



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 12:21 AM UTC

PDB ID : 6I9F / pdb_00006i9f
BMRB ID : 18632
Title : Solution structure of As-p18 reveals that nematode fatty acid binding proteins exhibit unusual structural features
Authors : Ibanez Shimabukuro, M.; Rey Burusco, M.F.; Kennedy, M.W.; Corsico, B.; Smith, B.O.
Deposited on : 2018-11-23

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

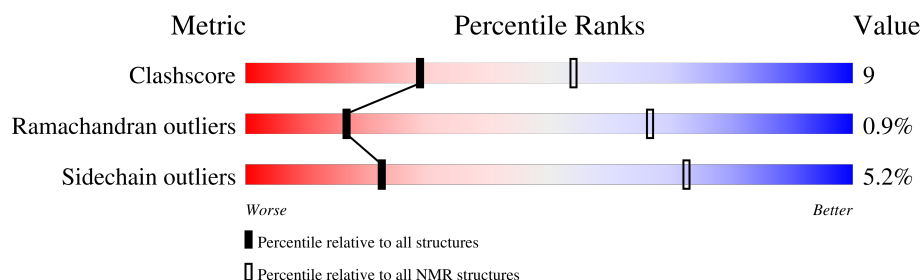
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	155	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:143 (142)	0.69	3

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2599 atoms, of which 1287 are hydrogens and 0 are deuteriums.

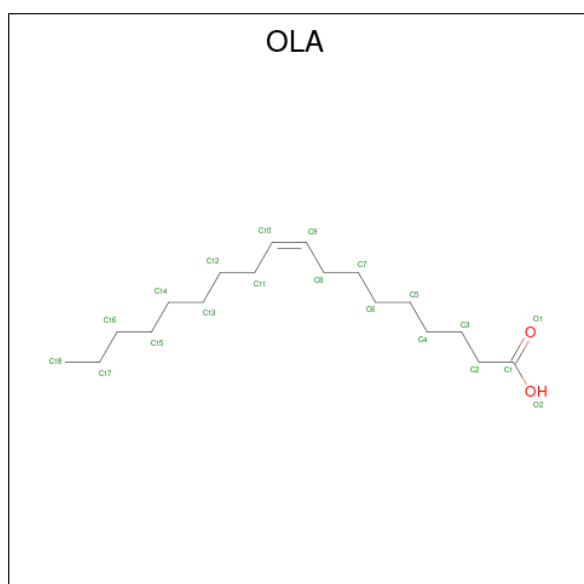
- Molecule 1 is a protein called Fatty acid-binding protein homolog.

Mol	Chain	Residues	Atoms						Trace
1	A	155	Total	C	H	N	O	S	0
			2546	811	1254	231	245	5	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P55776
A	-10	ARG	-	expression tag	UNP P55776
A	-9	GLY	-	expression tag	UNP P55776
A	-8	SER	-	expression tag	UNP P55776
A	-7	HIS	-	expression tag	UNP P55776
A	-6	HIS	-	expression tag	UNP P55776
A	-5	HIS	-	expression tag	UNP P55776
A	-4	HIS	-	expression tag	UNP P55776
A	-3	HIS	-	expression tag	UNP P55776
A	-2	HIS	-	expression tag	UNP P55776
A	-1	GLY	-	expression tag	UNP P55776
A	0	SER	-	expression tag	UNP P55776

- Molecule 2 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).



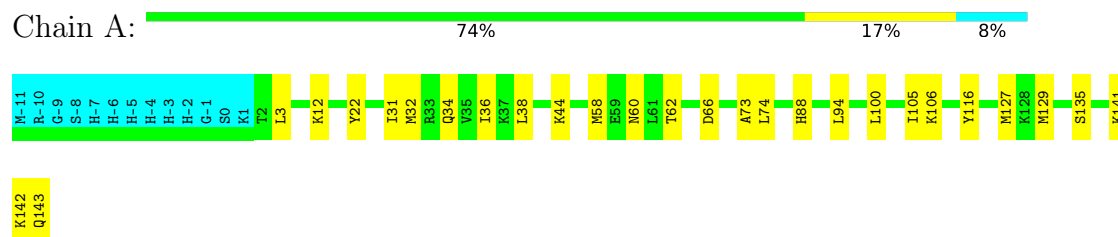
Mol	Chain	Residues	Atoms			
			Total	C	H	O
2	A	1	53	18	33	2

4 Residue-property plots [i](#)

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: Fatty acid-binding protein homolog

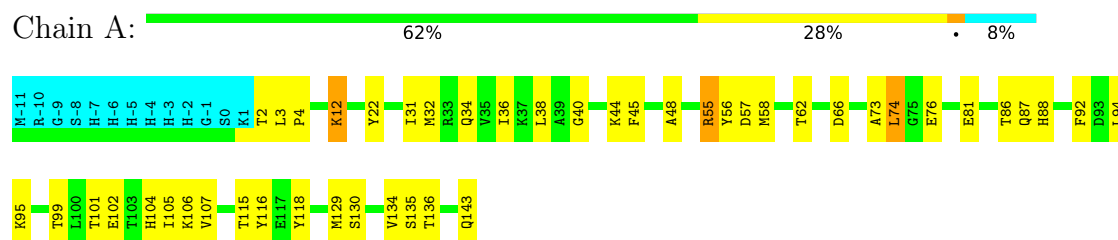


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

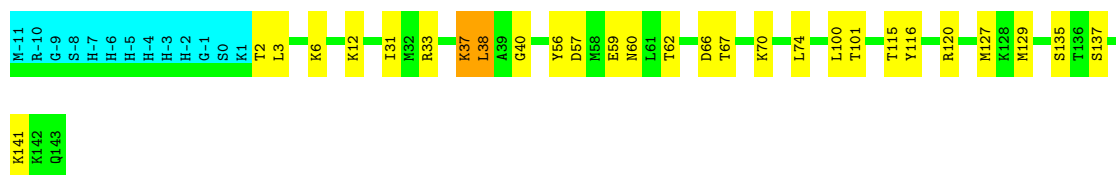
- Molecule 1: Fatty acid-binding protein homolog



4.2.2 Score per residue for model 2

- Molecule 1: Fatty acid-binding protein homolog

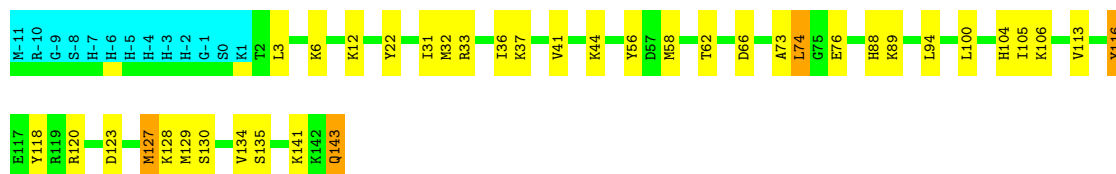




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Fatty acid-binding protein homolog

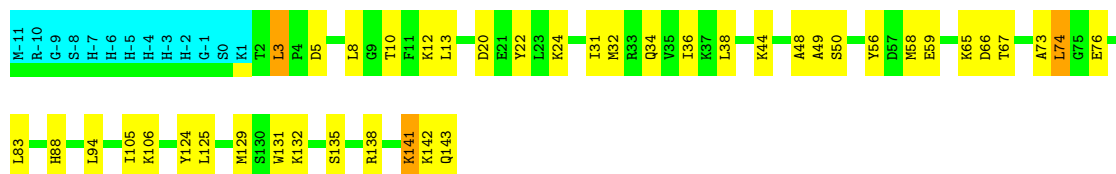
Chain A: 67% 22% 8%



4.2.4 Score per residue for model 4

- Molecule 1: Fatty acid-binding protein homolog

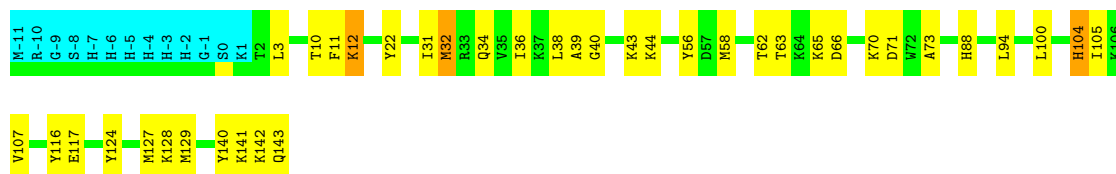
Chain A: 65% 25% 8%



4.2.5 Score per residue for model 5

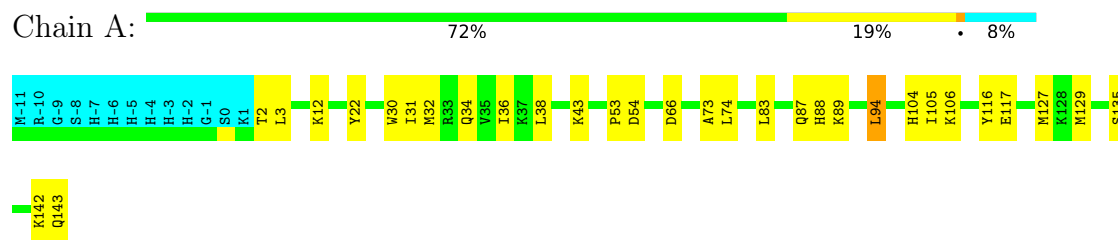
- Molecule 1: Fatty acid-binding protein homolog

