	7	0.11
(2,1510)	1:116:A:LEU:HD21	1:54:A:LEU:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1461)	1:71:A:HIS:HA	1:67:A:ILE:HG21	8	0.11
(2,1444)	1:43:A:THR:HG22	1:39:A:LEU:HB2	15	0.11
(2,1439)	1:102:A:MET:HE3	1:106:A:TYR:HD2	4	0.11
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	1	0.11
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	4	0.11
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	5	0.11
(2,1402)	1:35:A:LEU:HD11	1:65:A:GLN:HB2	5	0.11
(2,1394)	1:156:A:LEU:HD23	1:152:A:TYR:HA	15	0.11
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	15	0.11
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	4	0.11
(2,1355)	1:131:A:ARG:HG2	1:131:A:ARG:HD3	9	0.11
(2,1349)	1:20:A:LEU:HD11	1:23:A:THR:H	10	0.11
(2,1341)	1:140:A:SER:HB3	1:140:A:SER:H	14	0.11
(2,1331)	1:89:A:VAL:HG23	1:89:A:VAL:HA	10	0.11
(2,1331)	1:89:A:VAL:HG21	1:89:A:VAL:HA	11	0.11
(2,1331)	1:89:A:VAL:HG22	1:89:A:VAL:HA	15	0.11
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	4	0.11
(2,1320)	1:104:A:VAL:HB	1:184:A:ALA:HB1	3	0.11
(2,1308)	1:142:A:LEU:HD23	1:61:A:PHE:HD1	14	0.11
(2,1296)	1:139:A:SER:HB2	1:117:A:ILE:HD12	5	0.11
(2,1279)	1:59:A:ILE:HG21	1:112:A:ASP:HB3	8	0.11
(2,1261)	1:17:A:MET:HE2	1:21:A:LEU:HD21	4	0.11
(2,1255)	1:17:A:MET:HE3	1:82:A:TYR:HE2	8	0.11
(2,1255)	1:17:A:MET:HE1	1:82:A:TYR:HE2	10	0.11
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD11	13	0.11
(2,1224)	1:53:A:ILE:HA	1:60:A:ILE:HD12	14	0.11
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG21	4	0.11
(2,1207)	1:42:A:MET:HA	1:49:A:ILE:HG23	13	0.11
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	3	0.11
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	5	0.11
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	10	0.11
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	15	0.11
(2,1185)	1:97:A:ALA:HA	1:97:A:ALA:HB3	2	0.11
(2,1147)	1:135:A:ALA:HA	1:134:A:LEU:HD12	4	0.11
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	2	0.11
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	3	0.11
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	7	0.11
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	8	0.11
(2,1141)	1:43:A:THR:HG23	1:43:A:THR:HB	9	0.11
(2,1141)	1:43:A:THR:HG23	1:43:A:THR:HB	11	0.11
(2,1141)	1:43:A:THR:HG22	1:43:A:THR:HB	13	0.11
(2,1141)	1:43:A:THR:HG22	1:43:A:THR:HB	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1141)	1:43:A:THR:HG23	1:43:A:THR:HB	15	0.11
(2,1133)	1:66:A:GLU:HB2	1:66:A:GLU:HA	10	0.11
(2,1122)	1:7:A:GLU:HG2	1:7:A:GLU:HA	15	0.11
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	5	0.11
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	9	0.11
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	10	0.11
(2,1099)	1:22:A:GLN:HA	1:22:A:GLN:HG2	4	0.11
(2,1094)	1:150:A:THR:HG23	1:151:A:LYS:HA	8	0.11
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	4	0.11
(2,1081)	1:40:A:TRP:HD1	1:40:A:TRP:HA	15	0.11
(2,1038)	1:49:A:ILE:HD12	1:54:A:LEU:HA	4	0.11
(2,928)	1:29:A:ARG:HD2	1:29:A:ARG:H	10	0.11
(2,913)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	9	0.11
(2,879)	1:148:A:ARG:HG2	1:148:A:ARG:HD2	1	0.11
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD21	1	0.11
(2,760)	1:36:A:GLU:HG2	1:32:A:HIS:HD2	8	0.11
(2,760)	1:36:A:GLU:HG2	1:32:A:HIS:HD2	10	0.11