Chain A: 66% 23% 8%



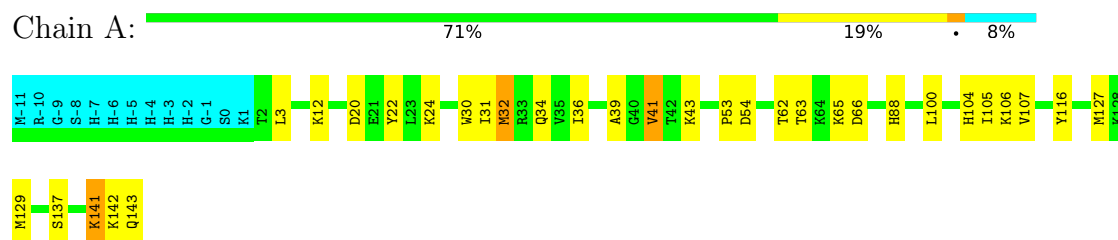
4.2.6 Score per residue for model 6

- Molecule 1: Fatty acid-binding protein homolog



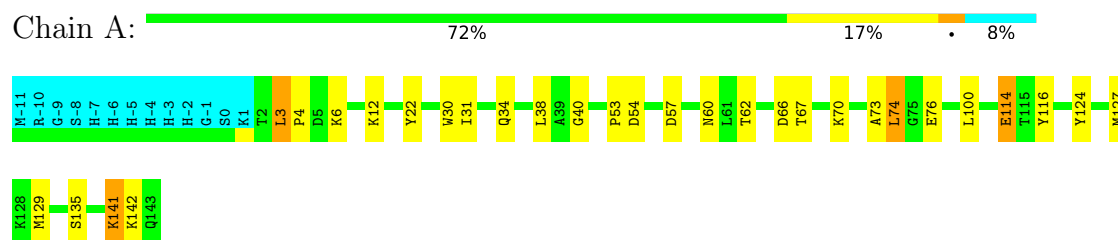
4.2.7 Score per residue for model 7

- Molecule 1: Fatty acid-binding protein homolog



4.2.8 Score per residue for model 8

- Molecule 1: Fatty acid-binding protein homolog



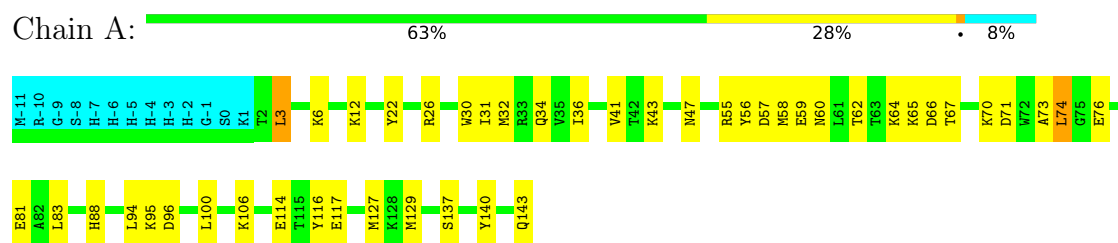
4.2.9 Score per residue for model 9

- Molecule 1: Fatty acid-binding protein homolog



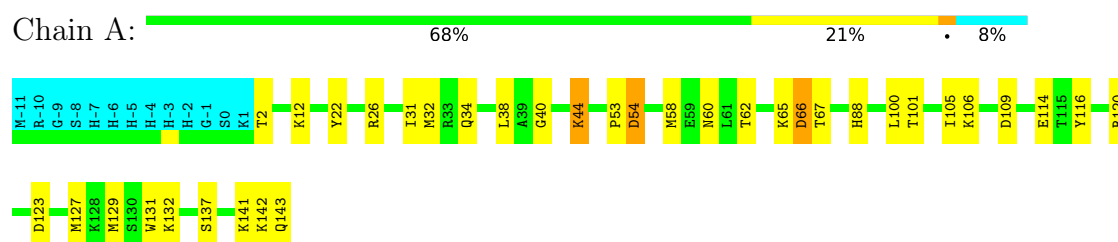
4.2.10 Score per residue for model 10

- Molecule 1: Fatty acid-binding protein homolog



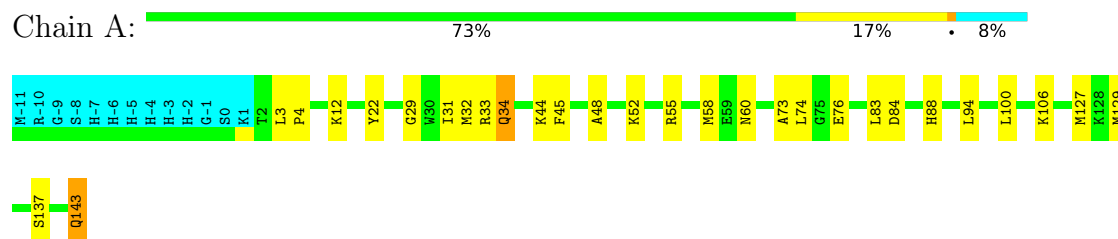
4.2.11 Score per residue for model 11

- Molecule 1: Fatty acid-binding protein homolog



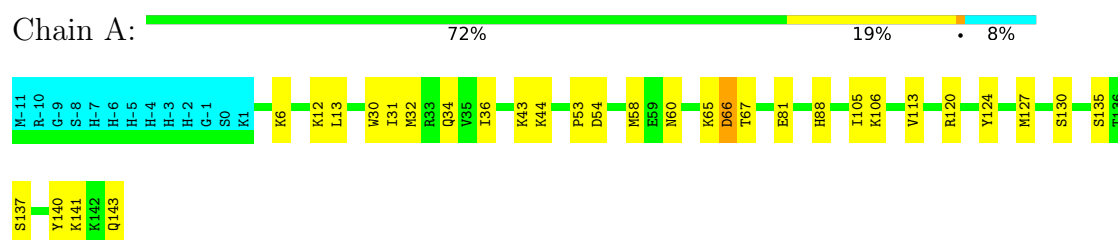
4.2.12 Score per residue for model 12

- Molecule 1: Fatty acid-binding protein homolog



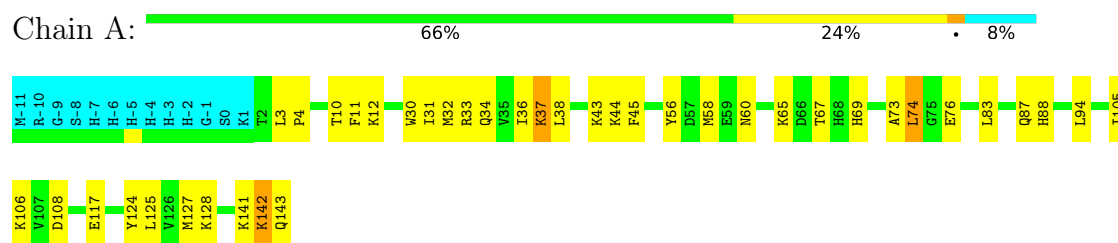
4.2.13 Score per residue for model 13

- Molecule 1: Fatty acid-binding protein homolog



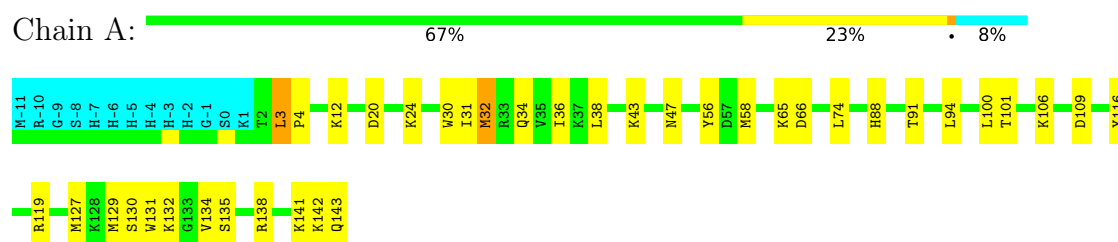
4.2.14 Score per residue for model 14

- Molecule 1: Fatty acid-binding protein homolog



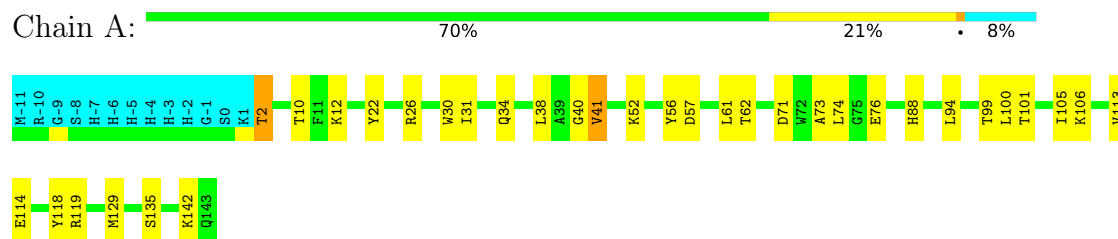
4.2.15 Score per residue for model 15

- Molecule 1: Fatty acid-binding protein homolog



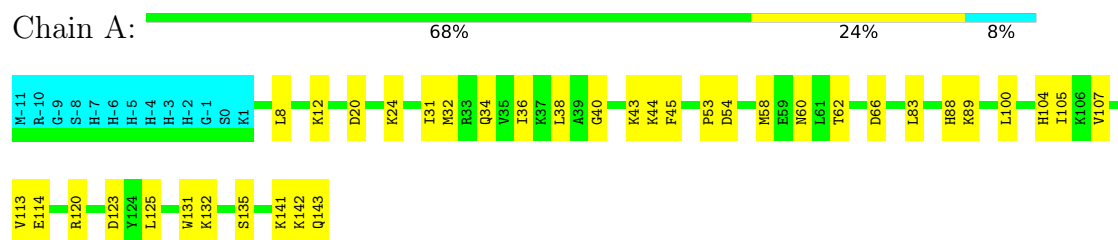
4.2.16 Score per residue for model 16

- Molecule 1: Fatty acid-binding protein homolog



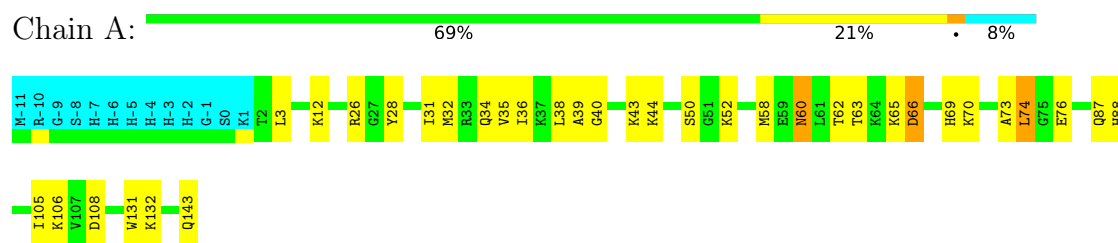
4.2.17 Score per residue for model 17

- Molecule 1: Fatty acid-binding protein homolog



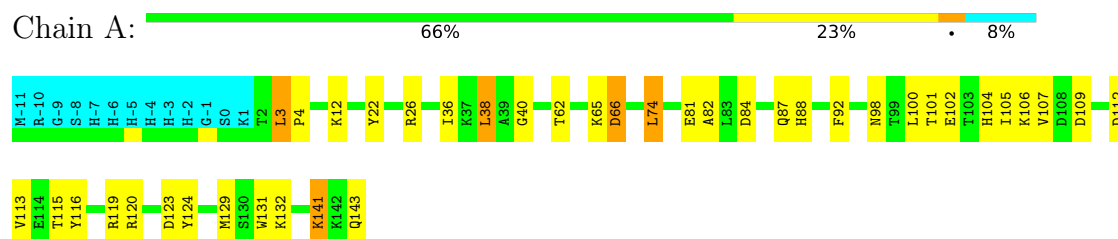
4.2.18 Score per residue for model 18

- Molecule 1: Fatty acid-binding protein homolog



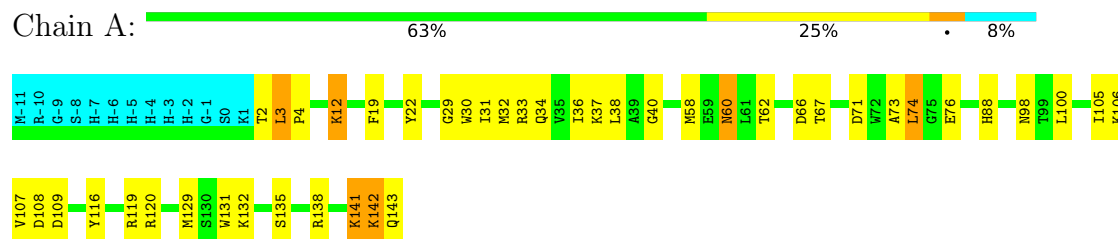
4.2.19 Score per residue for model 19

- Molecule 1: Fatty acid-binding protein homolog



4.2.20 Score per residue for model 20

- Molecule 1: Fatty acid-binding protein homolog



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
ARIA	structure calculation	2.3.1
CNS	structure calculation	1.2

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	3
Total number of shifts	5308
Number of shifts mapped to atoms	5308
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLA

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	0.44±0.03	0±0/1211 (0.0± 0.0%)	0.71±0.02	0±0/1628 (0.0± 0.0%)
All	All	0.44	2/24220 (0.0%)	0.71	0/32560 (0.0%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	116	TYR	CE1-CZ	7.53	1.56	1.38	3	1
1	A	116	TYR	CE2-CZ	-7.52	1.20	1.38	3	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1184	1153	1149	22±4
2	A	20	33	33	2±2
All	All	24080	23720	23640	448

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ALA:HB3	1:A:55:ARG:HD2	0.94	1.34	1	1
1:A:41:VAL:HB	1:A:62:THR:HG22	0.80	1.50	9	5
1:A:88:HIS:HA	1:A:107:VAL:HG13	0.72	1.62	5	3
2:A:1001:OLA:H31	2:A:1001:OLA:H182	0.70	1.64	4	1
1:A:88:HIS:HA	1:A:107:VAL:HG23	0.69	1.63	17	2
1:A:43:LYS:HE3	1:A:127:MET:SD	0.68	2.28	13	3
1:A:22:TYR:CE1	1:A:129:MET:HE3	0.68	2.24	8	1
2:A:1001:OLA:H141	2:A:1001:OLA:C10	0.65	2.21	20	3
1:A:31:ILE:HD12	1:A:31:ILE:H	0.65	1.52	7	2
1:A:31:ILE:H	1:A:31:ILE:HD12	0.64	1.53	18	5
1:A:3:LEU:HB2	1:A:56:TYR:CE1	0.64	2.28	3	6
1:A:2:THR:HA	1:A:56:TYR:OH	0.63	1.94	16	1
2:A:1001:OLA:H41	2:A:1001:OLA:H182	0.63	1.69	16	2
1:A:88:HIS:HB2	1:A:105:ILE:O	0.62	1.94	11	13
1:A:12:LYS:HB3	1:A:143:GLN:NE2	0.61	2.10	13	8
1:A:52:LYS:O	1:A:55:ARG:HB3	0.60	1.95	12	1
1:A:22:TYR:CE1	1:A:129:MET:HE2	0.60	2.31	7	12
1:A:32:MET:O	1:A:36:ILE:HG12	0.60	1.96	7	1
1:A:48:ALA:HB3	1:A:55:ARG:CG	0.60	2.27	12	1
1:A:39:ALA:HA	1:A:63:THR:OG1	0.60	1.96	18	2
1:A:124:TYR:CD2	1:A:141:LYS:HB3	0.59	2.32	13	4
1:A:74:LEU:HD11	1:A:94:LEU:HD23	0.59	1.74	6	2
1:A:34:GLN:O	1:A:38:LEU:HD23	0.58	1.98	6	12
1:A:116:TYR:CE1	1:A:129:MET:HE3	0.58	2.34	10	7
1:A:40:GLY:O	1:A:62:THR:HA	0.57	2.00	18	10
1:A:124:TYR:CE2	1:A:141:LYS:HB3	0.56	2.36	4	4
1:A:41:VAL:CB	1:A:62:THR:HG22	0.56	2.30	7	3
1:A:65:LYS:HG3	1:A:66:ASP:H	0.56	1.61	13	4
1:A:73:ALA:O	1:A:76:GLU:HB3	0.55	2.01	20	8
1:A:120:ARG:NH2	1:A:123:ASP:HA	0.55	2.17	19	4
1:A:44:LYS:O	1:A:58:MET:HA	0.55	2.02	3	9
1:A:32:MET:O	1:A:36:ILE:HG13	0.55	2.02	3	10
1:A:74:LEU:HD21	1:A:94:LEU:HD23	0.55	1.78	9	1
1:A:48:ALA:HB3	1:A:55:ARG:HB2	0.54	1.78	12	1
1:A:57:ASP:OD2	1:A:70:LYS:HA	0.54	2.02	8	3
1:A:88:HIS:CB	1:A:106:LYS:HA	0.54	2.32	15	14
1:A:127:MET:O	1:A:137:SER:HA	0.54	2.03	11	5
1:A:141:LYS:HD3	1:A:142:LYS:O	0.54	2.03	8	3
1:A:131:TRP:CD1	1:A:132:LYS:HG2	0.53	2.38	18	4
1:A:28:TYR:OH	2:A:1001:OLA:H141	0.53	2.03	18	1
1:A:88:HIS:CE1	1:A:104:HIS:HB2	0.53	2.39	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:LEU:HD22	1:A:83:LEU:H	0.53	1.63	10	3
1:A:60:ASN:HB2	1:A:67:THR:OG1	0.53	2.03	20	4
1:A:43:LYS:HE2	1:A:127:MET:SD	0.53	2.43	9	1
1:A:50:SER:OG	1:A:52:LYS:HE2	0.53	2.04	18	1
1:A:118:TYR:CE1	1:A:127:MET:HE1	0.52	2.39	3	1
1:A:73:ALA:O	1:A:76:GLU:HB2	0.52	2.04	16	2
1:A:43:LYS:HE2	1:A:127:MET:HE1	0.52	1.82	6	1
1:A:88:HIS:CE1	1:A:104:HIS:HB3	0.52	2.40	5	4
1:A:53:PRO:O	1:A:54:ASP:HB3	0.52	2.05	17	6
1:A:74:LEU:HD13	1:A:74:LEU:H	0.51	1.65	19	8
1:A:33:ARG:O	1:A:37:LYS:HG2	0.51	2.05	3	1
1:A:67:THR:HG23	1:A:83:LEU:HD13	0.51	1.82	10	2
1:A:48:ALA:HB3	1:A:55:ARG:CB	0.51	2.35	12	1
1:A:100:LEU:HD23	1:A:101:THR:N	0.51	2.21	15	5
1:A:8:LEU:HD23	1:A:45:PHE:HB3	0.51	1.82	17	1
1:A:3:LEU:HD23	1:A:4:PRO:HD2	0.50	1.83	12	7
1:A:11:PHE:HA	1:A:142:LYS:HA	0.50	1.83	14	3
1:A:19:PHE:CD1	1:A:138:ARG:HD2	0.50	2.42	20	1
1:A:12:LYS:HG2	1:A:142:LYS:O	0.50	2.06	11	2
1:A:12:LYS:HB3	1:A:143:GLN:CD	0.50	2.32	3	2
1:A:105:ILE:HG12	1:A:113:VAL:HG23	0.49	1.84	9	1
1:A:102:GLU:O	1:A:115:THR:HA	0.49	2.08	19	2
1:A:36:ILE:HG21	2:A:1001:OLA:H182	0.49	1.85	15	2
1:A:31:ILE:HD12	1:A:31:ILE:N	0.49	2.22	2	7
1:A:38:LEU:C	1:A:38:LEU:HD13	0.49	2.32	14	2
1:A:141:LYS:HD2	1:A:142:LYS:O	0.49	2.07	17	1
2:A:1001:OLA:H141	2:A:1001:OLA:C9	0.49	2.37	13	2
1:A:32:MET:HE1	2:A:1001:OLA:H132	0.49	1.85	5	2
1:A:117:GLU:O	1:A:127:MET:HA	0.49	2.06	5	3
1:A:12:LYS:HG2	1:A:143:GLN:HE21	0.49	1.66	14	2
1:A:131:TRP:CD1	1:A:132:LYS:HD3	0.49	2.43	19	4
1:A:36:ILE:CG2	2:A:1001:OLA:H182	0.49	2.38	15	1
1:A:5:ASP:HA	1:A:8:LEU:HD12	0.49	1.85	4	1
1:A:2:THR:HA	1:A:56:TYR:HH	0.48	1.68	16	1
1:A:81:GLU:HA	1:A:87:GLN:NE2	0.48	2.23	19	1
1:A:12:LYS:O	1:A:12:LYS:HD3	0.48	2.08	20	2
1:A:12:LYS:CG	1:A:143:GLN:HE21	0.48	2.21	10	1
1:A:12:LYS:N	1:A:141:LYS:O	0.48	2.47	14	11
1:A:33:ARG:O	1:A:37:LYS:HG3	0.48	2.09	14	1
1:A:48:ALA:O	1:A:50:SER:N	0.48	2.47	4	1
1:A:65:LYS:O	1:A:83:LEU:HD12	0.48	2.09	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:SER:HA	1:A:134:VAL:O	0.47	2.08	1	4
1:A:124:TYR:CE2	1:A:141:LYS:HE3	0.47	2.44	14	2
1:A:36:ILE:HG21	2:A:1001:OLA:H183	0.47	1.85	18	1
1:A:13:LEU:HD23	1:A:140:TYR:CE2	0.47	2.44	13	1
1:A:67:THR:HG22	1:A:81:GLU:O	0.47	2.10	10	3
1:A:106:LYS:HB2	1:A:109:ASP:O	0.47	2.09	15	4
1:A:43:LYS:HE3	1:A:60:ASN:ND2	0.47	2.24	18	1
1:A:88:HIS:HA	1:A:107:VAL:CG2	0.47	2.39	17	2
1:A:6:LYS:O	1:A:120:ARG:HD3	0.47	2.09	13	2
1:A:58:MET:HE1	1:A:60:ASN:OD1	0.47	2.10	17	3
1:A:33:ARG:O	1:A:37:LYS:HD2	0.47	2.09	2	1
1:A:30:TRP:O	1:A:34:GLN:HG2	0.47	2.10	14	8
1:A:20:ASP:OD1	1:A:24:LYS:HE3	0.47	2.09	15	3
1:A:10:THR:HG23	1:A:143:GLN:HB2	0.46	1.87	5	2
1:A:45:PHE:CE2	1:A:58:MET:HG3	0.46	2.45	12	3
1:A:10:THR:O	1:A:142:LYS:HA	0.46	2.10	4	1
1:A:127:MET:SD	1:A:140:TYR:HE2	0.46	2.33	10	1
1:A:104:HIS:CE1	1:A:114:GLU:HB3	0.46	2.45	17	2
1:A:127:MET:HE2	2:A:1001:OLA:O2	0.46	2.11	15	1
1:A:106:LYS:CG	1:A:112:ASP:HB3	0.46	2.41	19	1
1:A:36:ILE:HA	2:A:1001:OLA:H9	0.46	1.88	18	6
1:A:48:ALA:HA	1:A:57:ASP:OD1	0.46	2.10	1	1
1:A:31:ILE:O	1:A:34:GLN:HG3	0.46	2.10	12	1
1:A:20:ASP:OD1	1:A:24:LYS:HE2	0.45	2.10	4	1
1:A:58:MET:HE3	1:A:60:ASN:OD1	0.45	2.11	20	1
1:A:95:LYS:HE3	1:A:99:THR:HG21	0.45	1.86	1	1
1:A:95:LYS:HG3	1:A:96:ASP:OD1	0.45	2.11	10	1
1:A:84:ASP:HA	2:A:1001:OLA:H142	0.45	1.88	12	1
1:A:141:LYS:HG3	1:A:142:LYS:O	0.45	2.10	15	2
1:A:65:LYS:HE2	1:A:83:LEU:O	0.45	2.12	4	1
1:A:32:MET:HE2	2:A:1001:OLA:H132	0.45	1.89	12	2
1:A:22:TYR:O	1:A:26:ARG:HB2	0.45	2.11	19	1
1:A:82:ALA:HB1	1:A:84:ASP:OD1	0.45	2.11	19	1
1:A:59:GLU:HG3	1:A:67:THR:O	0.45	2.11	9	4
1:A:115:THR:O	1:A:129:MET:HG3	0.45	2.12	2	1
1:A:106:LYS:HB3	1:A:108:ASP:OD2	0.44	2.12	14	2
1:A:128:LYS:HE2	1:A:130:SER:OG	0.44	2.11	3	1
1:A:26:ARG:HA	1:A:131:TRP:CD1	0.44	2.48	11	2
1:A:10:THR:OG1	1:A:44:LYS:HG2	0.44	2.11	14	1
1:A:89:LYS:CG	1:A:105:ILE:HB	0.44	2.42	3	2
1:A:10:THR:O	1:A:142:LYS:HD2	0.44	2.13	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:VAL:HA	1:A:61:LEU:O	0.44	2.12	16	1
1:A:3:LEU:HD21	1:A:100:LEU:HD12	0.44	1.90	15	1
1:A:88:HIS:HB2	1:A:106:LYS:HA	0.44	1.89	12	3
1:A:52:LYS:HD2	1:A:71:ASP:OD1	0.44	2.13	16	1
1:A:98:ASN:OD1	1:A:120:ARG:HB3	0.44	2.12	20	1
1:A:74:LEU:CD2	1:A:94:LEU:HD23	0.43	2.43	9	1
1:A:3:LEU:HB2	1:A:56:TYR:CZ	0.43	2.48	2	2
1:A:48:ALA:HB3	1:A:55:ARG:HG3	0.43	1.89	12	1
1:A:32:MET:HE1	2:A:1001:OLA:H111	0.43	1.89	18	1
1:A:12:LYS:HG3	1:A:142:LYS:O	0.43	2.13	5	2
1:A:127:MET:SD	1:A:140:TYR:CE2	0.43	3.11	10	1
1:A:43:LYS:HD2	1:A:58:MET:CE	0.43	2.43	18	1
1:A:92:PHE:HA	1:A:101:THR:O	0.43	2.13	1	1
1:A:37:LYS:HG3	1:A:38:LEU:HD22	0.43	1.89	20	1
1:A:13:LEU:HD11	1:A:138:ARG:NH2	0.43	2.28	4	1
1:A:140:TYR:OH	2:A:1001:OLA:O1	0.43	2.35	5	1
1:A:58:MET:SD	1:A:69:HIS:HD2	0.43	2.37	18	1
1:A:44:LYS:O	1:A:58:MET:HG2	0.43	2.13	14	2
1:A:43:LYS:HZ1	2:A:1001:OLA:C1	0.43	2.27	17	2
1:A:6:LYS:N	1:A:6:LYS:HD2	0.43	2.29	3	1
1:A:116:TYR:HB3	1:A:127:MET:HE3	0.43	1.89	7	1
1:A:105:ILE:HA	1:A:113:VAL:HG12	0.42	1.89	16	1
1:A:129:MET:HB2	1:A:136:THR:CG2	0.42	2.44	1	1
1:A:47:ASN:HA	1:A:56:TYR:CD2	0.42	2.49	10	2
1:A:98:ASN:O	1:A:119:ARG:HA	0.42	2.13	19	1
1:A:38:LEU:HD13	1:A:38:LEU:C	0.42	2.38	2	1
1:A:116:TYR:N	1:A:116:TYR:CD1	0.42	2.88	3	1
1:A:117:GLU:CG	1:A:128:LYS:HB3	0.42	2.44	5	1
1:A:73:ALA:HB3	1:A:76:GLU:CG	0.42	2.43	16	1
1:A:116:TYR:CD1	1:A:116:TYR:N	0.42	2.87	2	1
1:A:138:ARG:HD3	2:A:1001:OLA:O1	0.42	2.14	15	1
1:A:121:ASP:HB3	1:A:126:VAL:HG21	0.42	1.92	9	1
1:A:55:ARG:HD3	1:A:71:ASP:OD2	0.42	2.14	10	1
1:A:106:LYS:HE2	1:A:108:ASP:OD2	0.42	2.15	20	1
1:A:36:ILE:HG12	2:A:1001:OLA:C9	0.42	2.45	13	1
1:A:43:LYS:NZ	1:A:127:MET:HE1	0.42	2.30	14	1
1:A:32:MET:HA	1:A:35:VAL:CG2	0.42	2.45	18	1
1:A:74:LEU:HD22	1:A:74:LEU:N	0.42	2.30	18	1
1:A:88:HIS:CA	1:A:107:VAL:HG23	0.41	2.40	17	1
1:A:12:LYS:HD2	1:A:143:GLN:NE2	0.41	2.30	7	1
1:A:83:LEU:O	2:A:1001:OLA:H132	0.41	2.15	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:THR:HA	1:A:118:TYR:O	0.41	2.15	1	2
1:A:13:LEU:HB2	1:A:140:TYR:CE1	0.41	2.51	13	1
1:A:29:GLY:O	1:A:33:ARG:HG3	0.41	2.16	20	2
1:A:77:GLU:HA	1:A:90:ILE:O	0.41	2.14	9	1
1:A:36:ILE:HG12	2:A:1001:OLA:H10	0.41	1.93	6	1
1:A:12:LYS:HG2	1:A:143:GLN:CD	0.41	2.40	19	1
1:A:12:LYS:HD3	1:A:12:LYS:O	0.41	2.16	1	1
1:A:6:LYS:HD2	1:A:6:LYS:H	0.41	1.75	3	1
1:A:83:LEU:H	1:A:83:LEU:HD22	0.41	1.75	6	1
1:A:22:TYR:OH	1:A:114:GLU:HG3	0.41	2.15	8	1
1:A:116:TYR:HB3	1:A:127:MET:SD	0.41	2.56	8	1
1:A:65:LYS:HD3	1:A:66:ASP:N	0.41	2.31	10	1
1:A:58:MET:SD	1:A:69:HIS:CD2	0.41	3.14	14	1
1:A:117:GLU:HG2	1:A:128:LYS:O	0.41	2.16	14	1
1:A:43:LYS:HD2	1:A:58:MET:HE1	0.41	1.93	15	1
1:A:39:ALA:O	1:A:63:THR:HG21	0.41	2.15	7	1
1:A:86:THR:OG1	1:A:88:HIS:HD2	0.41	1.99	9	1
1:A:48:ALA:CB	1:A:55:ARG:HB2	0.40	2.47	12	1
1:A:81:GLU:HA	1:A:86:THR:O	0.40	2.16	1	1
1:A:26:ARG:NH2	1:A:114:GLU:HB2	0.40	2.32	10	1
1:A:129:MET:O	1:A:135:SER:HA	0.40	2.17	20	1
1:A:116:TYR:HB3	1:A:127:MET:HE2	0.40	1.92	6	1
1:A:31:ILE:H	1:A:31:ILE:CD1	0.40	2.27	7	1
1:A:32:MET:HE2	1:A:36:ILE:HD11	0.40	1.94	7	1
1:A:124:TYR:CZ	1:A:141:LYS:HE3	0.40	2.52	9	1
1:A:105:ILE:HG12	1:A:113:VAL:HG12	0.40	1.93	3	1
1:A:36:ILE:HG23	2:A:1001:OLA:C6	0.40	2.46	5	1
1:A:26:ARG:NH1	1:A:114:GLU:HB2	0.40	2.32	16	1
1:A:36:ILE:CG2	2:A:1001:OLA:H183	0.40	2.47	18	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	141/155 (91%)	128±3 (91±2%)	12±2 (9±2%)	1±1 (1±1%)	16	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2820/3100 (91%)	2554 (91%)	242 (9%)	24 (1%)	16	66

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	66	ASP	16
1	A	142	LYS	3
1	A	49	ALA	1
1	A	30	TRP	1
1	A	54	ASP	1
1	A	113	VAL	1
1	A	71	ASP	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	128/139 (92%)	120±4 (94±3%)	7±1 (5±1%)	22	72
All	All	2534/2780 (91%)	2401 (95%)	133 (5%)	22	72

All 37 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	31	ILE	11
1	A	135	SER	11
1	A	74	LEU	10
1	A	94	LEU	9
1	A	3	LEU	9
1	A	100	LEU	8
1	A	2	THR	6
1	A	32	MET	6
1	A	143	GLN	5
1	A	141	LYS	5
1	A	12	LYS	4
1	A	87	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	60	ASN	4
1	A	125	LEU	3
1	A	65	LYS	3
1	A	70	LYS	3
1	A	41	VAL	3
1	A	119	ARG	3
1	A	55	ARG	2
1	A	37	LYS	2
1	A	38	LEU	2
1	A	104	HIS	2
1	A	6	LYS	2
1	A	114	GLU	2
1	A	113	VAL	2
1	A	127	MET	1
1	A	71	ASP	1
1	A	137	SER	1
1	A	101	THR	1
1	A	64	LYS	1
1	A	44	LYS	1
1	A	34	GLN	1
1	A	130	SER	1
1	A	91	THR	1
1	A	57	ASP	1
1	A	89	LYS	1
1	A	92	PHE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	OLA	A	1001	-	19,19,19	0.49±0.03	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	OLA	A	1001	-	19,19,19	0.64±0.03	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLA	A	1001	-	-	0±0,17,17,17	-

There are no bond-length outliers.

There are no bond-angle outliers.

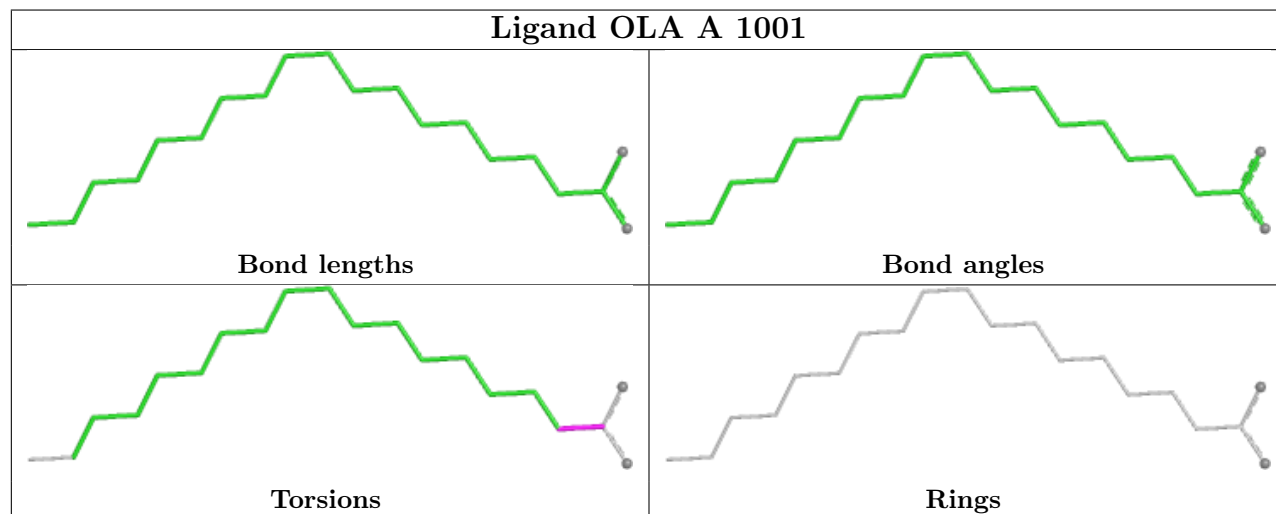
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 83% for the well-defined parts and 79% 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	1770
Number of shifts mapped to atoms	1770
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	-0.16 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	-0.18 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	138	-0.57 ± 0.42	None needed (imprecise)

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 83%, i.e. 1657 atoms were assigned a chemical shift out of a possible 1994. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	563/710 (79%)	285/288 (99%)	142/284 (50%)	136/138 (99%)
Sidechain	944/1084 (87%)	635/691 (92%)	299/344 (87%)	10/49 (20%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	150/200 (75%)	76/96 (79%)	70/93 (75%)	4/11 (36%)
Overall	1657/1994 (83%)	996/1075 (93%)	511/721 (71%)	150/198 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1719 atoms were assigned a chemical shift out of a possible 2174. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	581/777 (75%)	294/316 (93%)	149/310 (48%)	138/151 (91%)
Sidechain	984/1149 (86%)	662/733 (90%)	312/363 (86%)	10/53 (19%)
Aromatic	154/248 (62%)	78/120 (65%)	72/105 (69%)	4/23 (17%)
Overall	1719/2174 (79%)	1034/1169 (88%)	533/778 (69%)	152/227 (67%)

7.1.4 Statistically unusual chemical shifts ⓘ

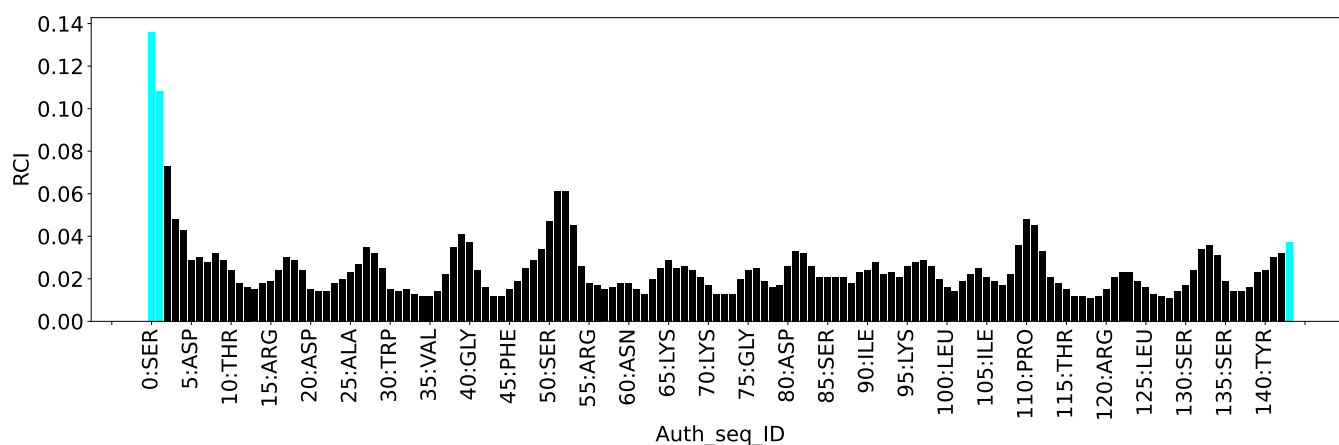
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	62	THR	HG1	6.74	0.08 – 2.19	26.6
1	A	136	THR	HG1	4.39	0.08 – 2.19	15.4
1	A	67	THR	HG1	4.23	0.08 – 2.19	14.7
1	A	56	TYR	HB2	-0.49	1.09 – 4.72	-9.4
1	A	90	ILE	HB	-0.23	0.35 – 3.22	-7.0
1	A	102	GLU	HG3	1.04	1.20 – 3.30	-5.8
1	A	138	ARG	CB	40.21	21.74 – 39.52	5.4
1	A	26	ARG	HD2	1.93	1.97 – 4.26	-5.2
1	A	90	ILE	HG12	-0.73	-0.69 – 3.24	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_2*

7.2.1 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	1770
Number of shifts mapped to atoms	1770
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	-0.18 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	-0.18 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	138	-0.57 ± 0.48	None needed (imprecise)

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 83%, i.e. 1657 atoms were assigned a chemical shift out of a possible 1994. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	563/710 (79%)	285/288 (99%)	142/284 (50%)	136/138 (99%)
Sidechain	944/1084 (87%)	635/691 (92%)	299/344 (87%)	10/49 (20%)
Aromatic	150/200 (75%)	76/96 (79%)	70/93 (75%)	4/11 (36%)
Overall	1657/1994 (83%)	996/1075 (93%)	511/721 (71%)	150/198 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1719 atoms were assigned a chemical shift out of a possible 2174. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	581/777 (75%)	294/316 (93%)	149/310 (48%)	138/151 (91%)
Sidechain	984/1149 (86%)	662/733 (90%)	312/363 (86%)	10/53 (19%)
Aromatic	154/248 (62%)	78/120 (65%)	72/105 (69%)	4/23 (17%)
Overall	1719/2174 (79%)	1034/1169 (88%)	533/778 (69%)	152/227 (67%)

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.

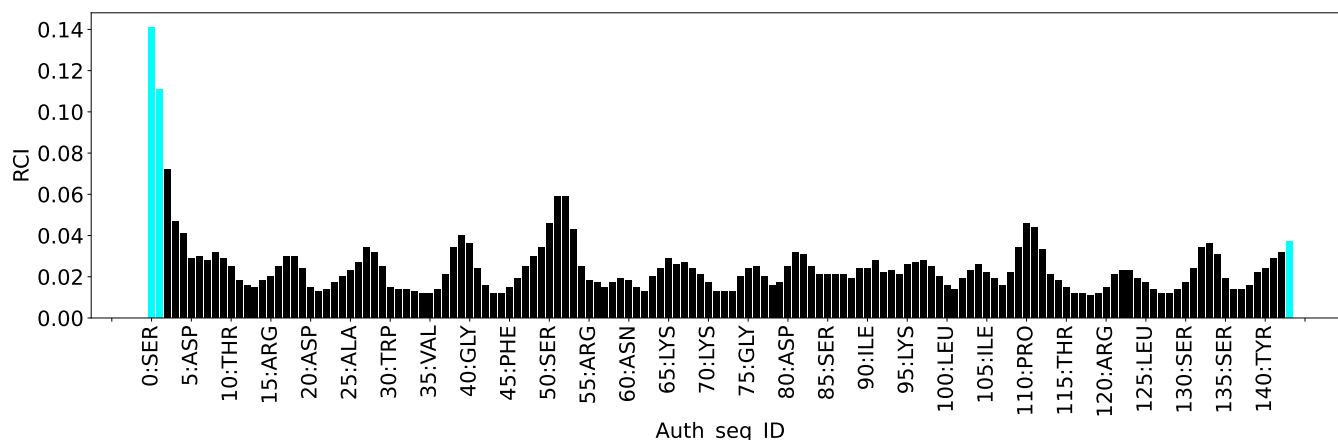
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	A	62	THR	HG1	6.72	0.08 – 2.19	26.5
2	A	136	THR	HG1	4.39	0.08 – 2.19	15.4
2	A	67	THR	HG1	4.25	0.08 – 2.19	14.8
2	A	56	TYR	HB2	-0.49	1.09 – 4.72	-9.4
2	A	90	ILE	HB	-0.23	0.35 – 3.22	-7.0
2	A	102	GLU	HG3	1.04	1.20 – 3.30	-5.8
2	A	138	ARG	CB	40.21	21.74 – 39.52	5.4
2	A	26	ARG	HD2	1.93	1.97 – 4.26	-5.2
2	A	90	ILE	HG12	-0.73	-0.69 – 3.24	-5.1

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:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1_2_3*

7.3.1 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	1768
Number of shifts mapped to atoms	1768
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.3.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	-0.17 ± 0.17	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\beta$	140	-0.17 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	137	-0.55 ± 0.50	None needed (imprecise)

7.3.3 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 83%, i.e. 1655 atoms were assigned a chemical shift out of a possible 1994. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	561/710 (79%)	284/288 (99%)	142/284 (50%)	135/138 (98%)
Sidechain	944/1084 (87%)	635/691 (92%)	299/344 (87%)	10/49 (20%)
Aromatic	150/200 (75%)	76/96 (79%)	70/93 (75%)	4/11 (36%)
Overall	1655/1994 (83%)	995/1075 (93%)	511/721 (71%)	149/198 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1717 atoms were assigned a chemical shift out of a possible 2174. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	579/777 (75%)	293/316 (93%)	149/310 (48%)	137/151 (91%)
Sidechain	984/1149 (86%)	662/733 (90%)	312/363 (86%)	10/53 (19%)
Aromatic	154/248 (62%)	78/120 (65%)	72/105 (69%)	4/23 (17%)
Overall	1717/2174 (79%)	1033/1169 (88%)	533/778 (69%)	151/227 (67%)

7.3.4 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
3	A	62	THR	HG1	6.73	0.08 – 2.19	26.5
3	A	136	THR	HG1	4.39	0.08 – 2.19	15.4
3	A	67	THR	HG1	4.23	0.08 – 2.19	14.7
3	A	56	TYR	HB2	-0.49	1.09 – 4.72	-9.4
3	A	90	ILE	HB	-0.23	0.35 – 3.22	-7.0
3	A	102	GLU	HG3	1.04	1.20 – 3.30	-5.8
3	A	138	ARG	CB	40.21	21.74 – 39.52	5.4