(2,739)	1:86:A:PRO:HB3	1:89:A:VAL:HG22	6	0.11
(2,704)	1:18:A:ALA:HB2	1:21:A:LEU:HB3	14	0.11
(2,685)	1:119:A:GLU:HB3	1:118:A:LEU:HD21	2	0.11
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	8	0.11
(2,643)	1:105:A:THR:HG23	1:106:A:TYR:HD2	14	0.11
(2,642)	1:150:A:THR:HG23	1:154:A:LEU:HG	5	0.11
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	1	0.11
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	3	0.11
(2,635)	1:176:A:VAL:HG13	1:176:A:VAL:HB	6	0.11
(2,635)	1:176:A:VAL:HG11	1:176:A:VAL:HB	10	0.11
(2,635)	1:176:A:VAL:HG13	1:176:A:VAL:HB	11	0.11
(2,635)	1:176:A:VAL:HG12	1:176:A:VAL:HB	12	0.11
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	8	0.11
(2,632)	1:64:A:ILE:HG21	1:39:A:LEU:HB2	11	0.11
(2,603)	1:28:A:VAL:HG22	1:72:A:ASN:HB3	8	0.11
(2,595)	1:28:A:VAL:HG22	1:28:A:VAL:H	3	0.11
(2,554)	1:67:A:ILE:HG22	1:31:A:LEU:HD21	6	0.11
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	2	0.11
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	3	0.11
(2,553)	1:16:A:ILE:HG21	1:16:A:ILE:H	12	0.11
(2,552)	1:67:A:ILE:HG22	1:68:A:TYR:H	6	0.11
(2,541)	1:116:A:LEU:HD22	1:116:A:LEU:HB3	2	0.11
(2,541)	1:116:A:LEU:HD21	1:116:A:LEU:HB3	4	0.11
(2,475)	1:59:A:ILE:HG21	1:116:A:LEU:HB3	5	0.11
(2,468)	1:178:A:LEU:HD23	1:175:A:GLU:HA	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,444)	1:31:A:LEU:HD13	1:30:A:ASP:HB2	3	0.11
(2,420)	1:53:A:ILE:HD13	1:60:A:ILE:HG13	4	0.11
(2,420)	1:53:A:ILE:HD13	1:60:A:ILE:HG13	10	0.11
(2,420)	1:53:A:ILE:HD11	1:60:A:ILE:HG13	13	0.11
(2,420)	1:53:A:ILE:HD12	1:60:A:ILE:HG13	14	0.11
(2,406)	1:156:A:LEU:HD13	1:93:A:PHE:HZ	3	0.11
(2,401)	1:35:A:LEU:HD21	1:31:A:LEU:HB3	9	0.11
(2,392)	1:39:A:LEU:HD22	1:42:A:MET:HB2	15	0.11
(2,389)	1:39:A:LEU:HD21	1:41:A:GLU:H	11	0.11
(2,379)	1:142:A:LEU:HD22	1:138:A:ILE:HD12	7	0.11
(2,379)	1:142:A:LEU:HD21	1:138:A:ILE:HD11	11	0.11
(2,369)	1:138:A:ILE:HD11	1:60:A:ILE:HG23	6	0.11
(2,365)	1:60:A:ILE:HG21	1:53:A:ILE:HB	4	0.11
(2,362)	1:156:A:LEU:HD22	1:152:A:TYR:HB2	2	0.11
(2,334)	1:42:A:MET:HE3	1:53:A:ILE:HD12	2	0.11
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD13	4	0.11
(2,334)	1:42:A:MET:HE1	1:53:A:ILE:HD12	12	0.11
(2,329)	1:89:A:VAL:HG11	1:17:A:MET:HE1	1	0.11
(2,329)	1:89:A:VAL:HG13	1:17:A:MET:HE3	3	0.11
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE1	9	0.11
(2,329)	1:89:A:VAL:HG13	1:17:A:MET:HE2	12	0.11
(2,329)	1:89:A:VAL:HG12	1:17:A:MET:HE3	13	0.11
(2,329)	1:89:A:VAL:HG11	1:17:A:MET:HE2	14	0.11
(2,325)	1:17:A:MET:HE1	1:83:A:GLU:HA	5	0.11
(2,292)	1:38:A:TYR:HA	1:138:A:ILE:HD13	8	0.11
(2,267)	1:183:A:LYS:HA	1:186:A:ASP:HB2	3	0.11
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG21	7	0.11
(2,170)	1:37:A:THR:HG21	1:33:A:GLU:HG3	11	0.11
(2,156)	1:7:A:GLU:HG2	1:8:A:PHE:H	8	0.11
(2,139)	1:36:A:GLU:HG3	1:32:A:HIS:HE1	12	0.11
(2,139)	1:36:A:GLU:HG3	1:32:A:HIS:HE1	14	0.11
(2,139)	1:36:A:GLU:HG3	1:32:A:HIS:HE1	15	0.11
(2,134)	1:18:A:ALA:HB3	1:22:A:GLN:HB2	1	0.11
(2,134)	1:18:A:ALA:HB3	1:22:A:GLN:HB2	2	0.11
(2,134)	1:18:A:ALA:HB3	1:22:A:GLN:HB2	12	0.11
(2,133)	1:23:A:THR:HG23	1:22:A:GLN:HB2	8	0.11
(2,112)	1:177:A:MET:HE3	1:100:A:PHE:HE2	8	0.11
(2,102)	1:28:A:VAL:HG13	1:72:A:ASN:HB3	12	0.11
(2,92)	1:116:A:LEU:HD13	1:115:A:GLN:HB2	1	0.11
(2,92)	1:116:A:LEU:HD11	1:115:A:GLN:HB2	2	0.11