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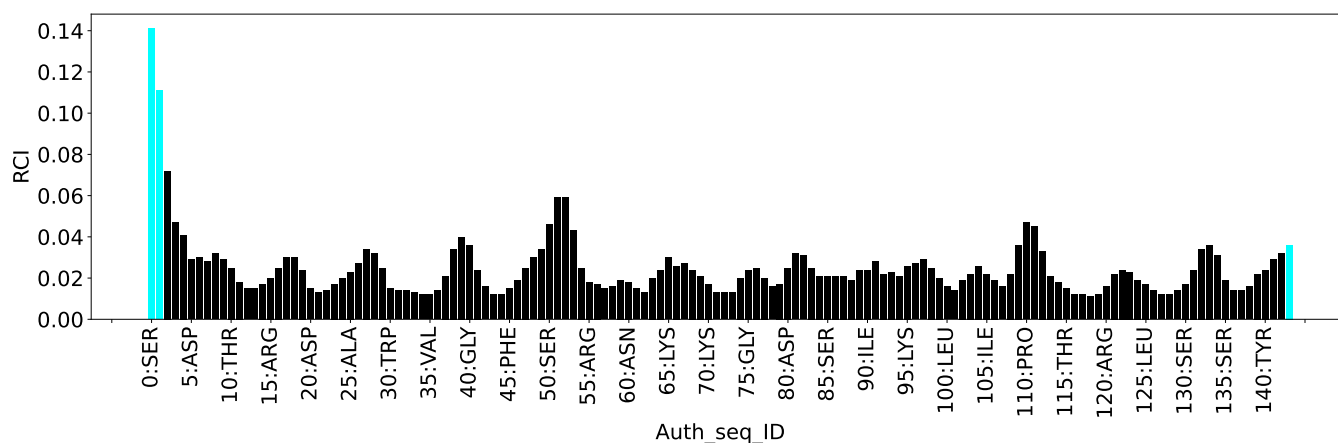
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
3	A	26	ARG	HD2	1.93	1.97 – 4.26	-5.2
3	A	90	ILE	HG12	-0.73	-0.69 – 3.24	-5.1

7.3.5 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	4637
Intra-residue ($ i-j =0$)	1789
Sequential ($ i-j =1$)	942
Medium range ($ i-j >1$ and $ i-j <5$)	457
Long range ($ i-j \geq 5$)	1219
Inter-chain	122
Hydrogen bond restraints	108
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	29.7
Number of long range restraints per residue ¹	8.4

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)	79.5	0.2
0.2-0.5 (Medium)	183.2	0.5
>0.5 (Large)	257.0	4.02

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

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

9 Distance violation analysis ⓘ

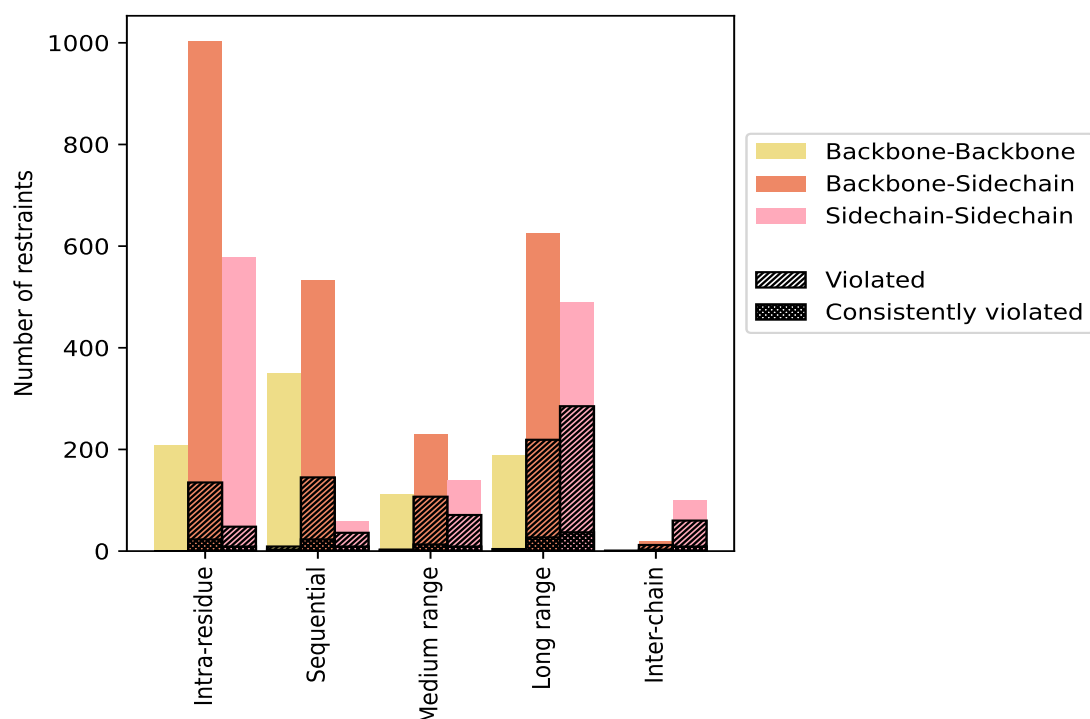
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1789	38.6	183	10.2	3.9	32	1.8	0.7
Backbone-Backbone	208	4.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1003	21.6	135	13.5	2.9	23	2.3	0.5
Sidechain-Sidechain	578	12.5	48	8.3	1.0	9	1.6	0.2
Sequential ($i-j =1$)	942	20.3	190	20.2	4.1	35	3.7	0.8
Backbone-Backbone	350	7.5	9	2.6	0.2	3	0.9	0.1
Backbone-Sidechain	533	11.5	145	27.2	3.1	23	4.3	0.5
Sidechain-Sidechain	59	1.3	36	61.0	0.8	9	15.3	0.2
Medium range ($i-j >1$ & $i-j <5$)	457	9.9	176	38.5	3.8	23	5.0	0.5
Backbone-Backbone	111	2.4	3	2.7	0.1	1	0.9	0.0
Backbone-Sidechain	206	4.4	102	49.5	2.2	13	6.3	0.3
Sidechain-Sidechain	140	3.0	71	50.7	1.5	9	6.4	0.2
Long range ($i-j \geq 5$)	1219	26.3	501	41.1	10.8	62	5.1	1.3
Backbone-Backbone	188	4.1	4	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	542	11.7	212	39.1	4.6	25	4.6	0.5
Sidechain-Sidechain	489	10.5	285	58.3	6.1	37	7.6	0.8
Inter-chain	122	2.6	73	59.8	1.6	12	9.8	0.3
Backbone-Backbone	2	0.0	1	50.0	0.0	0	0.0	0.0
Backbone-Sidechain	20	0.4	12	60.0	0.3	3	15.0	0.1
Sidechain-Sidechain	100	2.2	60	60.0	1.3	9	9.0	0.2
Hydrogen bond	108	2.3	12	11.1	0.3	2	1.9	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4637	100.0	1135	24.5	24.5	166	3.6	3.6
Backbone-Backbone	859	18.5	17	2.0	0.4	4	0.5	0.1
Backbone-Sidechain	2412	52.0	618	25.6	13.3	89	3.7	1.9
Sidechain-Sidechain	1366	29.5	500	36.6	10.8	73	5.3	1.6

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	98	107	85	214	36	540	0.76	3.37	0.66	0.54
2	102	99	79	227	35	542	0.73	3.27	0.63	0.52
3	99	90	81	214	28	512	0.66	2.83	0.54	0.5
4	102	99	77	195	31	504	0.67	4.02	0.56	0.5
5	95	89	76	234	39	533	0.73	3.46	0.63	0.51
6	97	88	77	217	31	510	0.65	3.56	0.57	0.47
7	103	97	86	204	32	522	0.66	3.12	0.55	0.49
8	99	102	84	207	34	526	0.66	3.27	0.57	0.47
9	96	107	77	193	40	513	0.69	3.47	0.58	0.5
10	94	98	79	227	30	528	0.69	2.85	0.57	0.5

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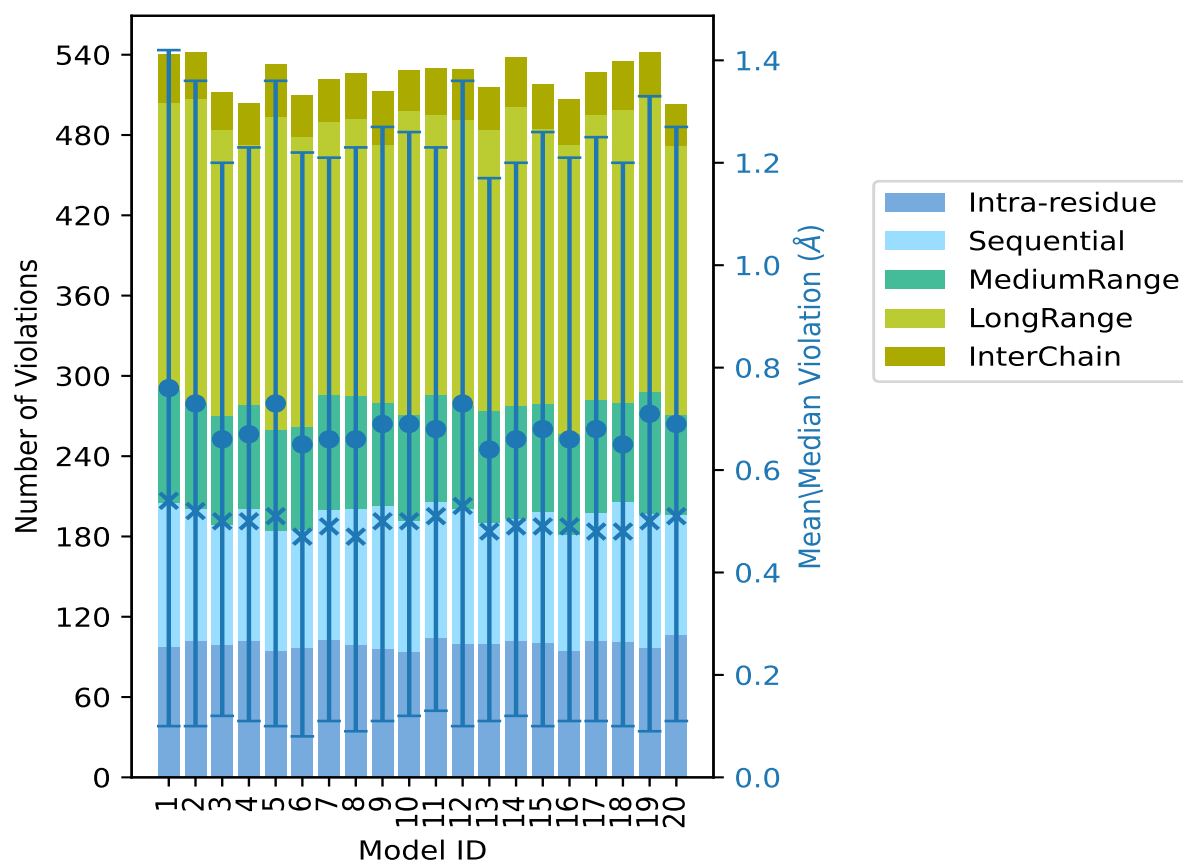
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	104	102	80	209	35	530	0.68	3.35	0.55	0.51
12	100	101	77	213	38	529	0.73	3.58	0.63	0.53
13	100	90	84	210	32	516	0.64	3.03	0.53	0.48
14	102	91	85	223	37	538	0.66	2.82	0.54	0.49
15	101	98	80	206	33	518	0.68	3.7	0.58	0.49
16	95	86	76	216	34	507	0.66	2.96	0.55	0.49
17	102	96	84	213	32	527	0.68	3.13	0.57	0.48
18	101	105	74	219	36	535	0.65	2.8	0.55	0.48
19	97	100	91	220	34	542	0.71	3.76	0.62	0.5
20	107	89	75	201	31	503	0.69	3.6	0.58	0.51

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

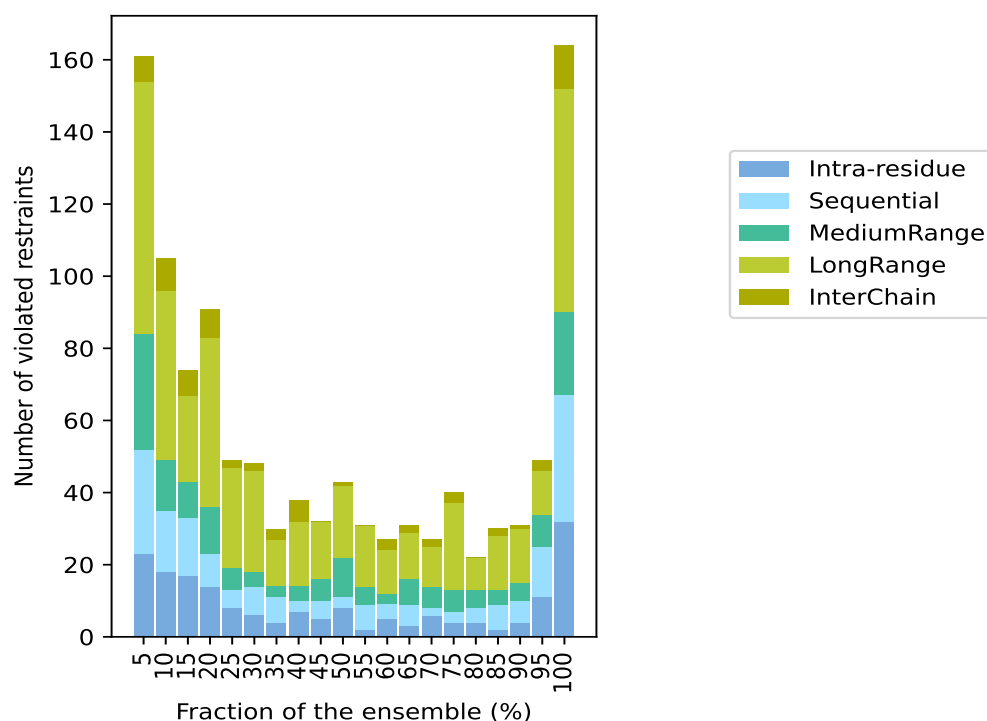
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3406(IR:1606, SQ:752, MR:281, LR:718, IC:49) restraints are 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	%
23	29	32	70	7	161	1	5.0
18	17	14	47	9	105	2	10.0
17	16	10	24	7	74	3	15.0
14	9	13	47	8	91	4	20.0
8	5	6	28	2	49	5	25.0
6	8	4	28	2	48	6	30.0
4	7	3	13	3	30	7	35.0
7	3	4	18	6	38	8	40.0
5	5	6	16	0	32	9	45.0
8	3	11	20	1	43	10	50.0
2	7	5	17	0	31	11	55.0
5	4	3	12	3	27	12	60.0
3	6	7	13	2	31	13	65.0
6	2	6	11	2	27	14	70.0
4	3	6	24	3	40	15	75.0
4	4	5	9	0	22	16	80.0
2	7	4	15	2	30	17	85.0
4	6	5	15	1	31	18	90.0
11	14	9	12	3	49	19	95.0
32	35	23	62	12	164	20	100.0