(2,86)	1:67:A:ILE:HG22	1:106:A:TYR:HD2	11	0.11
(2,73)	1:76:A:LEU:HD22	1:80:A:GLU:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,73)	1:76:A:LEU:HD22	1:80:A:GLU:H	15	0.11
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	6	0.11
(2,61)	1:155:A:LEU:HD23	1:21:A:LEU:H	15	0.11
(2,57)	1:142:A:LEU:HD12	1:61:A:PHE:HE1	2	0.11
(2,42)	1:53:A:ILE:HG21	1:120:A:HIS:HD2	14	0.11
(2,19)	1:79:A:LEU:HD13	1:92:A:CYS:HG	7	0.11
(2,18)	1:79:A:LEU:HD13	1:92:A:CYS:HB2	12	0.11
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	14	0.11
(1,122)	1:153:A:GLN:O	1:157:A:LYS:N	4	0.11
(1,33)	1:30:A:ASP:O	1:34:A:CYS:H	3	0.11
(1,11)	1:19:A:GLU:O	1:23:A:THR:H	3	0.11
(2,4821)	1:160:A:LEU:HB3	1:174:A:LEU:H	10	0.1
(2,4790)	1:108:A:LYS:HD3	1:108:A:LYS:H	15	0.1
(2,4785)	1:56:A:LYS:HE3	1:56:A:LYS:H	13	0.1
(2,4767)	1:8:A:PHE:HD2	1:9:A:PRO:HG3	12	0.1
(2,4748)	1:106:A:TYR:HD1	1:110:A:LYS:HB2	10	0.1
(2,4696)	1:24:A:GLU:H	1:25:A:LYS:HB2	2	0.1
(2,4658)	1:87:A:GLU:HG3	1:88:A:ASP:H	11	0.1
(2,4599)	1:173:A:GLY:H	1:94:A:VAL:HB	12	0.1
(2,4595)	1:152:A:TYR:H	1:154:A:LEU:HB2	11	0.1
(2,4594)	1:148:A:ARG:H	1:151:A:LYS:HB3	6	0.1
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	2	0.1
(2,4593)	1:134:A:LEU:H	1:141:A:TYR:HE2	12	0.1
(2,4546)	1:67:A:ILE:HG22	1:67:A:ILE:HB	6	0.1
(2,4529)	1:60:A:ILE:HG22	1:113:A:SER:HB2	4	0.1
(2,4422)	1:56:A:LYS:HE2	1:56:A:LYS:HG2	11	0.1
(2,4421)	1:56:A:LYS:HE3	1:56:A:LYS:HD2	8	0.1
(2,4421)	1:56:A:LYS:HE3	1:56:A:LYS:HD2	9	0.1
(2,4421)	1:56:A:LYS:HE3	1:56:A:LYS:HD2	13	0.1
(2,4419)	1:103:A:TYR:HB2	1:104:A:VAL:HG11	12	0.1
(2,4393)	1:130:A:GLN:HB2	1:131:A:ARG:HG2	1	0.1
(2,4358)	1:177:A:MET:HE3	1:173:A:GLY:HA3	1	0.1
(2,4294)	1:164:A:GLU:HB2	1:164:A:GLU:HG3	10	0.1
(2,4265)	1:142:A:LEU:HD13	1:110:A:LYS:HB2	7	0.1
(2,4169)	1:128:A:ILE:H	1:128:A:ILE:HD12	3	0.1
(2,4164)	1:125:A:PHE:HE2	1:126:A:ASP:H	14	0.1
(2,4116)	1:79:A:LEU:HD13	1:78:A:GLU:H	9	0.1
(2,4063)	1:19:A:GLU:H	1:155:A:LEU:HD23	3	0.1
(2,4058)	1:16:A:ILE:HD13	1:15:A:PHE:H	2	0.1
(2,4047)	1:156:A:LEU:HD12	1:159:A:LEU:H	14	0.1
(2,4043)	1:12:A:LYS:HB3	1:12:A:LYS:H	12	0.1
(2,4043)	1:12:A:LYS:HB3	1:12:A:LYS:H	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,3998)	1:49:A:ILE:HD11	1:54:A:LEU:H	14	0.1
(2,3992)	1:35:A:LEU:HD23	1:65:A:GLN:H	9	0.1
(2,3981)	1:53:A:ILE:HG23	1:121:A:ALA:H	14	0.1
(2,3979)	1:18:A:ALA:HB1	1:22:A:GLN:H	3	0.1
(2,3978)	1:23:A:THR:HG23	1:22:A:GLN:H	10	0.1
(2,3978)	1:23:A:THR:HG21	1:22:A:GLN:H	11	0.1
(2,3942)	1:102:A:MET:HE2	1:102:A:MET:H	15	0.1
(2,3920)	1:42:A:MET:HE2	1:42:A:MET:H	2	0.1
(2,3920)	1:42:A:MET:HE3	1:42:A:MET:H	4	0.1
(2,3920)	1:42:A:MET:HE1	1:42:A:MET:H	14	0.1
(2,3891)	1:133:A:GLY:H	1:134:A:LEU:HD13	7	0.1
(2,3875)	1:39:A:LEU:HD22	1:43:A:THR:H	10	0.1
(2,3837)	1:182:A:LYS:HD2	1:182:A:LYS:H	3	0.1
(2,3830)	1:177:A:MET:HE1	1:178:A:LEU:H	15	0.1
(2,3812)	1:154:A:LEU:HB3	1:154:A:LEU:H	9	0.1
(2,3808)	1:143:A:ILE:HG23	1:144:A:LYS:H	10	0.1
(2,3782)	1:124:A:PHE:H	1:123:A:THR:HG22	7	0.1
(2,3745)	1:97:A:ALA:HB2	1:98:A:ASP:H	11	0.1
(2,3745)	1:97:A:ALA:HB2	1:98:A:ASP:H	12	0.1
(2,3721)	1:83:A:GLU:HG3	1:84:A:GLN:H	4	0.1
(2,3657)	1:33:A:GLU:HB3	1:33:A:GLU:H	15	0.1
(2,3635)	1:12:A:LYS:HA	1:13:A:LYS:H	5	0.1
(2,3554)	1:152:A:TYR:HD1	1:155:A:LEU:HD12	5	0.1
(2,3546)	1:68:A:TYR:HE1	1:29:A:ARG:HA	7	0.1
(2,3477)	1:103:A:TYR:HE1	1:149:A:VAL:HG22	11	0.1
(2,3447)	1:40:A:TRP:HZ3	1:46:A:VAL:HG23	6	0.1
(2,3446)	1:40:A:TRP:HZ3	1:41:A:GLU:HA	11	0.1
(2,3397)	1:72:A:ASN:H	1:71:A:HIS:H	2	0.1
(2,3376)	1:153:A:GLN:HE22	1:149:A:VAL:HG22	10	0.1
(2,3361)	1:147:A:GLN:HE22	1:147:A:GLN:HE21	12	0.1
(2,3341)	1:188:A:MET:H	1:185:A:ASN:HB2	9	0.1
(2,3335)	1:71:A:HIS:H	1:67:A:ILE:HA	15	0.1
(2,3260)	1:161:A:THR:HG23	1:158:A:GLU:H	10	0.1
(2,3182)	1:15:A:PHE:HB2	1:15:A:PHE:H	4	0.1
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	3	0.1
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	5	0.1
(2,3093)	1:39:A:LEU:H	1:39:A:LEU:HB3	8	0.1
(2,3089)	1:36:A:GLU:HG2	1:37:A:THR:H	14	0.1
(2,3089)	1:36:A:GLU:HG2	1:37:A:THR:H	15	0.1
(2,3036)	1:22:A:GLN:H	1:23:A:THR:H	3	0.1
(2,2976)	1:182:A:LYS:H	1:181:A:PRO:HD2	7	0.1
(2,2765)	1:162:A:CYS:H	1:160:A:LEU:H	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2752)	1:129:A:GLN:H	1:126:A:ASP:HA	12	0.1
(2,2752)	1:129:A:GLN:H	1:126:A:ASP:HA	15	0.1
(2,2686)	1:114:A:ASN:H	1:112:A:ASP:HB2	5	0.1
(2,2686)	1:114:A:ASN:H	1:112:A:ASP:HB2	11	0.1
(2,2669)	1:112:A:ASP:H	1:110:A:LYS:H	5	0.1
(2,2551)	1:88:A:ASP:H	1:82:A:TYR:HD1	14	0.1
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	6	0.1
(2,2516)	1:84:A:GLN:H	1:83:A:GLU:HB3	11	0.1
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	1	0.1
(2,2508)	1:36:A:GLU:HG2	1:36:A:GLU:H	5	0.1
(2,2500)	1:81:A:LYS:H	1:79:A:LEU:HB3	2	0.1
(2,2484)	1:17:A:MET:H	1:15:A:PHE:HB3	15	0.1
(2,2455)	1:73:A:ASN:HB2	1:74:A:ILE:H	1	0.1
(2,2366)	1:63:A:ASN:HA	1:64:A:ILE:H	10	0.1
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	4	0.1
(2,2321)	1:56:A:LYS:H	1:54:A:LEU:HA	12	0.1
(2,2313)	1:54:A:LEU:HD23	1:55:A:ASN:HD22	6	0.1
(2,2288)	1:21:A:LEU:HD11	1:22:A:GLN:H	4	0.1
(2,2287)	1:22:A:GLN:H	1:20:A:LEU:HB2	3	0.1
(2,2287)	1:22:A:GLN:H	1:20:A:LEU:HB2	12	0.1
(2,2274)	1:189:A:HIS:H	1:188:A:MET:HB3	6	0.1
(2,2243)	1:132:A:HIS:H	1:133:A:GLY:HA2	8	0.1
(2,2224)	1:124:A:PHE:H	1:124:A:PHE:HE2	7	0.1
(2,2087)	1:91:A:HIS:HA	1:94:A:VAL:H	12	0.1
(2,2076)	1:92:A:CYS:H	1:90:A:GLY:H	1	0.1
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	3	0.1
(2,2010)	1:27:A:TYR:H	1:27:A:TYR:HB3	8	0.1
(2,2005)	1:15:A:PHE:H	1:15:A:PHE:HA	1	0.1
(2,2005)	1:15:A:PHE:H	1:15:A:PHE:HA	12	0.1
(2,1993)	1:70:A:PHE:H	1:67:A:ILE:HG21	11	0.1
(2,1991)	1:35:A:LEU:HD21	1:68:A:TYR:H	8	0.1
(2,1833)	1:13:A:LYS:H	1:13:A:LYS:HB2	11	0.1
(2,1831)	1:131:A:ARG:HE	1:131:A:ARG:H	10	0.1
(2,1764)	1:83:A:GLU:H	1:81:A:LYS:HB3	3	0.1
(2,1732)	1:69:A:ASP:H	1:72:A:ASN:HB3	8	0.1
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	10	0.1
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	14	0.1
(2,1724)	1:176:A:VAL:H	1:174:A:LEU:HG	15	0.1
(2,1693)	1:38:A:TYR:H	1:38:A:TYR:HB2	13	0.1
(2,1684)	1:18:A:ALA:HA	1:22:A:GLN:H	14	0.1
(2,1672)	1:133:A:GLY:H	1:130:A:GLN:HG3	12	0.1
(2,1645)	1:174:A:LEU:H	1:178:A:LEU:HG	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1638)	1:42:A:MET:H	1:124:A:PHE:HZ	6	0.1
(2,1619)	1:91:A:HIS:H	1:88:A:ASP:HA	6	0.1
(2,1606)	1:68:A:TYR:H	1:68:A:TYR:HE2	2	0.1
(2,1592)	1:135:A:ALA:HB3	1:129:A:GLN:HE22	5	0.1
(2,1511)	1:38:A:TYR:HE2	1:142:A:LEU:HD22	6	0.1
(2,1461)	1:71:A:HIS:HA	1:67:A:ILE:HG22	6	0.1
(2,1439)	1:102:A:MET:HE1	1:106:A:TYR:HD2	15	0.1
(2,1422)	1:116:A:LEU:HD23	1:60:A:ILE:HA	2	0.1
(2,1407)	1:109:A:ASN:HB3	1:109:A:ASN:H	7	0.1