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

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

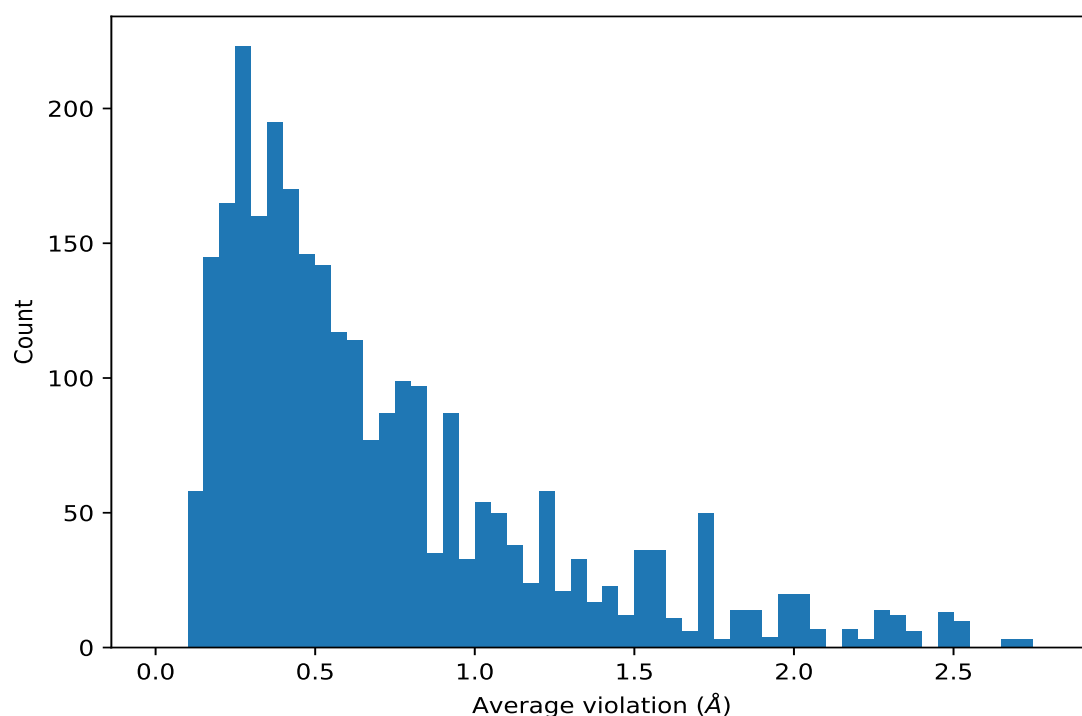
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	20	2.74	0.31	2.73
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD13	20	2.74	0.31	2.73
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD12	20	2.74	0.31	2.73
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	20	2.67	0.31	2.66
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	20	2.67	0.31	2.66
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	20	2.67	0.31	2.66
(2,89)	1:3:A:LEU:HD22	1:9:A:GLY:H	20	2.54	0.37	2.64
(2,89)	1:125:A:LEU:HD12	1:139:A:TYR:H	20	2.54	0.37	2.64
(2,89)	1:3:A:LEU:HD21	1:46:A:ARG:H	20	2.54	0.37	2.64
(2,89)	1:125:A:LEU:HD11	1:9:A:GLY:H	20	2.54	0.37	2.64
(2,89)	1:3:A:LEU:HD23	1:46:A:ARG:H	20	2.54	0.37	2.64
(2,89)	1:3:A:LEU:HD22	1:46:A:ARG:H	20	2.54	0.37	2.64
(2,89)	1:125:A:LEU:HD11	1:139:A:TYR:H	20	2.54	0.37	2.64
(2,89)	1:125:A:LEU:HD13	1:139:A:TYR:H	20	2.54	0.37	2.64
(2,89)	1:125:A:LEU:HD12	1:9:A:GLY:H	20	2.54	0.37	2.64
(2,89)	1:125:A:LEU:HD13	1:9:A:GLY:H	20	2.54	0.37	2.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,756)	1:94:A:LEU:HD11	1:3:A:LEU:HD11	20	2.47	0.81	2.52
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD11	20	2.47	0.81	2.52
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD11	20	2.47	0.81	2.52
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD13	20	2.47	0.81	2.52
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD13	20	2.47	0.81	2.52
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD12	20	2.47	0.81	2.52
(1,756)	1:94:A:LEU:HD11	1:3:A:LEU:HD13	20	2.47	0.81	2.52
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	20	2.35	0.42	2.44
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	20	2.35	0.42	2.44
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	20	2.35	0.42	2.44
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	20	2.32	0.28	2.33
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD12	20	2.32	0.28	2.33
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD13	20	2.32	0.28	2.33
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H131	20	2.32	0.4	2.52
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H131	20	2.32	0.4	2.52
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	20	2.32	0.4	2.52
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H161	20	2.32	0.4	2.52
(2,1649)	1:23:A:LEU:HD12	2:1001:A:OLA:H161	20	2.32	0.4	2.52
(2,1649)	1:23:A:LEU:HD12	2:1001:A:OLA:H131	20	2.32	0.4	2.52
(2,88)	1:3:A:LEU:HD23	1:45:A:PHE:HA	20	2.27	0.46	2.19
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	20	2.27	0.46	2.19
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD11	20	2.27	0.46	2.19
(2,88)	1:3:A:LEU:HD21	1:45:A:PHE:HA	20	2.27	0.46	2.19
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD13	20	2.27	0.46	2.19
(2,465)	1:87:A:GLN:HG2	1:107:A:VAL:HG13	20	2.26	0.8	2.35
(2,465)	1:87:A:GLN:HG2	1:107:A:VAL:HG11	20	2.26	0.8	2.35
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG12	20	2.26	0.8	2.35
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB2	20	2.26	0.8	2.35
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB3	20	2.26	0.8	2.35
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG13	20	2.26	0.8	2.35
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG11	20	2.26	0.8	2.35
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB1	20	2.26	0.8	2.35
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG21	20	2.18	0.52	2.37
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG22	20	2.18	0.52	2.37
(2,489)	1:58:A:MET:HE1	1:90:A:ILE:HG21	20	2.18	0.52	2.37
(2,489)	1:90:A:ILE:HG21	1:58:A:MET:HG2	20	2.18	0.52	2.37
(2,489)	1:90:A:ILE:HG23	1:58:A:MET:HG2	20	2.18	0.52	2.37
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG23	20	2.18	0.52	2.37
(2,489)	1:58:A:MET:HE1	1:90:A:ILE:HG22	20	2.18	0.52	2.37
(1,2810)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	20	2.02	0.08	2.02
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	20	2.02	0.08	2.02
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	20	2.02	0.08	2.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2810)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	20	2.02	0.08	2.02
(1,2810)	2:1001:A:OLA:H181	1:23:A:LEU:HD12	20	2.02	0.08	2.02
(1,2810)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	20	2.02	0.08	2.02
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	20	2.02	0.08	2.02
(1,2810)	2:1001:A:OLA:H181	1:23:A:LEU:HD11	20	2.02	0.08	2.02
(2,493)	1:90:A:ILE:HD13	1:81:A:GLU:HG2	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD13	1:79:A:GLN:HG3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD11	1:81:A:GLU:HB3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD12	1:79:A:GLN:HG3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD11	1:79:A:GLN:HG3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD11	1:87:A:GLN:HB2	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD13	1:81:A:GLU:HB2	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD12	1:79:A:GLN:HB3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD11	1:79:A:GLN:HB3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD11	1:114:A:GLU:HB3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD13	1:81:A:GLU:HB3	20	2.0	0.3	1.99
(2,493)	1:90:A:ILE:HD13	1:87:A:GLN:HB2	20	2.0	0.3	1.99
(2,81)	1:3:A:LEU:HD22	1:45:A:PHE:HB2	20	1.97	0.5	2.16
(2,81)	1:3:A:LEU:HD23	1:2:A:THR:HB	20	1.97	0.5	2.16
(2,81)	1:125:A:LEU:HD11	1:13:A:LEU:HA	20	1.97	0.5	2.16
(2,81)	1:125:A:LEU:HD12	1:45:A:PHE:HB2	20	1.97	0.5	2.16
(2,81)	1:125:A:LEU:HD11	1:45:A:PHE:HB2	20	1.97	0.5	2.16
(2,81)	1:3:A:LEU:HD23	1:45:A:PHE:HB2	20	1.97	0.5	2.16
(2,81)	1:125:A:LEU:HD13	1:13:A:LEU:HA	20	1.97	0.5	2.16
(2,81)	1:3:A:LEU:HD22	1:2:A:THR:HB	20	1.97	0.5	2.16
(2,81)	1:125:A:LEU:HD13	1:45:A:PHE:HB2	20	1.97	0.5	2.16
(2,81)	1:3:A:LEU:HD21	1:45:A:PHE:HB2	20	1.97	0.5	2.16
(1,2829)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	20	1.95	0.08	1.95
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	20	1.95	0.08	1.95
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	20	1.95	0.08	1.95
(1,2829)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	20	1.95	0.08	1.95
(1,2829)	2:1001:A:OLA:H181	1:23:A:LEU:HD12	20	1.95	0.08	1.95
(1,2829)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	20	1.95	0.08	1.95
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	20	1.95	0.08	1.95
(1,2829)	2:1001:A:OLA:H181	1:23:A:LEU:HD11	20	1.95	0.08	1.95
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	20	1.94	0.31	1.93
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	20	1.94	0.31	1.93
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	20	1.94	0.31	1.93
(1,2077)	1:23:A:LEU:HD13	1:26:A:ARG:H	20	1.86	0.09	1.83
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	20	1.86	0.09	1.83
(1,2077)	1:23:A:LEU:HD12	1:26:A:ARG:H	20	1.86	0.09	1.83
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	20	1.85	0.42	1.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	20	1.85	0.42	1.94
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	20	1.85	0.42	1.94
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD11	20	1.84	0.68	2.2
(2,72)	1:3:A:LEU:HD11	1:58:A:MET:HG2	20	1.84	0.68	2.2
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD13	20	1.84	0.68	2.2
(2,72)	1:3:A:LEU:HD13	1:74:A:LEU:HB2	20	1.84	0.68	2.2
(2,72)	1:3:A:LEU:HD12	1:58:A:MET:HG2	20	1.84	0.68	2.2
(2,72)	1:3:A:LEU:HD12	1:74:A:LEU:HB2	20	1.84	0.68	2.2
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD12	20	1.84	0.68	2.2
(2,72)	1:4:A:PRO:HB3	1:3:A:LEU:HD13	20	1.84	0.68	2.2
(2,72)	1:3:A:LEU:HD13	1:58:A:MET:HG2	20	1.84	0.68	2.2
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	20	1.81	0.34	1.92
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD11	20	1.81	0.34	1.92
(2,79)	1:3:A:LEU:HD12	1:55:A:ARG:HA	20	1.81	0.34	1.92
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD13	20	1.81	0.34	1.92
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD12	20	1.81	0.34	1.92
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD23	20	1.74	0.66	1.78
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD13	20	1.74	0.66	1.78
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD21	20	1.74	0.66	1.78
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD11	20	1.74	0.66	1.78
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD22	20	1.74	0.66	1.78
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD12	20	1.74	0.66	1.78
(2,463)	1:90:A:ILE:HG13	1:87:A:GLN:HB3	20	1.72	0.6	1.69
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG11	20	1.72	0.6	1.69
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB2	20	1.72	0.6	1.69
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG12	20	1.72	0.6	1.69
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB1	20	1.72	0.6	1.69
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG13	20	1.72	0.6	1.69
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB3	20	1.72	0.6	1.69
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG23	20	1.72	0.53	1.82
(2,553)	1:132:A:LYS:HE2	1:134:A:VAL:HG23	20	1.72	0.53	1.82
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG22	20	1.72	0.53	1.82
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG21	20	1.72	0.53	1.82
(2,553)	1:103:A:THR:HG21	1:89:A:LYS:HE2	20	1.72	0.53	1.82
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG22	20	1.72	0.53	1.82
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG23	20	1.72	0.53	1.82
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG21	20	1.72	0.53	1.82
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	20	1.67	0.2	1.68
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	20	1.67	0.2	1.68
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG22	20	1.67	0.2	1.68
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD13	20	1.62	0.11	1.62
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	20	1.62	0.11	1.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD12	20	1.62	0.11	1.62
(1,2793)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	20	1.59	0.08	1.6
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	20	1.59	0.08	1.6
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	20	1.59	0.08	1.6
(1,2793)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	20	1.59	0.08	1.6
(1,2793)	2:1001:A:OLA:H181	1:23:A:LEU:HD12	20	1.59	0.08	1.6
(1,2793)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	20	1.59	0.08	1.6
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	20	1.59	0.08	1.6
(1,2793)	2:1001:A:OLA:H181	1:23:A:LEU:HD11	20	1.59	0.08	1.6
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	20	1.56	0.21	1.57
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD22	20	1.56	0.21	1.57
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD21	20	1.56	0.21	1.57
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD21	1:8:A:LEU:HD21	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD22	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD23	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD21	1:8:A:LEU:HD22	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD21	1:8:A:LEU:HD23	20	1.55	0.18	1.5
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD23	20	1.55	0.18	1.5
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	20	1.55	0.33	1.62
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	20	1.55	0.33	1.62
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG11	20	1.55	0.33	1.62
(2,734)	1:58:A:MET:HE1	1:100:A:LEU:HD22	20	1.55	0.65	1.4
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD21	20	1.55	0.65	1.4
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD22	20	1.55	0.65	1.4
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD23	20	1.55	0.65	1.4
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD23	20	1.55	0.65	1.4
(2,734)	1:58:A:MET:HE1	1:100:A:LEU:HD21	20	1.55	0.65	1.4
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD21	20	1.55	0.65	1.4
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD22	20	1.55	0.65	1.4
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD21	1:8:A:LEU:HD21	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD22	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD23	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD21	1:8:A:LEU:HD22	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD21	1:8:A:LEU:HD23	20	1.53	0.18	1.47
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD23	20	1.53	0.18	1.47
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD13	20	1.52	0.51	1.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD13	20	1.52	0.51	1.4
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD12	20	1.52	0.51	1.4
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD13	20	1.52	0.51	1.4
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD11	20	1.52	0.51	1.4
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD11	20	1.52	0.51	1.4
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD12	20	1.52	0.51	1.4
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD11	20	1.52	0.51	1.4
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	20	1.51	0.17	1.53
(2,175)	1:16:A:ASP:HB2	1:15:A:ARG:HG2	20	1.51	0.17	1.53
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	20	1.5	0.47	1.57
(1,386)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	20	1.5	0.47	1.57
(1,386)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	20	1.5	0.47	1.57
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	20	1.46	0.47	1.54
(1,290)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	20	1.46	0.47	1.54
(1,290)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	20	1.46	0.47	1.54
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	20	1.46	0.21	1.46
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD22	20	1.46	0.21	1.46
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD21	20	1.46	0.21	1.46
(2,391)	1:35:A:VAL:HG21	1:64:A:LYS:HD2	20	1.45	0.39	1.42
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG21	20	1.45	0.39	1.42
(2,391)	1:35:A:VAL:HG22	1:64:A:LYS:HD2	20	1.45	0.39	1.42
(2,391)	1:35:A:VAL:HG23	1:64:A:LYS:HD2	20	1.45	0.39	1.42
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG22	20	1.45	0.39	1.42
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG23	20	1.45	0.39	1.42
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	20	1.41	0.23	1.5
(2,77)	1:74:A:LEU:HA	1:3:A:LEU:HD11	20	1.41	0.23	1.5
(2,77)	1:74:A:LEU:HA	1:3:A:LEU:HD13	20	1.41	0.23	1.5
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD12	20	1.41	0.23	1.5
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD11	20	1.41	0.23	1.5
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	20	1.41	0.23	1.42
(2,1589)	1:32:A:MET:HB3	2:1001:A:OLA:H183	20	1.41	0.23	1.42
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H183	20	1.41	0.23	1.42
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H183	20	1.41	0.23	1.42
(2,1589)	1:32:A:MET:HB3	2:1001:A:OLA:H181	20	1.41	0.23	1.42
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H181	20	1.41	0.23	1.42
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H182	20	1.41	0.23	1.42
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H182	20	1.41	0.23	1.42
(2,1589)	1:26:A:ARG:HD2	2:1001:A:OLA:H182	20	1.41	0.23	1.42
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HD22	20	1.37	0.45	1.27
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	20	1.37	0.45	1.27
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HB2	20	1.37	0.45	1.27
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HD23	20	1.37	0.45	1.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HD22	20	1.37	0.45	1.27
(2,613)	1:125:A:LEU:HD23	1:100:A:LEU:HB2	20	1.37	0.45	1.27
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HD23	20	1.37	0.45	1.27
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HD21	20	1.37	0.45	1.27
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD13	20	1.33	0.03	1.33
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	20	1.33	0.03	1.33
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD12	20	1.33	0.03	1.33
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	20	1.33	0.77	1.01
(1,430)	1:23:A:LEU:HD22	1:37:A:LYS:HG2	20	1.33	0.77	1.01
(1,430)	1:23:A:LEU:HD21	1:37:A:LYS:HG2	20	1.33	0.77	1.01
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD23	20	1.32	0.82	1.32
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	20	1.32	0.82	1.32
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD21	20	1.32	0.82	1.32
(2,540)	1:7:A:PHE:HA	1:100:A:LEU:HD23	20	1.32	0.82	1.32
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG21	20	1.3	0.1	1.25
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG22	20	1.3	0.1	1.25
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	20	1.3	0.1	1.25
(2,485)	1:90:A:ILE:HG22	1:78:A:PHE:HB2	20	1.3	0.1	1.25
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD13	20	1.29	0.11	1.28
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	20	1.29	0.11	1.28
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD12	20	1.29	0.11	1.28
(2,730)	1:58:A:MET:HE2	1:43:A:LYS:H	20	1.26	0.3	1.3
(2,730)	1:58:A:MET:HE3	1:43:A:LYS:H	20	1.26	0.3	1.3
(2,730)	1:58:A:MET:HE1	1:69:A:HIS:H	20	1.26	0.3	1.3
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	20	1.26	0.3	1.3
(2,730)	1:58:A:MET:HE3	1:69:A:HIS:H	20	1.26	0.3	1.3
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	20	1.24	0.12	1.25
(2,216)	1:23:A:LEU:HD23	1:22:A:TYR:HB2	20	1.24	0.12	1.25
(2,216)	1:23:A:LEU:HD23	1:33:A:ARG:HD3	20	1.24	0.12	1.25
(2,216)	1:23:A:LEU:HD22	1:33:A:ARG:HD3	20	1.24	0.12	1.25
(2,216)	1:23:A:LEU:HD22	1:22:A:TYR:HB2	20	1.24	0.12	1.25
(2,1217)	1:63:A:THR:H	1:38:A:LEU:HB3	20	1.23	0.31	1.25
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	20	1.23	0.31	1.25
(2,1217)	1:65:A:LYS:HD2	1:63:A:THR:H	20	1.23	0.31	1.25
(2,1217)	1:63:A:THR:H	1:83:A:LEU:HG	20	1.23	0.31	1.25
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	20	1.19	0.16	1.13
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HG3	20	1.19	0.16	1.13
(2,230)	1:25:A:ALA:HB1	1:26:A:ARG:HB3	20	1.19	0.16	1.13
(2,230)	1:25:A:ALA:HB1	1:26:A:ARG:HG3	20	1.19	0.16	1.13
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HB3	20	1.19	0.16	1.13
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HB3	20	1.19	0.16	1.13
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD11	20	1.16	0.63	1.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD13	20	1.16	0.63	1.06
(1,632)	1:74:A:LEU:HD12	1:3:A:LEU:HD11	20	1.16	0.63	1.06
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD11	20	1.16	0.63	1.06
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD12	20	1.16	0.63	1.06
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD12	20	1.16	0.63	1.06
(1,632)	1:74:A:LEU:HD12	1:3:A:LEU:HD13	20	1.16	0.63	1.06
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD13	20	1.16	0.63	1.06
(1,632)	1:74:A:LEU:HD12	1:3:A:LEU:HD12	20	1.16	0.63	1.06
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	20	1.14	0.26	1.13
(2,386)	1:35:A:VAL:HG21	1:64:A:LYS:HG2	20	1.14	0.26	1.13
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG22	20	1.14	0.26	1.13
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG23	20	1.14	0.26	1.13
(2,386)	1:35:A:VAL:HG23	1:64:A:LYS:HG2	20	1.14	0.26	1.13
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG21	20	1.12	0.22	1.16
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	20	1.12	0.22	1.16
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	20	1.12	0.22	1.16
(2,1646)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	20	1.09	0.38	1.13
(2,1646)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	20	1.09	0.38	1.13
(2,1646)	1:36:A:ILE:HD11	1:23:A:LEU:HB2	20	1.09	0.38	1.13
(2,1646)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	20	1.09	0.38	1.13
(2,1646)	1:36:A:ILE:HD11	1:33:A:ARG:HG3	20	1.09	0.38	1.13
(2,1646)	1:36:A:ILE:HD12	1:33:A:ARG:HG3	20	1.09	0.38	1.13
(2,1646)	1:36:A:ILE:HD12	2:1001:A:OLA:H112	20	1.09	0.38	1.13
(2,1646)	2:1001:A:OLA:H111	1:36:A:ILE:HD11	20	1.09	0.38	1.13
(2,1646)	1:36:A:ILE:HD13	1:33:A:ARG:HG3	20	1.09	0.38	1.13
(2,1646)	2:1001:A:OLA:H111	1:36:A:ILE:HD12	20	1.09	0.38	1.13
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	20	1.09	0.17	1.09
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	20	1.09	0.17	1.09
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG12	20	1.09	0.17	1.09
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE2	20	1.04	0.22	1.0
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE1	20	1.04	0.22	1.0
(1,1192)	1:23:A:LEU:HD12	1:32:A:MET:HE1	20	1.04	0.22	1.0
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE3	20	1.04	0.22	1.0
(1,1192)	1:23:A:LEU:HD12	1:32:A:MET:HE3	20	1.04	0.22	1.0
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE1	20	1.04	0.22	1.0
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE3	20	1.04	0.22	1.0
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE2	20	1.04	0.22	1.0
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG23	20	1.04	0.21	1.15
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG21	20	1.04	0.21	1.15
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG21	20	1.04	0.21	1.15
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG22	20	1.04	0.21	1.15
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG22	20	1.04	0.21	1.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG23	20	1.04	0.21	1.15
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	20	1.02	0.27	0.98
(2,1648)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	20	1.02	0.27	0.98
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	20	1.02	0.27	0.98
(2,1648)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	20	1.02	0.27	0.98
(2,1648)	1:36:A:ILE:HD11	2:1001:A:OLA:H152	20	1.02	0.27	0.98
(2,1648)	2:1001:A:OLA:H172	1:36:A:ILE:HD12	20	1.02	0.27	0.98
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	20	1.02	0.27	0.98
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	20	1.02	0.27	0.98
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H152	20	1.02	0.27	0.98
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD13	20	1.02	0.13	0.98
(1,186)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	20	1.02	0.13	0.98
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD11	20	1.02	0.13	0.98
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	20	1.02	0.13	0.98
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD13	20	1.02	0.13	0.98
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD11	20	1.02	0.13	0.98
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD12	20	1.02	0.13	0.98
(1,186)	1:3:A:LEU:HD21	1:8:A:LEU:HD11	20	1.02	0.13	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD13	20	0.98	0.03	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	20	0.98	0.03	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD12	20	0.98	0.03	0.98
(2,667)	1:136:A:THR:HG21	1:135:A:SER:HB2	20	0.98	0.2	1.0
(2,667)	1:130:A:SER:HB2	1:136:A:THR:HG21	20	0.98	0.2	1.0
(2,667)	1:136:A:THR:HG22	1:135:A:SER:HB2	20	0.98	0.2	1.0
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG21	20	0.98	0.2	1.0
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG22	20	0.98	0.2	1.0
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG23	20	0.98	0.2	1.0
(2,667)	1:136:A:THR:HG23	1:135:A:SER:HB2	20	0.98	0.2	1.0
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG22	20	0.92	0.04	0.9
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	20	0.92	0.04	0.9
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG23	20	0.92	0.04	0.9
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	20	0.91	0.32	0.78
(2,636)	1:134:A:VAL:HG13	1:130:A:SER:HB3	20	0.91	0.32	0.78
(2,636)	1:134:A:VAL:HG12	1:130:A:SER:HB3	20	0.91	0.32	0.78
(2,636)	1:134:A:VAL:HG11	1:130:A:SER:HB3	20	0.91	0.32	0.78
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	20	0.91	0.32	0.94
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	20	0.91	0.32	0.94
(2,620)	1:124:A:TYR:HD2	1:126:A:VAL:HG13	20	0.91	0.32	0.94
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG11	20	0.91	0.32	0.94
(2,707)	1:41:A:VAL:HG12	1:62:A:THR:HG1	20	0.91	0.2	0.89
(2,707)	1:41:A:VAL:HG11	1:62:A:THR:HG1	20	0.91	0.2	0.89
(2,707)	1:67:A:THR:HG22	1:62:A:THR:HG1	20	0.91	0.2	0.89