(2,1386)	1:33:A:GLU:HG2	1:29:A:ARG:HD3	8	0.1
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	2	0.1
(2,1378)	1:178:A:LEU:HG	1:176:A:VAL:H	12	0.1
(2,1369)	1:156:A:LEU:HD13	1:170:A:LEU:HB3	12	0.1
(2,1367)	1:6:A:PRO:HA	1:6:A:PRO:HG3	14	0.1
(2,1362)	1:80:A:GLU:HG3	1:77:A:LYS:HA	5	0.1
(2,1331)	1:89:A:VAL:HG22	1:89:A:VAL:HA	13	0.1
(2,1328)	1:183:A:LYS:HE2	1:187:A:ALA:H	11	0.1
(2,1279)	1:59:A:ILE:HG23	1:112:A:ASP:HB3	14	0.1
(2,1261)	1:17:A:MET:HE1	1:21:A:LEU:HD21	3	0.1
(2,1261)	1:17:A:MET:HE2	1:21:A:LEU:HD23	11	0.1
(2,1261)	1:17:A:MET:HE3	1:21:A:LEU:HD23	15	0.1
(2,1211)	1:161:A:THR:HB	1:161:A:THR:HG23	5	0.1
(2,1194)	1:3:A:LEU:HA	1:3:A:LEU:HB2	14	0.1
(2,1173)	1:121:A:ALA:HA	1:125:A:PHE:HE2	9	0.1
(2,1151)	1:43:A:THR:HA	1:39:A:LEU:HD22	1	0.1
(2,1141)	1:43:A:THR:HG21	1:43:A:THR:HB	1	0.1
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG23	2	0.1
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG23	3	0.1
(2,1140)	1:141:A:TYR:HA	1:143:A:ILE:HG22	11	0.1
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD11	13	0.1
(2,1121)	1:150:A:THR:HB	1:154:A:LEU:HD11	15	0.1
(2,1112)	1:119:A:GLU:HA	1:119:A:GLU:HG2	14	0.1
(2,1038)	1:49:A:ILE:HD12	1:54:A:LEU:HA	5	0.1
(2,1037)	1:143:A:ILE:HG22	1:140:A:SER:HB2	15	0.1
(2,927)	1:29:A:ARG:HD2	1:30:A:ASP:H	6	0.1
(2,913)	1:81:A:LYS:HE2	1:81:A:LYS:HG3	11	0.1
(2,862)	1:66:A:GLU:HG2	1:102:A:MET:HE2	1	0.1
(2,848)	1:143:A:ILE:HD12	1:146:A:VAL:HB	2	0.1
(2,796)	1:64:A:ILE:HG23	1:65:A:GLN:HB2	6	0.1
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD22	5	0.1
(2,782)	1:80:A:GLU:HB2	1:76:A:LEU:HD22	13	0.1
(2,778)	1:108:A:LYS:HB2	1:105:A:THR:HA	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,710)	1:49:A:ILE:HB	1:49:A:ILE:HD12	12	0.1
(2,690)	1:184:A:ALA:HB1	1:185:A:ASN:HB3	2	0.1
(2,668)	1:77:A:LYS:HG3	1:80:A:GLU:HG2	14	0.1
(2,642)	1:150:A:THR:HG23	1:154:A:LEU:HG	8	0.1
(2,635)	1:176:A:VAL:HG13	1:176:A:VAL:HB	14	0.1
(2,601)	1:28:A:VAL:HG23	1:71:A:HIS:HB2	11	0.1
(2,491)	1:178:A:LEU:HD12	1:174:A:LEU:HB2	2	0.1
(2,477)	1:59:A:ILE:HG21	1:60:A:ILE:HD11	10	0.1
(2,468)	1:178:A:LEU:HD22	1:175:A:GLU:HA	4	0.1
(2,442)	1:31:A:LEU:HD11	1:68:A:TYR:HA	2	0.1
(2,398)	1:35:A:LEU:HD22	1:68:A:TYR:HD2	6	0.1
(2,337)	1:102:A:MET:HE2	1:66:A:GLU:HA	12	0.1
(2,334)	1:42:A:MET:HE3	1:53:A:ILE:HD13	11	0.1
(2,329)	1:89:A:VAL:HG13	1:17:A:MET:HE2	2	0.1
(2,316)	1:20:A:LEU:HD13	1:152:A:TYR:HB3	12	0.1
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG21	2	0.1
(2,264)	1:48:A:GLU:HA	1:49:A:ILE:HG21	8	0.1
(2,221)	1:83:A:GLU:HA	1:21:A:LEU:HG	13	0.1
(2,206)	1:60:A:ILE:HA	1:113:A:SER:HG	5	0.1
(2,188)	1:92:A:CYS:HB2	1:91:A:HIS:H	5	0.1
(2,166)	1:78:A:GLU:HG3	1:95:A:THR:HG22	6	0.1
(2,140)	1:36:A:GLU:HG3	1:37:A:THR:H	15	0.1
(2,139)	1:36:A:GLU:HG3	1:32:A:HIS:HE1	1	0.1
(2,112)	1:177:A:MET:HE2	1:100:A:PHE:HE2	9	0.1
(2,65)	1:117:A:ILE:HG23	1:117:A:ILE:HB	1	0.1
(2,65)	1:117:A:ILE:HG22	1:117:A:ILE:HB	11	0.1
(2,65)	1:117:A:ILE:HG22	1:117:A:ILE:HB	12	0.1
(2,42)	1:53:A:ILE:HG23	1:120:A:HIS:HD2	10	0.1
(2,39)	1:31:A:LEU:HD13	1:34:A:CYS:H	11	0.1
(2,14)	1:75:A:PHE:HD1	1:79:A:LEU:HD12	8	0.1
(2,14)	1:75:A:PHE:HD1	1:79:A:LEU:HD13	15	0.1
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	7	0.1
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	8	0.1
(1,147)	1:181:A:PRO:O	1:185:A:ASN:H	12	0.1