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,707)	1:41:A:VAL:HG13	1:62:A:THR:HG1	20	0.91	0.2	0.89
(2,707)	1:67:A:THR:HG21	1:62:A:THR:HG1	20	0.91	0.2	0.89
(2,707)	1:67:A:THR:HG23	1:62:A:THR:HG1	20	0.91	0.2	0.89
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	20	0.9	0.55	0.54
(2,740)	1:31:A:ILE:HD13	1:30:A:TRP:HZ2	20	0.9	0.55	0.54
(2,740)	1:31:A:ILE:HD11	1:30:A:TRP:HZ2	20	0.9	0.55	0.54
(2,740)	1:30:A:TRP:HZ2	1:31:A:ILE:HG23	20	0.9	0.55	0.54
(2,740)	1:30:A:TRP:HZ2	1:31:A:ILE:HG21	20	0.9	0.55	0.54
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	20	0.9	0.23	0.86
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	20	0.9	0.23	0.86
(1,557)	1:63:A:THR:HG21	1:40:A:GLY:HA2	20	0.9	0.23	0.86
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	20	0.87	0.24	0.72
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD11	20	0.87	0.24	0.72
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD12	20	0.87	0.24	0.72
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	20	0.86	0.21	0.82
(2,114)	1:8:A:LEU:HD22	1:5:A:ASP:HA	20	0.86	0.21	0.82
(2,114)	1:8:A:LEU:HD23	1:5:A:ASP:HA	20	0.86	0.21	0.82
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	20	0.85	0.24	0.97
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD11	20	0.85	0.24	0.97
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD13	20	0.85	0.24	0.97
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	20	0.84	0.89	0.49
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	20	0.84	0.89	0.49
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG13	20	0.84	0.89	0.49
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE2	20	0.84	0.32	0.8
(2,841)	1:129:A:MET:HE3	1:114:A:GLU:HG3	20	0.84	0.32	0.8
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE1	20	0.84	0.32	0.8
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE3	20	0.84	0.32	0.8
(2,841)	1:129:A:MET:HE2	1:114:A:GLU:HG3	20	0.84	0.32	0.8
(2,841)	1:129:A:MET:HE1	1:114:A:GLU:HG3	20	0.84	0.32	0.8
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	20	0.83	0.27	0.78
(2,293)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	20	0.83	0.27	0.78
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	20	0.83	0.27	0.78
(2,293)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	20	0.83	0.27	0.78
(2,293)	1:36:A:ILE:HD11	2:1001:A:OLA:H152	20	0.83	0.27	0.78
(2,293)	2:1001:A:OLA:H172	1:36:A:ILE:HD12	20	0.83	0.27	0.78
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	20	0.83	0.27	0.78
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	20	0.83	0.27	0.78
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H152	20	0.83	0.27	0.78
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	20	0.8	0.26	0.77
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG23	20	0.8	0.26	0.77
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG22	20	0.8	0.26	0.77
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	20	0.8	0.18	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG21	20	0.8	0.18	0.8
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG23	20	0.8	0.18	0.8
(2,848)	1:91:A:THR:HG23	1:91:A:THR:H	20	0.8	0.18	0.8
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD12	20	0.8	0.3	0.74
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	20	0.8	0.3	0.74
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD11	20	0.8	0.3	0.74
(2,836)	1:49:A:ALA:HB3	1:48:A:ALA:HA	20	0.79	0.12	0.78
(2,836)	1:49:A:ALA:HB1	1:48:A:ALA:HA	20	0.79	0.12	0.78
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	20	0.79	0.12	0.78
(2,836)	1:49:A:ALA:HB2	1:50:A:SER:HB3	20	0.79	0.12	0.78
(2,836)	1:49:A:ALA:HB3	1:50:A:SER:HB3	20	0.79	0.12	0.78
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	20	0.78	0.27	0.74
(2,1605)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	20	0.78	0.27	0.74
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	20	0.78	0.27	0.74
(2,1605)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	20	0.78	0.27	0.74
(2,1605)	1:36:A:ILE:HD11	2:1001:A:OLA:H152	20	0.78	0.27	0.74
(2,1605)	2:1001:A:OLA:H172	1:36:A:ILE:HD12	20	0.78	0.27	0.74
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	20	0.78	0.27	0.74
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	20	0.78	0.27	0.74
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H152	20	0.78	0.27	0.74
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	20	0.78	0.21	0.78
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	20	0.78	0.21	0.78
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB2	20	0.78	0.21	0.78
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	20	0.78	0.07	0.78
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	20	0.78	0.07	0.78
(1,1474)	1:105:A:ILE:HD13	1:106:A:LYS:H	20	0.78	0.07	0.78
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG23	20	0.77	0.26	0.77
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG22	20	0.77	0.26	0.77
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	20	0.77	0.26	0.77
(2,24)	1:94:A:LEU:HD13	1:4:A:PRO:HB2	20	0.77	0.26	0.77
(2,24)	1:4:A:PRO:HB2	1:94:A:LEU:HD23	20	0.77	0.26	0.77
(2,24)	1:94:A:LEU:HD11	1:4:A:PRO:HB2	20	0.77	0.26	0.77
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	20	0.77	0.29	0.72
(2,107)	1:120:A:ARG:HB2	1:7:A:PHE:HB3	20	0.77	0.29	0.72
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE1	20	0.73	0.25	0.74
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	20	0.73	0.25	0.74
(1,1220)	1:118:A:TYR:HD2	1:58:A:MET:HE3	20	0.73	0.25	0.74
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE3	20	0.73	0.25	0.74
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD13	20	0.72	0.28	0.7
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	20	0.72	0.28	0.7
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD12	20	0.72	0.28	0.7
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	20	0.72	0.24	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	20	0.72	0.24	0.74
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD13	20	0.72	0.24	0.74
(1,1464)	1:8:A:LEU:HD11	1:45:A:PHE:HB2	20	0.71	0.1	0.74
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	20	0.71	0.1	0.74
(1,1464)	1:8:A:LEU:HD12	1:45:A:PHE:HB2	20	0.71	0.1	0.74
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	20	0.71	0.12	0.7
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB2	20	0.71	0.12	0.7
(2,437)	1:86:A:THR:HB	1:82:A:ALA:HB2	20	0.71	0.12	0.7
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB3	20	0.71	0.12	0.7
(2,437)	1:86:A:THR:HB	1:82:A:ALA:HB1	20	0.71	0.12	0.7
(2,1274)	1:113:A:VAL:HG13	1:105:A:ILE:H	20	0.71	0.07	0.73
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	20	0.71	0.07	0.73
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG22	20	0.71	0.07	0.73
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG23	20	0.71	0.07	0.73
(2,786)	1:32:A:MET:HE2	1:36:A:ILE:HA	20	0.7	0.15	0.72
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	20	0.7	0.15	0.72
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	20	0.7	0.15	0.72
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	20	0.7	0.07	0.69
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	20	0.7	0.07	0.69
(2,502)	1:90:A:ILE:HD11	1:90:A:ILE:H	20	0.7	0.07	0.69
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG21	20	0.68	0.08	0.68
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	20	0.68	0.08	0.68
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG23	20	0.68	0.08	0.68
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	20	0.68	0.05	0.69
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	20	0.68	0.05	0.69
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB1	20	0.68	0.05	0.69
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	20	0.67	0.19	0.69
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG22	20	0.67	0.19	0.69
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG23	20	0.67	0.19	0.69
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	20	0.67	0.2	0.74
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	20	0.67	0.2	0.74
(2,188)	1:134:A:VAL:HG12	1:21:A:GLU:HG2	20	0.67	0.2	0.74
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	20	0.66	0.15	0.66
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	20	0.66	0.15	0.66
(1,2593)	1:67:A:THR:HG23	1:84:A:ASP:H	20	0.66	0.15	0.66
(1,558)	1:63:A:THR:HG22	1:62:A:THR:H	20	0.66	0.05	0.65
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	20	0.66	0.05	0.65
(1,558)	1:63:A:THR:HG21	1:62:A:THR:H	20	0.66	0.05	0.65
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	20	0.66	0.21	0.7
(1,288)	1:23:A:LEU:HD21	1:33:A:ARG:HA	20	0.66	0.21	0.7
(1,288)	1:23:A:LEU:HD23	1:33:A:ARG:HA	20	0.66	0.21	0.7
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	20	0.66	0.1	0.65