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

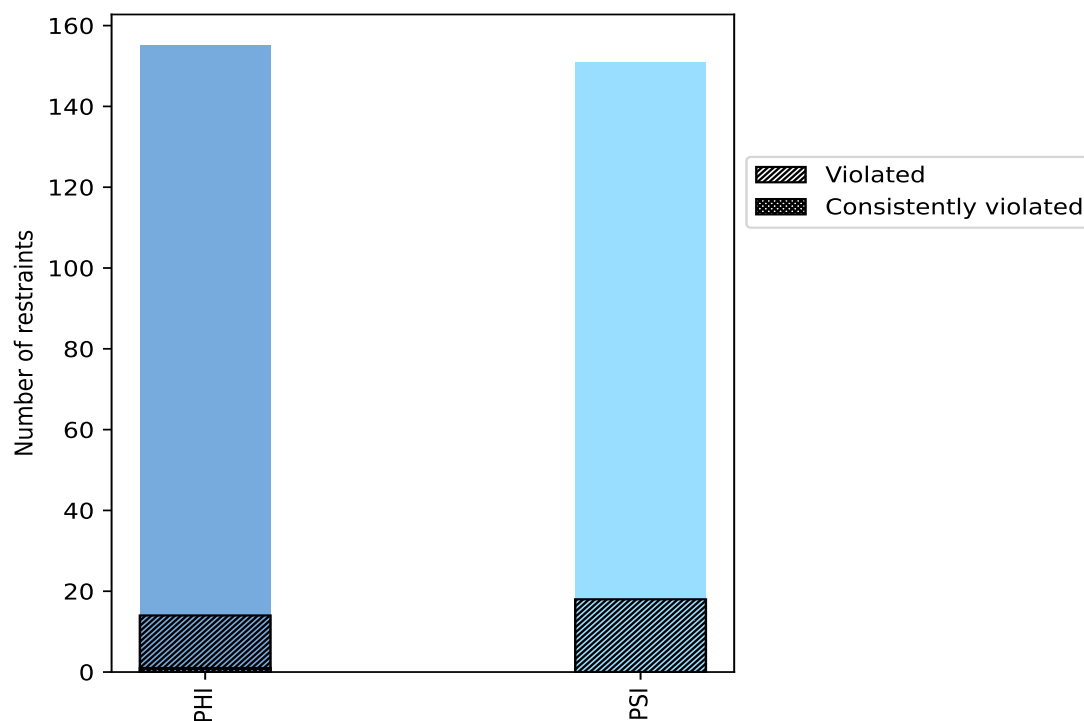
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	155	50.7	14	9.0	4.6	1	0.6	0.3
PSI	151	49.3	18	11.9	5.9	0	0.0	0.0
Total	306	100.0	32	10.5	10.5	1	0.3	0.3

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



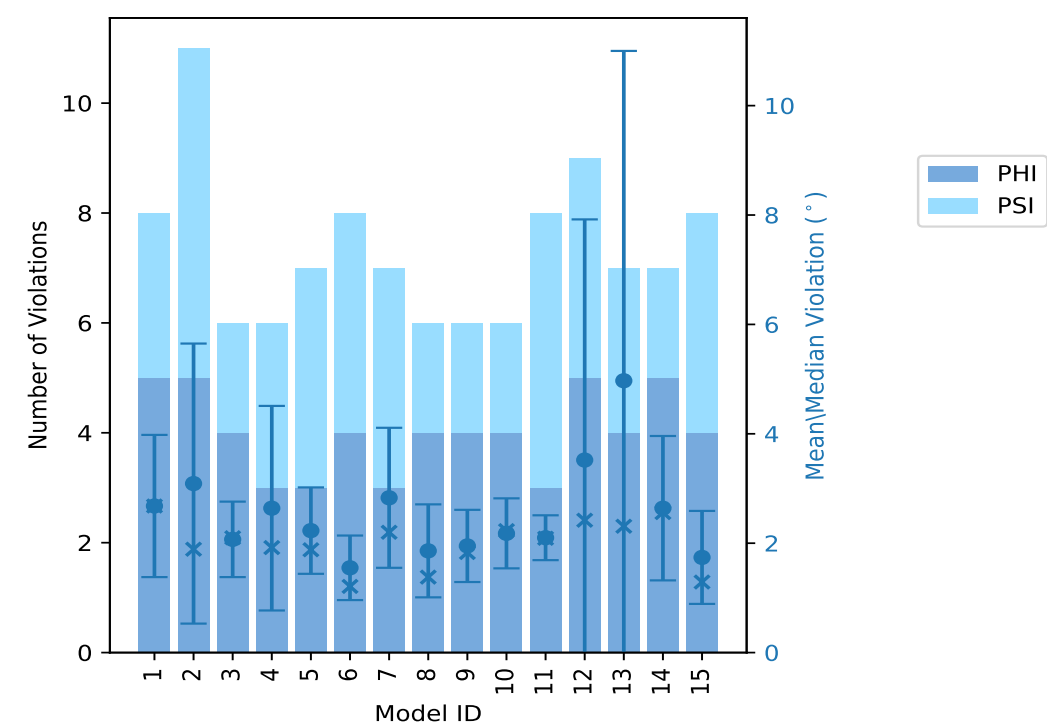
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model ⓘ

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	5	3	8	2.68	4.52	1.3	2.68
2	5	6	11	3.09	9.3	2.56	1.89
3	4	2	6	2.07	3.03	0.69	2.1
4	3	3	6	2.64	6.72	1.87	1.92
5	3	4	7	2.23	3.51	0.79	1.88
6	4	4	8	1.55	2.94	0.59	1.21
7	3	4	7	2.83	5.44	1.28	2.2
8	4	2	6	1.86	3.47	0.85	1.38
9	4	2	6	1.95	3.14	0.66	1.83
10	4	2	6	2.18	2.98	0.64	2.23
11	3	5	8	2.1	2.77	0.41	2.09
12	5	4	9	3.52	15.85	4.4	2.42
13	4	3	7	4.97	19.47	6.03	2.31
14	5	2	7	2.64	5.66	1.32	2.56
15	4	4	8	1.74	3.7	0.85	1.29

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

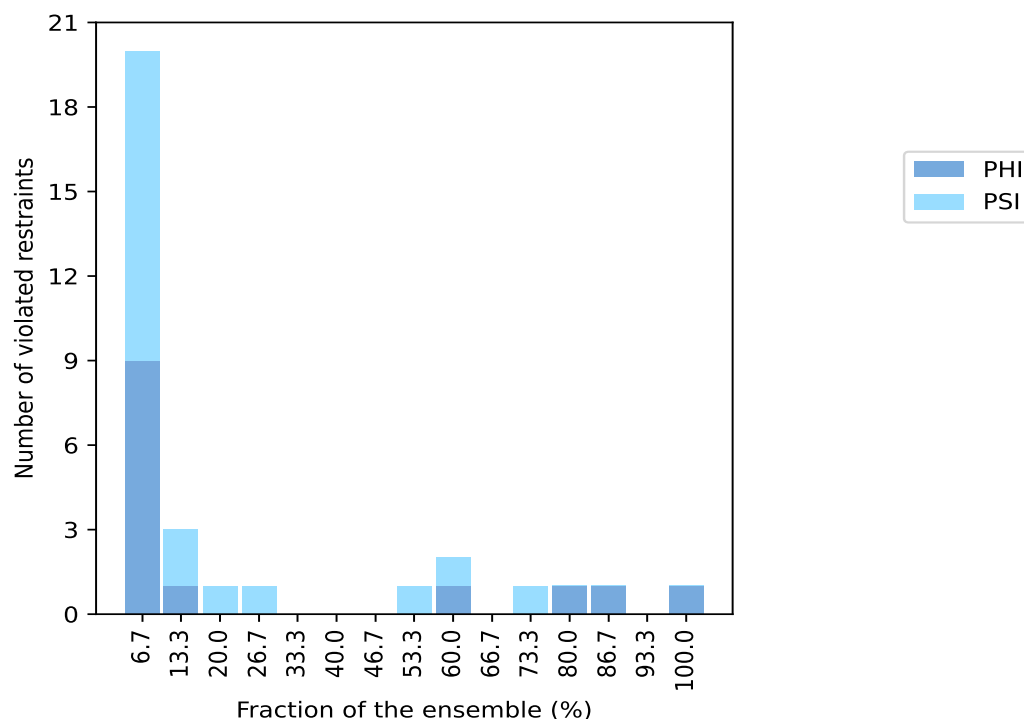
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
9	11	20	1	6.7
1	2	3	2	13.3
0	1	1	3	20.0
0	1	1	4	26.7
0	0	0	5	33.3
0	0	0	6	40.0
0	0	0	7	46.7
0	1	1	8	53.3
1	1	2	9	60.0
0	0	0	10	66.7
0	1	1	11	73.3
1	0	1	12	80.0
1	0	1	13	86.7
0	0	0	14	93.3
1	0	1	15	100.0

¹ Number of models with violations

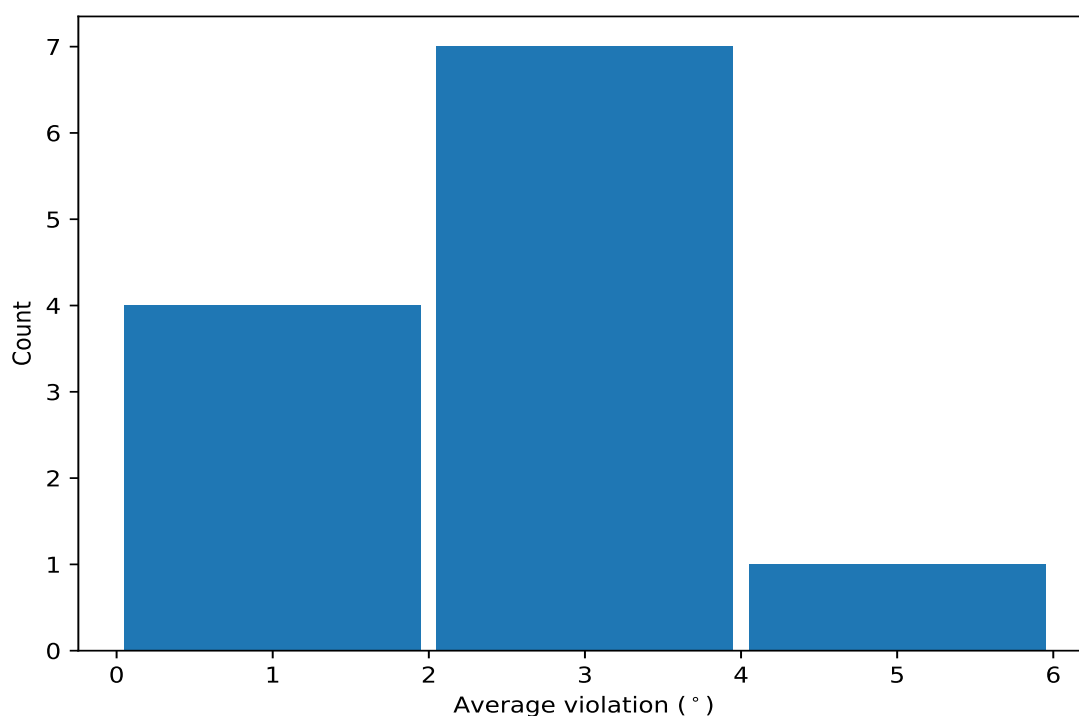
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

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

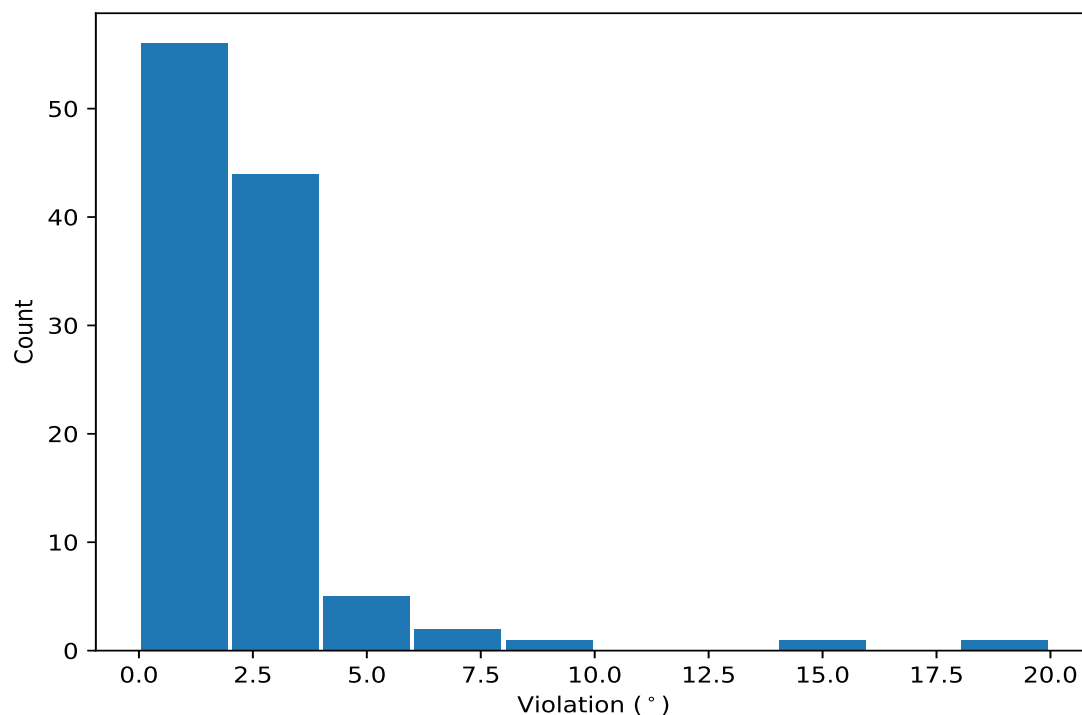
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	15	2.24	0.56	2.29
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	13	2.45	0.81	2.31
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	12	1.52	0.3	1.46
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	11	2.09	0.67	2.05
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	9	2.39	1.46	1.88
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	9	2.03	0.59	2.2
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	8	2.56	1.86	2.04
(1,270)	1:162:A:CYS:N	1:162:A:CYS:CA	1:162:A:CYS:C	1:163:A:CYS:N	4	2.11	0.69	2.09
(1,111)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:PHE:N	3	1.53	0.36	1.62
(1,50)	1:38:A:TYR:C	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	2	5.37	0.29	5.37
(1,4)	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	1:16:A:ILE:N	2	1.75	0.68	1.75
(1,125)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:TYR:N	2	1.29	0.08	1.29

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,254)	1:154:A:LEU:N	1:154:A:LEU:CA	1:154:A:LEU:C	1:155:A:LEU:N	13	19.47
(1,134)	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	1:88:A:ASP:N	12	15.85
(1,157)	1:100:A:PHE:C	1:101:A:GLN:N	1:101:A:GLN:CA	1:101:A:GLN:C	2	9.3
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	2	7.31
(1,252)	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	1:154:A:LEU:N	4	6.72
(1,50)	1:38:A:TYR:C	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	14	5.66
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	7	5.44
(1,50)	1:38:A:TYR:C	1:39:A:LEU:N	1:39:A:LEU:CA	1:39:A:LEU:C	13	5.08
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	1	4.52
(1,306)	1:187:A:ALA:N	1:187:A:ALA:CA	1:187:A:ALA:C	1:188:A:MET:N	1	4.21
(1,116)	1:76:A:LEU:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	7	3.73