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG21	20	0.66	0.1	0.65
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	20	0.66	0.1	0.65
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG22	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG22	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG23	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG22	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG23	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG23	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG21	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG21	20	0.64	0.17	0.68
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG21	20	0.64	0.17	0.68
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	20	0.64	0.2	0.69
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE1	20	0.64	0.2	0.69
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE3	20	0.64	0.2	0.69
(2,1313)	1:125:A:LEU:HA	1:124:A:TYR:H	20	0.63	0.09	0.62
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	20	0.63	0.09	0.62
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG23	20	0.62	0.32	0.59
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	20	0.62	0.32	0.59
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	20	0.62	0.32	0.59
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD22	20	0.62	0.08	0.65
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	20	0.62	0.08	0.65
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD21	20	0.62	0.08	0.65
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	20	0.61	0.23	0.57
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	20	0.61	0.23	0.57
(2,56)	1:63:A:THR:HG21	1:40:A:GLY:HA2	20	0.61	0.23	0.57
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	20	0.6	0.24	0.72
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD11	20	0.6	0.24	0.72
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD13	20	0.6	0.24	0.72
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	20	0.59	0.08	0.59
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	20	0.59	0.08	0.59
(2,558)	1:105:A:ILE:HD13	1:105:A:ILE:HA	20	0.59	0.08	0.59
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	20	0.59	0.18	0.62
(2,1328)	1:36:A:ILE:H	1:34:A:GLN:HB3	20	0.59	0.18	0.62
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	20	0.56	0.1	0.58
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG23	20	0.56	0.1	0.58
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG22	20	0.56	0.1	0.58
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	20	0.56	0.29	0.5
(2,178)	1:134:A:VAL:HG13	1:18:A:ASN:HB2	20	0.56	0.29	0.5
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	20	0.56	0.29	0.5
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	20	0.56	0.33	0.52
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	20	0.56	0.33	0.52
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HG	20	0.56	0.33	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,729)	1:66:A:ASP:HA	1:59:A:GLU:HB3	20	0.56	0.33	0.52
(2,561)	1:106:A:LYS:HA	1:105:A:ILE:HG22	20	0.55	0.21	0.56
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG12	20	0.55	0.21	0.56
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG13	20	0.55	0.21	0.56
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG11	20	0.55	0.21	0.56
(2,561)	1:106:A:LYS:HA	1:105:A:ILE:HG21	20	0.55	0.21	0.56
(2,561)	1:106:A:LYS:HA	1:105:A:ILE:HG23	20	0.55	0.21	0.56
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	20	0.55	0.4	0.46
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	20	0.55	0.4	0.46
(1,923)	1:125:A:LEU:HD23	1:118:A:TYR:HB2	20	0.55	0.4	0.46
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	20	0.54	0.02	0.55
(2,115)	1:8:A:LEU:HD21	1:8:A:LEU:HB2	20	0.54	0.02	0.55
(2,115)	1:8:A:LEU:HD22	1:8:A:LEU:HB2	20	0.54	0.02	0.55
(2,115)	1:8:A:LEU:HD21	1:56:A:TYR:HB3	20	0.54	0.02	0.55
(2,119)	1:8:A:LEU:HD11	1:9:A:GLY:H	20	0.54	0.19	0.5
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	20	0.54	0.19	0.5
(2,119)	1:8:A:LEU:HD12	1:9:A:GLY:H	20	0.54	0.19	0.5
(2,119)	1:8:A:LEU:HD13	1:46:A:ARG:H	20	0.54	0.19	0.5
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	20	0.52	0.09	0.52
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	20	0.52	0.09	0.52
(1,1292)	1:111:A:THR:HG21	1:112:A:ASP:H	20	0.52	0.09	0.52
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	20	0.51	0.04	0.51
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	20	0.51	0.04	0.51
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG12	20	0.51	0.04	0.51
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	20	0.51	0.04	0.51
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	20	0.51	0.04	0.51
(1,1344)	1:105:A:ILE:HD11	1:105:A:ILE:H	20	0.51	0.04	0.51
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE2	20	0.5	0.04	0.49
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	20	0.5	0.04	0.49
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE3	20	0.5	0.04	0.49
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	20	0.5	0.16	0.49
(2,929)	1:116:A:TYR:H	1:129:A:MET:HB2	20	0.5	0.16	0.49
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG22	20	0.5	0.16	0.49
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG21	20	0.5	0.16	0.49
(2,1670)	2:1001:A:OLA:H82	2:1001:A:OLA:H182	20	0.49	0.18	0.48
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	20	0.49	0.18	0.48
(2,1670)	2:1001:A:OLA:H182	2:1001:A:OLA:H21	20	0.49	0.18	0.48
(2,1670)	2:1001:A:OLA:H181	2:1001:A:OLA:H21	20	0.49	0.18	0.48
(2,1670)	2:1001:A:OLA:H82	2:1001:A:OLA:H181	20	0.49	0.18	0.48
(2,1670)	2:1001:A:OLA:H183	2:1001:A:OLA:H21	20	0.49	0.18	0.48
(2,1670)	2:1001:A:OLA:H82	2:1001:A:OLA:H183	20	0.49	0.18	0.48
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H183	20	0.49	0.18	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	20	0.48	0.12	0.48
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	20	0.48	0.12	0.48
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	20	0.48	0.03	0.48
(1,2833)	2:1001:A:OLA:H183	1:36:A:ILE:HA	20	0.48	0.03	0.48
(1,2833)	2:1001:A:OLA:H181	1:36:A:ILE:HA	20	0.48	0.03	0.48
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	20	0.48	0.05	0.48
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG22	20	0.48	0.05	0.48
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG23	20	0.48	0.05	0.48
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	20	0.48	0.11	0.48
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG23	20	0.48	0.11	0.48
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG21	20	0.48	0.11	0.48
(2,118)	1:8:A:LEU:HD11	1:8:A:LEU:HA	20	0.47	0.02	0.47
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	20	0.47	0.02	0.47
(2,118)	1:8:A:LEU:HD12	1:8:A:LEU:HA	20	0.47	0.02	0.47
(2,118)	1:8:A:LEU:HD13	1:47:A:ASN:HA	20	0.47	0.02	0.47
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	20	0.47	0.05	0.47
(1,878)	1:115:A:THR:H	1:115:A:THR:HG22	20	0.47	0.05	0.47
(1,878)	1:115:A:THR:H	1:115:A:THR:HG23	20	0.47	0.05	0.47
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	20	0.47	0.04	0.45
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	20	0.47	0.04	0.45
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	20	0.46	0.11	0.46
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	20	0.46	0.11	0.46
(2,288)	1:36:A:ILE:HD12	1:37:A:LYS:H	20	0.46	0.11	0.46
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	20	0.43	0.15	0.44
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB2	20	0.43	0.15	0.44
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	20	0.43	0.15	0.44
(1,1580)	1:8:A:LEU:HD12	1:8:A:LEU:H	20	0.43	0.02	0.43
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	20	0.43	0.02	0.43
(1,1580)	1:8:A:LEU:HD13	1:8:A:LEU:H	20	0.43	0.02	0.43
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG21	20	0.43	0.05	0.44
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	20	0.43	0.05	0.44
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	20	0.43	0.05	0.44
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	20	0.4	0.04	0.38
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	20	0.4	0.04	0.38
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD11	20	0.4	0.06	0.42
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	20	0.4	0.06	0.42
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD13	20	0.4	0.06	0.42
(2,1678)	1:10:A:THR:HG21	1:44:A:LYS:HG2	20	0.39	0.23	0.28
(2,1678)	1:10:A:THR:HG22	1:44:A:LYS:HG2	20	0.39	0.23	0.28
(2,1678)	1:83:A:LEU:HB2	1:67:A:THR:HG22	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H151	2:1001:A:OLA:H142	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H161	2:1001:A:OLA:H152	20	0.39	0.23	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1678)	1:10:A:THR:HG23	1:44:A:LYS:HG2	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H122	2:1001:A:OLA:H142	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H122	2:1001:A:OLA:H141	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H141	2:1001:A:OLA:H152	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H152	2:1001:A:OLA:H142	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H61	2:1001:A:OLA:H161	20	0.39	0.23	0.28
(2,1678)	2:1001:A:OLA:H121	2:1001:A:OLA:H131	20	0.39	0.23	0.28
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	20	0.38	0.1	0.38
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD23	20	0.38	0.1	0.38
(2,112)	1:8:A:LEU:HD22	1:47:A:ASN:HD21	20	0.38	0.1	0.38
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD21	20	0.38	0.1	0.38
(2,112)	1:8:A:LEU:HD21	1:47:A:ASN:HD21	20	0.38	0.1	0.38
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	20	0.38	0.07	0.37
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG23	20	0.38	0.07	0.37
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG22	20	0.38	0.07	0.37
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	20	0.37	0.04	0.36
(2,610)	1:125:A:LEU:HD21	1:125:A:LEU:H	20	0.37	0.04	0.36
(2,610)	1:125:A:LEU:HD22	1:125:A:LEU:H	20	0.37	0.04	0.36
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	20	0.37	0.21	0.33
(2,98)	1:8:A:LEU:HD22	1:5:A:ASP:HA	20	0.37	0.21	0.33
(2,98)	1:8:A:LEU:HD23	1:5:A:ASP:HA	20	0.37	0.21	0.33
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	20	0.36	0.09	0.34
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	20	0.36	0.09	0.34
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	20	0.36	0.12	0.34
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	20	0.36	0.12	0.34
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG21	20	0.36	0.12	0.34
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG23	20	0.35	0.18	0.28
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	20	0.35	0.18	0.28
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	20	0.35	0.18	0.28
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	20	0.34	0.08	0.35
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	20	0.34	0.08	0.35
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB1	20	0.34	0.11	0.32
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB3	20	0.34	0.11	0.32
(2,416)	1:77:A:GLU:H	1:73:A:ALA:HB3	20	0.34	0.11	0.32
(2,416)	1:77:A:GLU:H	1:73:A:ALA:HB2	20	0.34	0.11	0.32
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB2	20	0.34	0.11	0.32
(2,416)	1:77:A:GLU:H	1:73:A:ALA:HB1	20	0.34	0.11	0.32
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	20	0.32	0.02	0.33
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG23	20	0.32	0.19	0.19
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	20	0.32	0.19	0.19
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	20	0.32	0.19	0.19
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	20	0.32	0.06	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H181	20	0.32	0.06	0.32
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H182	20	0.32	0.06	0.32
(1,687)	1:86:A:THR:HG21	1:87:A:GLN:H	20	0.32	0.09	0.32
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	20	0.32	0.09	0.32
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	20	0.32	0.09	0.32
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	20	0.29	0.04	0.3
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	20	0.29	0.04	0.3
(2,228)	1:25:A:ALA:HB1	1:26:A:ARG:HA	20	0.29	0.04	0.3
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	20	0.29	0.05	0.29
(1,1297)	1:8:A:LEU:HD23	1:8:A:LEU:H	20	0.29	0.05	0.29
(1,1297)	1:8:A:LEU:HD21	1:8:A:LEU:H	20	0.29	0.05	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	20	0.29	0.04	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG21	20	0.29	0.04	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	20	0.29	0.04	0.29
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	20	0.28	0.06	0.26
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB3	20	0.28	0.06	0.26
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB1	20	0.28	0.06	0.26
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	20	0.28	0.05	0.28
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB3	20	0.28	0.05	0.28
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB2	20	0.28	0.05	0.28
(2,479)	1:90:A:ILE:HG21	1:78:A:PHE:H	20	0.28	0.07	0.26
(2,479)	1:90:A:ILE:HG22	1:78:A:PHE:H	20	0.28	0.07	0.26
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG23	20	0.28	0.07	0.26
(2,479)	1:90:A:ILE:HG23	1:78:A:PHE:H	20	0.28	0.07	0.26
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG22	20	0.28	0.07	0.26
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	20	0.28	0.02	0.27
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	20	0.26	0.03	0.26
(1,2789)	2:1001:A:OLA:H183	1:36:A:ILE:HA	20	0.26	0.03	0.26
(1,2789)	2:1001:A:OLA:H181	1:36:A:ILE:HA	20	0.26	0.03	0.26
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG23	20	0.26	0.02	0.27
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	20	0.26	0.02	0.27
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG22	20	0.26	0.02	0.27
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	20	0.25	0.01	0.25
(2,218)	1:23:A:LEU:HD23	1:23:A:LEU:HB2	20	0.25	0.01	0.25
(2,218)	1:23:A:LEU:HD22	1:23:A:LEU:HB2	20	0.25	0.01	0.25
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	20	0.25	0.04	0.25
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	20	0.25	0.04	0.25
(1,307)	1:25:A:ALA:HB1	1:27:A:GLY:H	20	0.25	0.04	0.25
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	20	0.25	0.03	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	20	0.24	0.0	0.24
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	20	0.23	0.03	0.24
(2,875)	1:-5:A:HIS:HA	1:-5:A:HIS:HB2	20	0.23	0.03	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	20	0.23	0.03	0.23
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	20	0.22	0.05	0.23
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	20	0.22	0.06	0.21
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG23	20	0.22	0.06	0.21
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG22	20	0.22	0.06	0.21
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	20	0.2	0.03	0.2
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HA	20	0.17	0.02	0.17
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HB	20	0.17	0.02	0.17
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HB	20	0.17	0.02	0.17
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HB	20	0.17	0.02	0.17
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HA	20	0.17	0.02	0.17
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HA	20	0.17	0.02	0.17
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	20	0.16	0.0	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	20	0.16	0.02	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	20	0.16	0.02	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG23	20	0.16	0.02	0.16
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	19	1.88	0.16	1.92
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	19	1.88	0.16	1.92
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG11	19	1.88	0.16	1.92
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	19	1.56	0.56	1.57
(2,278)	1:35:A:VAL:HG21	2:1001:A:OLA:H10	19	1.56	0.56	1.57
(2,278)	1:35:A:VAL:HG23	2:1001:A:OLA:H10	19	1.56	0.56	1.57
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD22	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:83:A:LEU:HD22	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:83:A:LEU:HD13	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD11	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD12	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD23	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD21	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD13	19	1.53	0.67	1.49
(2,1376)	1:59:A:GLU:H	1:83:A:LEU:HD11	19	1.53	0.67	1.49
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	19	1.26	0.1	1.26
(2,70)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	19	1.26	0.1	1.26
(2,70)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	19	1.26	0.1	1.26
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	19	1.22	0.05	1.23
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD11	19	1.22	0.05	1.23
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD13	19	1.22	0.05	1.23
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE1	19	1.22	0.26	1.22
(2,784)	1:35:A:VAL:HG21	1:32:A:MET:HE1	19	1.22	0.26	1.22
(2,784)	1:35:A:VAL:HG23	1:32:A:MET:HE3	19	1.22	0.26	1.22
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE2	19	1.22	0.26	1.22
(2,784)	1:32:A:MET:HE2	1:31:A:ILE:HG23	19	1.22	0.26	1.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,784)	1:32:A:MET:HE2	1:31:A:ILE:HG22	19	1.22	0.26	1.22
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE3	19	1.22	0.26	1.22
(2,784)	1:35:A:VAL:HG21	1:32:A:MET:HE3	19	1.22	0.26	1.22
(2,784)	1:35:A:VAL:HG23	1:32:A:MET:HE2	19	1.22	0.26	1.22
(2,784)	1:32:A:MET:HE3	1:31:A:ILE:HG23	19	1.22	0.26	1.22
(2,60)	1:0:A:SER:HB2	1:1:A:LYS:HD2	19	1.2	0.43	1.31
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	19	1.2	0.43	1.31
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	19	1.2	0.04	1.2
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	19	1.2	0.04	1.2
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG11	19	1.2	0.04	1.2
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	19	1.06	0.25	1.03
(1,131)	1:3:A:LEU:HD11	1:7:A:PHE:HD2	19	1.06	0.25	1.03
(1,131)	1:3:A:LEU:HD13	1:7:A:PHE:HD2	19	1.06	0.25	1.03
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	19	1.02	0.81	0.61
(1,429)	1:23:A:LEU:HD22	1:37:A:LYS:HG3	19	1.02	0.81	0.61
(1,429)	1:23:A:LEU:HD21	1:37:A:LYS:HG3	19	1.02	0.81	0.61
(2,59)	1:0:A:SER:HB3	1:2:A:THR:HG21	19	0.92	0.34	0.89
(2,59)	1:0:A:SER:HB3	1:2:A:THR:HG23	19	0.92	0.34	0.89
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	19	0.92	0.34	0.89
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG22	19	0.92	0.34	0.89
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG21	19	0.92	0.34	0.89
(2,59)	1:94:A:LEU:HB3	1:0:A:SER:HB3	19	0.92	0.34	0.89
(1,1088)	1:61:A:LEU:HD23	1:62:A:THR:H	19	0.86	0.67	0.5
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	19	0.86	0.67	0.5
(1,1088)	1:61:A:LEU:HD22	1:62:A:THR:H	19	0.86	0.67	0.5
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	19	0.85	0.1	0.84
(1,1087)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	19	0.85	0.1	0.84
(1,1087)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	19	0.85	0.1	0.84
(2,840)	1:129:A:MET:HE3	1:114:A:GLU:HG3	19	0.83	0.41	0.86
(2,840)	1:129:A:MET:HE1	1:22:A:TYR:HB2	19	0.83	0.41	0.86
(2,840)	1:129:A:MET:HE1	1:114:A:GLU:HG3	19	0.83	0.41	0.86
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	19	0.83	0.41	0.86
(2,840)	1:129:A:MET:HE2	1:22:A:TYR:HB2	19	0.83	0.41	0.86
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD23	19	0.81	0.12	0.78
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD22	19	0.81	0.12	0.78
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	19	0.81	0.12	0.78
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	19	0.78	0.1	0.78
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	19	0.75	0.05	0.76
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD11	19	0.75	0.05	0.76
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD13	19	0.75	0.05	0.76
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	19	0.74	0.35	0.67
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG11	19	0.74	0.35	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG12	19	0.74	0.35	0.67
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	19	0.73	0.29	0.8
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	19	0.73	0.29	0.8
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG21	19	0.73	0.29	0.8
(1,1080)	1:56:A:TYR:HD2	1:2:A:THR:HG21	19	0.73	0.29	0.8
(1,1080)	1:56:A:TYR:HD2	1:2:A:THR:HG23	19	0.73	0.29	0.8
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	19	0.65	0.24	0.77
(2,731)	1:58:A:MET:HE1	1:61:A:LEU:H	19	0.65	0.24	0.77
(2,731)	1:58:A:MET:HE3	1:61:A:LEU:H	19	0.65	0.24	0.77
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	19	0.62	0.14	0.64
(1,1226)	1:49:A:ALA:HB3	1:51:A:GLY:H	19	0.62	0.14	0.64
(1,1226)	1:49:A:ALA:HB2	1:51:A:GLY:H	19	0.62	0.14	0.64
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG21	19	0.61	0.06	0.61
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	19	0.61	0.06	0.61
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG22	19	0.61	0.06	0.61
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	19	0.57	0.07	0.57
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	19	0.57	0.07	0.57
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG11	19	0.57	0.07	0.57
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	19	0.52	0.31	0.49
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	19	0.52	0.31	0.49
(1,548)	1:62:A:THR:HG22	1:60:A:ASN:HB2	19	0.52	0.31	0.49
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	19	0.52	0.1	0.51
(1,397)	1:35:A:VAL:HG22	1:36:A:ILE:H	19	0.52	0.1	0.51
(1,397)	1:35:A:VAL:HG21	1:36:A:ILE:H	19	0.52	0.1	0.51
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	19	0.48	0.04	0.48
(2,290)	1:36:A:ILE:HD12	1:36:A:ILE:HA	19	0.48	0.04	0.48
(2,290)	1:36:A:ILE:HD11	1:36:A:ILE:HA	19	0.48	0.04	0.48
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	19	0.48	0.11	0.48
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	19	0.48	0.11	0.48
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG21	19	0.45	0.06	0.45
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	19	0.45	0.06	0.45
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG22	19	0.45	0.06	0.45
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	19	0.44	0.25	0.41
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	19	0.44	0.09	0.43
(1,1225)	1:127:A:MET:HE3	1:128:A:LYS:H	19	0.44	0.09	0.43
(1,1225)	1:127:A:MET:HE1	1:128:A:LYS:H	19	0.44	0.09	0.43
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG22	19	0.43	0.12	0.43
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	19	0.43	0.12	0.43
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG23	19	0.43	0.12	0.43
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	19	0.39	0.07	0.41
(2,551)	1:114:A:GLU:H	1:103:A:THR:HG22	19	0.39	0.07	0.41
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG11	19	0.39	0.07	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG13	19	0.39	0.07	0.41
(1,1105)	1:58:A:MET:HE1	1:92:A:PHE:HE2	19	0.37	0.05	0.36
(1,1105)	1:58:A:MET:HE2	1:92:A:PHE:HE2	19	0.37	0.05	0.36
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	19	0.37	0.05	0.36
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	19	0.36	0.08	0.37
(2,41)	1:54:A:ASP:H	1:53:A:PRO:HG3	19	0.36	0.08	0.37
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE3	19	0.36	0.2	0.25
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	19	0.36	0.2	0.25
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE1	19	0.36	0.2	0.25
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	19	0.35	0.04	0.36
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG13	19	0.35	0.04	0.36
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG11	19	0.35	0.04	0.36
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	19	0.33	0.1	0.33
(2,1556)	1:35:A:VAL:HG22	1:36:A:ILE:H	19	0.33	0.1	0.33
(2,1556)	1:35:A:VAL:HG21	1:36:A:ILE:H	19	0.33	0.1	0.33
(1,805)	1:101:A:THR:HG22	1:102:A:GLU:H	19	0.32	0.04	0.34
(1,805)	1:101:A:THR:HG23	1:102:A:GLU:H	19	0.32	0.04	0.34
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	19	0.32	0.04	0.34
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	19	0.32	0.1	0.34
(2,1539)	1:125:A:LEU:HA	1:120:A:ARG:H	19	0.32	0.1	0.34
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	19	0.29	0.12	0.28
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	19	0.28	0.03	0.28
(2,750)	1:104:A:HIS:HB3	1:104:A:HIS:HE1	19	0.28	0.03	0.28
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	19	0.27	0.09	0.24
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD11	19	0.27	0.09	0.24
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD13	19	0.27	0.09	0.24
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG22	19	0.27	0.06	0.28
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	19	0.27	0.06	0.28
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG23	19	0.27	0.06	0.28
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	19	0.26	0.09	0.26
(2,1153)	1:80:A:ASP:H	1:88:A:HIS:HB3	19	0.26	0.09	0.26
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	19	0.23	0.04	0.23
(1,1064)	1:36:A:ILE:HD12	1:36:A:ILE:HA	19	0.23	0.04	0.23
(1,1064)	1:36:A:ILE:HD11	1:36:A:ILE:HA	19	0.23	0.04	0.23
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	19	0.22	0.03	0.22
(2,676)	1:121:A:ASP:HB2	1:139:A:TYR:HE2	19	0.22	0.03	0.22
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	19	0.21	0.02	0.21
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	19	0.21	0.02	0.21
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG22	19	0.21	0.02	0.21
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	19	0.19	0.09	0.15
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	19	0.19	0.09	0.15
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE1	19	0.19	0.09	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	19	0.19	0.06	0.19
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H181	19	0.19	0.06	0.19
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H182	19	0.19	0.06	0.19
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	18	1.44	0.33	1.49
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	18	1.44	0.33	1.49
(1,924)	1:125:A:LEU:HD22	1:140:A:TYR:HB3	18	1.44	0.33	1.49
(2,82)	1:125:A:LEU:HD11	1:120:A:ARG:HD3	18	1.31	0.45	1.42
(2,82)	1:125:A:LEU:HD13	1:120:A:ARG:HD3	18	1.31	0.45	1.42
(2,82)	1:125:A:LEU:HD12	1:120:A:ARG:HD3	18	1.31	0.45	1.42
(2,82)	1:125:A:LEU:HD12	1:119:A:ARG:HD2	18	1.31	0.45	1.42
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	18	1.2	0.61	1.08
(2,330)	1:41:A:VAL:HG23	1:43:A:LYS:HE3	18	1.2	0.61	1.08
(2,330)	1:41:A:VAL:HG21	1:43:A:LYS:HE3	18	1.2	0.61	1.08
(2,616)	1:125:A:LEU:HD23	1:11:A:PHE:HD2	18	1.14	0.3	1.19
(2,616)	1:125:A:LEU:HD22	1:11:A:PHE:HD2	18	1.14	0.3	1.19
(2,616)	1:125:A:LEU:HD21	1:118:A:TYR:HE1	18	1.14	0.3	1.19
(2,616)	1:125:A:LEU:HD23	1:140:A:TYR:HD2	18	1.14	0.3	1.19
(2,616)	1:125:A:LEU:HD22	1:140:A:TYR:HD2	18	1.14	0.3	1.19
(2,616)	1:125:A:LEU:HD22	1:118:A:TYR:HE1	18	1.14	0.3	1.19
(2,616)	1:125:A:LEU:HD23	1:118:A:TYR:HE1	18	1.14	0.3	1.19
(2,616)	1:125:A:LEU:HD21	1:140:A:TYR:HD2	18	1.14	0.3	1.19
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	18	1.1	0.56	1.25
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	18	1.1	0.56	1.25
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	18	1.06	0.37	1.13
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	18	0.91	0.3	0.94
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	18	0.91	0.3	0.94
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	18	0.91	0.3	0.94
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	18	0.77	0.21	0.86
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG13	18	0.77	0.21	0.86
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG11	18	0.77	0.21	0.86
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	18	0.72	0.39	0.57
(2,1184)	1:143:A:GLN:HE22	1:61:A:LEU:HD21	18	0.72	0.39	0.57
(2,1184)	1:143:A:GLN:HE22	1:61:A:LEU:HD22	18	0.72	0.39	0.57
(2,1184)	1:61:A:LEU:HD11	1:143:A:GLN:HE22	18	0.72	0.39	0.57
(2,1184)	1:142:A:LYS:HG2	1:143:A:GLN:HE22	18	0.72	0.39	0.57
(2,1184)	1:61:A:LEU:HD12	1:143:A:GLN:HE22	18	0.72	0.39	0.57
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	18	0.7	0.33	0.74
(2,1591)	1:41:A:VAL:HG13	2:1001:A:OLA:H72	18	0.7	0.33	0.74
(2,1591)	1:41:A:VAL:HG12	2:1001:A:OLA:H72	18	0.7	0.33	0.74
(2,1591)	1:41:A:VAL:HG11	2:1001:A:OLA:H72	18	0.7	0.33	0.74
(2,496)	1:90:A:ILE:HD12	1:69:A:HIS:HA	18	0.7	0.23	0.7
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	18	0.7	0.23	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,496)	1:90:A:ILE:HD11	1:69:A:HIS:HA	18	0.7	0.23	0.7
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	18	0.68	0.32	0.63
(2,124)	1:10:A:THR:HB	1:44:A:LYS:HB2	18	0.68	0.32	0.63
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	18	0.56	0.22	0.66
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	18	0.56	0.22	0.66
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG23	18	0.56	0.22	0.66
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	18	0.56	0.17	0.61
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	18	0.56	0.17	0.61
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	18	0.56	0.17	0.61
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	18	0.55	0.3	0.43
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD11	18	0.55	0.3	0.43
(2,83)	1:120:A:ARG:HD2	1:125:A:LEU:HD12	18	0.55	0.3	0.43
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD13	18	0.55	0.3	0.43
(2,1521)	1:7:A:PHE:H	1:8:A:LEU:HB3	18	0.52	0.21	0.55
(2,1521)	1:7:A:PHE:H	1:120:A:ARG:HB2	18	0.52	0.21	0.55
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	18	0.52	0.21	0.55
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	18	0.51	0.14	0.54
(2,51)	1:48:A:ALA:HB2	1:56:A:TYR:HB3	18	0.51	0.14	0.54
(2,51)	1:48:A:ALA:HB3	1:56:A:TYR:HB3	18	0.51	0.14	0.54
(2,45)	1:49:A:ALA:HB1	1:48:A:ALA:HA	18	0.51	0.18	0.48
(2,45)	1:49:A:ALA:HB2	1:48:A:ALA:HA	18	0.51	0.18	0.48
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	18	0.51	0.18	0.48
(2,392)	1:1:A:LYS:HE2	1:1:A:LYS:HA	18	0.48	0.24	0.36
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	18	0.48	0.24	0.36
(2,392)	1:1:A:LYS:HA	1:1:A:LYS:HE3	18	0.48	0.24	0.36
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	18	0.47	0.16	0.51
(1,383)	1:23:A:LEU:HD21	1:33:A:ARG:HA	18	0.47	0.16	0.51
(1,383)	1:23:A:LEU:HD23	1:33:A:ARG:HA	18	0.47	0.16	0.51
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	18	0.44	0.09	0.46
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	18	0.44	0.09	0.46
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG21	18	0.44	0.09	0.46
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	18	0.41	0.17	0.43
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	18	0.41	0.17	0.43
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG22	18	0.41	0.17	0.43
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG23	18	0.39	0.13	0.4
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	18	0.39	0.13	0.4
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	18	0.39	0.13	0.4
(2,209)	1:23:A:LEU:HD12	1:36:A:ILE:HG22	18	0.38	0.17	0.36
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG22	18	0.38	0.17	0.36
(2,209)	1:23:A:LEU:HD11	1:36:A:ILE:HG21	18	0.38	0.17	0.36
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG23	18	0.38	0.17	0.36
(2,209)	1:23:A:LEU:HD11	1:36:A:ILE:HG22	18	0.38	0.17	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG21	18	0.38	0.17	0.36
(2,209)	1:23:A:LEU:HD12	1:36:A:ILE:HG21	18	0.38	0.17	0.36
(2,209)	1:23:A:LEU:HD11	1:36:A:ILE:HG23	18	0.38	0.17	0.36
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	18	0.33	0.11	0.32
(1,1386)	1:83:A:LEU:HD11	1:84:A:ASP:H	18	0.33	0.11	0.32
(1,1386)	1:83:A:LEU:HD12	1:84:A:ASP:H	18	0.33	0.11	0.32
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	18	0.32	0.14	0.32
(1,989)	1:134:A:VAL:HG13	1:22:A:TYR:HB3	18	0.32	0.14	0.32
(1,989)	1:134:A:VAL:HG11	1:22:A:TYR:HB3	18	0.32	0.14	0.32
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE2	18	0.3	0.11	0.3
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE3	18	0.3	0.11	0.3
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	18	0.3	0.11	0.3
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	18	0.25	0.06	0.24
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	18	0.25	0.06	0.24
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG11	18	0.25	0.06	0.24
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD22	18	0.24	0.07	0.25
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	18	0.24	0.07	0.25
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD21	18	0.24	0.07	0.25
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	18	0.22	0.06	0.22
(2,1390)	1:54:A:ASP:H	1:53:A:PRO:HG3	18	0.22	0.06	0.22
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	18	0.2	0.04	0.2
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	17	2.45	0.9	2.72
(1,2818)	1:83:A:LEU:HD22	1:62:A:THR:HG1	17	2.45	0.9	2.72
(1,2818)	1:83:A:LEU:HD23	1:62:A:THR:HG1	17	2.45	0.9	2.72
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	17	2.3	0.9	2.58
(1,2799)	1:83:A:LEU:HD22	1:62:A:THR:HG1	17	2.3	0.9	2.58
(1,2799)	1:83:A:LEU:HD23	1:62:A:THR:HG1	17	2.3	0.9	2.58
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD23	17	2.22	0.58	2.43
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	17	2.22	0.58	2.43
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD22	17	2.22	0.58	2.43
(2,93)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	17	1.32	0.33	1.4
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD11	17	1.32	0.33	1.4
(2,93)	1:120:A:ARG:HG2	1:125:A:LEU:HD12	17	1.32	0.33	1.4
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD13	17	1.32	0.33	1.4
(2,93)	1:125:A:LEU:HD12	1:127:A:MET:HG3	17	1.32	0.33	1.4
(2,93)	1:3:A:LEU:HD22	1:8:A:LEU:HD12	17	1.32	0.33	1.4
(2,93)	1:125:A:LEU:HD11	1:127:A:MET:HG3	17	1.32	0.33	1.4
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	17	1.32	0.33	1.4
(2,93)	1:3:A:LEU:HD21	1:8:A:LEU:HD11	17	1.32	0.33	1.4
(2,93)	1:3:A:LEU:HD22	1:8:A:LEU:HD13	17	1.32	0.33	1.4
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD12	17	1.22	0.39	1.2
(2,309)	1:65:A:LYS:H	1:83:A:LEU:HD22	17	1.22	0.39	1.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD11	17	1.22	0.39	1.2
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD13	17	1.22	0.39	1.2
(2,309)	1:65:A:LYS:H	1:83:A:LEU:HD23	17	1.22	0.39	1.2
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD23	17	1.07	0.41	1.12
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD22	17	1.07	0.41	1.12
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD22	17	1.07	0.41	1.12
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD21	17	1.07	0.41	1.12
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD23	17	1.07	0.41	1.12
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD21	17	1.07	0.41	1.12
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	17	1.06	0.24	1.14
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD23	17	0.97	0.74	0.77
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD21	17	0.97	0.74	0.77
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD22	17	0.97	0.74	0.77
(2,1029)	1:113:A:VAL:HG13	1:104:A:HIS:H	17	0.81	0.32	0.95
(2,1029)	1:113:A:VAL:HG11	1:104:A:HIS:H	17	0.81	0.32	0.95
(2,1029)	1:113:A:VAL:HG12	1:104:A:HIS:H	17	0.81	0.32	0.95
(2,1029)	1:105:A:ILE:HD13	1:104:A:HIS:H	17	0.81	0.32	0.95
(2,1029)	1:105:A:ILE:HD11	1:104:A:HIS:H	17	0.81	0.32	0.95
(2,1029)	1:105:A:ILE:HD12	1:104:A:HIS:H	17	0.81	0.32	0.95
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB3	17	0.81	0.29	0.78
(2,229)	1:25:A:ALA:HB3	1:132:A:LYS:HE2	17	0.81	0.29	0.78
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB1	17	0.81	0.29	0.78
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB2	17	0.81	0.29	0.78
(2,229)	1:25:A:ALA:HB2	1:132:A:LYS:HE2	17	0.81	0.29	0.78
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	17	0.8	0.23	0.77
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB1	17	0.8	0.23	0.77
(2,435)	1:104:A:HIS:HB2	1:82:A:ALA:HB1	17	0.8	0.23	0.77
(2,435)	1:104:A:HIS:HB2	1:82:A:ALA:HB2	17	0.8	0.23	0.77
(2,435)	1:88:A:HIS:HB3	1:82:A:ALA:HB3	17	0.8	0.23	0.77
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	17	0.65	0.29	0.62
(2,597)	1:118:A:TYR:HD2	1:102:A:GLU:HG3	17	0.65	0.29	0.62
(2,597)	1:118:A:TYR:HD2	1:99:A:THR:HG23	17	0.65	0.29	0.62
(2,597)	1:118:A:TYR:HD2	1:127:A:MET:HG3	17	0.65	0.29	0.62
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG3	17	0.61	0.03	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	17	0.61	0.03	0.6
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	17	0.59	0.24	0.53
(2,830)	2:1001:A:OLA:H81	1:36:A:ILE:HA	17	0.59	0.24	0.53
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD23	17	0.59	0.18	0.54
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD22	17	0.59	0.18	0.54
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD21	17	0.59	0.18	0.54
(2,1027)	1:39:A:ALA:H	1:36:A:ILE:HG21	17	0.59	0.18	0.54
(2,1027)	1:39:A:ALA:H	1:36:A:ILE:HG22	17	0.59	0.18	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,617)	1:125:A:LEU:HD23	1:127:A:MET:H	17	0.58	0.31	0.5
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD21	17	0.58	0.31	0.5
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD23	17	0.58	0.31	0.5
(2,617)	1:125:A:LEU:HD21	1:127:A:MET:H	17	0.58	0.31	0.5
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD22	17	0.58	0.31	0.5
(2,732)	1:58:A:MET:HE3	1:67:A:THR:HG1	17	0.53	0.16	0.53
(2,732)	1:58:A:MET:HE1	1:67:A:THR:HG1	17	0.53	0.16	0.53
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	17	0.53	0.16	0.53
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	17	0.52	0.16	0.49
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB3	17	0.52	0.16	0.49
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB1	17	0.52	0.16	0.49
(2,355)	1:57:A:ASP:HA	1:70:A:LYS:HG2	17	0.52	0.16	0.49
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD21	17	0.43	0.24	0.39
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	17	0.43	0.24	0.39
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD23	17	0.43	0.24	0.39
(2,517)	1:96:A:ASP:H	1:94:A:LEU:HD21	17	0.43	0.24	0.39
(2,517)	1:96:A:ASP:H	1:94:A:LEU:HD22	17	0.43	0.24	0.39
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	17	0.43	0.12	0.43
(1,629)	1:74:A:LEU:HD13	1:75:A:GLY:H	17	0.43	0.12	0.43
(1,629)	1:74:A:LEU:HD11	1:75:A:GLY:H	17	0.43	0.12	0.43
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	17	0.42	0.15	0.36
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG22	17	0.42	0.15	0.36
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG23	17	0.42	0.15	0.36
(2,552)	1:131:A:TRP:H	1:134:A:VAL:HG22	17	0.42	0.15	0.36
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	17	0.41	0.14	0.45
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	17	0.41	0.14	0.45
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	17	0.41	0.14	0.45
(2,787)	1:127:A:MET:HE2	1:117:A:GLU:H	17	0.39	0.13	0.42
(2,787)	1:39:A:ALA:HB1	1:40:A:GLY:H	17	0.39	0.13	0.42
(2,787)	1:39:A:ALA:HB3	1:40:A:GLY:H	17	0.39	0.13	0.42
(2,787)	1:39:A:ALA:HB2	1:40:A:GLY:H	17	0.39	0.13	0.42
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG3	17	0.36	0.03	0.35
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	17	0.36	0.03	0.35
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD22	17	0.31	0.08	0.29
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	17	0.31	0.08	0.29
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD21	17	0.31	0.08	0.29
(2,226)	1:134:A:VAL:HG22	1:25:A:ALA:HA	17	0.3	0.11	0.3
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	17	0.3	0.11	0.3
(2,226)	1:134:A:VAL:HG23	1:25:A:ALA:HA	17	0.3	0.11	0.3
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	17	0.25	0.07	0.25
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	17	0.24	0.09	0.23
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB2	17	0.24	0.09	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB1	17	0.24	0.09	0.23
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	17	0.17	0.04	0.16
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	17	0.16	0.04	0.16
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	16	1.73	0.56	1.8
(1,128)	1:100:A:LEU:HD23	1:3:A:LEU:HD11	16	1.73	0.56	1.8
(1,128)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	16	1.73	0.56	1.8
(1,128)	1:100:A:LEU:HD23	1:3:A:LEU:HD13	16	1.73	0.56	1.8
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	16	1.73	0.56	1.8
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD12	16	1.73	0.56	1.8
(1,128)	1:100:A:LEU:HD23	1:3:A:LEU:HD12	16	1.73	0.56	1.8
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	16	1.63	0.58	1.71
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG11	16	1.63	0.58	1.71
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG12	16	1.63	0.58	1.71
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	16	1.14	0.62	1.09
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG11	16	1.14	0.62	1.09
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG12	16	1.14	0.62	1.09
(2,825)	1:118:A:TYR:HD1	1:58:A:MET:HG3	16	1.09	0.41	0.9
(2,825)	1:118:A:TYR:HD1	1:127:A:MET:HG2	16	1.09	0.41	0.9
(2,825)	1:118:A:TYR:HD2	1:58:A:MET:HG3	16	1.09	0.41	0.9
(2,825)	1:118:A:TYR:HD2	1:127:A:MET:HG2	16	1.09	0.41	0.9
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD13	16	0.96	0.49	1.13
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD11	16	0.96	0.49	1.13
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD11	16	0.96	0.49	1.13
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD12	16	0.96	0.49	1.13
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD13	16	0.96	0.49	1.13
(1,1186)	1:127:A:MET:HE3	1:125:A:LEU:HD12	16	0.96	0.49	1.13
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD12	16	0.96	0.49	1.13
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	16	0.81	0.45	0.75
(2,422)	1:74:A:LEU:HD12	1:4:A:PRO:HD2	16	0.81	0.45	0.75
(2,422)	1:74:A:LEU:HD11	1:4:A:PRO:HD2	16	0.81	0.45	0.75
(2,1606)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	16	0.79	0.34	0.83
(2,1606)	1:36:A:ILE:HD11	1:23:A:LEU:HB2	16	0.79	0.34	0.83
(2,1606)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	16	0.79	0.34	0.83
(2,1606)	2:1001:A:OLA:H111	1:36:A:ILE:HD12	16	0.79	0.34	0.83
(2,1606)	1:36:A:ILE:HD13	2:1001:A:OLA:H112	16	0.79	0.34	0.83
(2,1606)	1:36:A:ILE:HD12	1:23:A:LEU:HB2	16	0.79	0.34	0.83
(2,1606)	1:36:A:ILE:HD12	2:1001:A:OLA:H112	16	0.79	0.34	0.83
(2,1606)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	16	0.79	0.34	0.83
(2,1606)	2:1001:A:OLA:H111	1:36:A:ILE:HD11	16	0.79	0.34	0.83
(2,1606)	1:36:A:ILE:HD13	1:23:A:LEU:HB2	16	0.79	0.34	0.83
(2,543)	1:58:A:MET:HE1	1:100:A:LEU:HD22	16	0.79	0.36	0.79
(2,543)	1:58:A:MET:HE2	1:100:A:LEU:HD21	16	0.79	0.36	0.79