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	15	3.7
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1	3.61
(1,266)	1:160:A:LEU:N	1:160:A:LEU:CA	1:160:A:LEU:C	1:161:A:THR:N	5	3.51

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	8	3.47
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	5	3.42
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1	3.32
(1,154)	1:99:A:LYS:N	1:99:A:LYS:CA	1:99:A:LYS:C	1:100:A:PHE:N	2	3.21
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	9	3.14
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	7	3.07
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	3	3.03
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	10	2.98
(1,270)	1:162:A:CYS:N	1:162:A:CYS:CA	1:162:A:CYS:C	1:163:A:CYS:N	6	2.94
(1,255)	1:154:A:LEU:C	1:155:A:LEU:N	1:155:A:LEU:CA	1:155:A:LEU:C	13	2.93
(1,268)	1:161:A:THR:N	1:161:A:THR:CA	1:161:A:THR:C	1:162:A:CYS:N	10	2.87
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	11	2.77
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	2	2.72
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	3	2.71
(1,270)	1:162:A:CYS:N	1:162:A:CYS:CA	1:162:A:CYS:C	1:163:A:CYS:N	12	2.63
(1,133)	1:86:A:PRO:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	12	2.59
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	14	2.59
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	14	2.58
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	14	2.56
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	4	2.53
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	12	2.51
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	8	2.48
(1,4)	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	1:16:A:ILE:N	11	2.43
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	12	2.42
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	10	2.38
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	2	2.36
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	9	2.36
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	13	2.31
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	11	2.31
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	3	2.29
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	7	2.2
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	15	2.18
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	4	2.15
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	11	2.14
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	15	2.13
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	14	2.11
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	10	2.08
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	11	2.05
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	1	2.04
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	9	2.02
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	6	1.99
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	11	1.94
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	12	1.94
(1,111)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:PHE:N	7	1.93
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	7	1.92
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	3	1.91
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	5	1.9
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	13	1.9
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	2	1.89
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	5	1.88
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	11	1.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	5	1.77
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	13	1.75
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	4	1.68
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	14	1.67
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	9	1.64
(1,111)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:PHE:N	2	1.62
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	12	1.58
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	5	1.56
(1,270)	1:162:A:CYS:N	1:162:A:CYS:CA	1:162:A:CYS:C	1:163:A:CYS:N	5	1.55
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	4	1.55
(1,27)	1:26:A:ALA:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	6	1.55
(1,152)	1:98:A:ASP:N	1:98:A:ASP:CA	1:98:A:ASP:C	1:99:A:LYS:N	2	1.53
(1,115)	1:76:A:LEU:N	1:76:A:LEU:CA	1:76:A:LEU:C	1:77:A:LYS:N	7	1.53
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	2	1.48
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	2	1.48
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	8	1.45
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	3	1.4
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	9	1.39
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	10	1.38
(1,125)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:TYR:N	1	1.37
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	10	1.36
(1,78)	1:55:A:ASN:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	13	1.34
(1,270)	1:162:A:CYS:N	1:162:A:CYS:CA	1:162:A:CYS:C	1:163:A:CYS:N	15	1.33
(1,269)	1:161:A:THR:C	1:162:A:CYS:N	1:162:A:CYS:CA	1:162:A:CYS:C	8	1.31
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	8	1.31
(1,109)	1:72:A:ASN:C	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	14	1.29
(1,174)	1:109:A:ASN:N	1:109:A:ASN:CA	1:109:A:ASN:C	1:110:A:LYS:N	11	1.28
(1,135)	1:88:A:ASP:C	1:89:A:VAL:N	1:89:A:VAL:CA	1:89:A:VAL:C	1	1.25
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	15	1.25
(1,125)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:TYR:N	6	1.21
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	6	1.21
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	4	1.2
(1,34)	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	1:31:A:LEU:N	6	1.2
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	6	1.18
(1,13)	1:19:A:GLU:C	1:20:A:LEU:N	1:20:A:LEU:CA	1:20:A:LEU:C	15	1.18
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	6	1.15
(1,110)	1:73:A:ASN:N	1:73:A:ASN:CA	1:73:A:ASN:C	1:74:A:ILE:N	9	1.15
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	1	1.14
(1,156)	1:100:A:PHE:N	1:100:A:PHE:CA	1:100:A:PHE:C	1:101:A:GLN:N	8	1.12
(1,141)	1:91:A:HIS:C	1:92:A:CYS:N	1:92:A:CYS:CA	1:92:A:CYS:C	2	1.12
(1,83)	1:58:A:HIS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	12	1.12
(1,126)	1:81:A:LYS:C	1:82:A:TYR:N	1:82:A:TYR:CA	1:82:A:TYR:C	15	1.1
(1,77)	1:55:A:ASN:N	1:55:A:ASN:CA	1:55:A:ASN:C	1:56:A:LYS:N	3	1.07
(1,4)	1:15:A:PHE:N	1:15:A:PHE:CA	1:15:A:PHE:C	1:16:A:ILE:N	15	1.07
(1,111)	1:74:A:ILE:N	1:74:A:ILE:CA	1:74:A:ILE:C	1:75:A:PHE:N	12	1.05