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,543)	1:100:A:LEU:HD23	1:74:A:LEU:HB2	16	0.79	0.36	0.79
(2,543)	1:100:A:LEU:HD22	1:58:A:MET:HG2	16	0.79	0.36	0.79
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD21	16	0.79	0.36	0.79
(2,543)	1:100:A:LEU:HD21	1:74:A:LEU:HB2	16	0.79	0.36	0.79
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD22	16	0.79	0.36	0.79
(2,543)	1:58:A:MET:HE3	1:100:A:LEU:HD21	16	0.79	0.36	0.79
(2,543)	1:58:A:MET:HE2	1:100:A:LEU:HD23	16	0.79	0.36	0.79
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD23	16	0.79	0.36	0.79
(2,543)	1:100:A:LEU:HD22	1:74:A:LEU:HB2	16	0.79	0.36	0.79
(1,448)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	16	0.76	0.24	0.83
(1,448)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	16	0.76	0.24	0.83
(1,448)	1:41:A:VAL:HG22	1:140:A:TYR:HE1	16	0.76	0.24	0.83
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	16	0.73	0.05	0.73
(1,194)	1:10:A:THR:H	1:10:A:THR:HG23	16	0.73	0.05	0.73
(1,194)	1:10:A:THR:H	1:10:A:THR:HG21	16	0.73	0.05	0.73
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	16	0.6	0.42	0.46
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD21	16	0.6	0.42	0.46
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD22	16	0.6	0.42	0.46
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	16	0.54	0.11	0.57
(2,927)	1:38:A:LEU:H	1:37:A:LYS:HB3	16	0.54	0.11	0.57
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	16	0.52	0.38	0.48
(2,528)	1:143:A:GLN:HA	1:141:A:LYS:HE3	16	0.52	0.38	0.48
(2,528)	1:141:A:LYS:HE3	1:141:A:LYS:HA	16	0.52	0.38	0.48
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE2	16	0.46	0.19	0.44
(2,782)	1:127:A:MET:HE2	1:116:A:TYR:HA	16	0.46	0.19	0.44
(2,782)	1:127:A:MET:HE3	1:116:A:TYR:HA	16	0.46	0.19	0.44
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE3	16	0.46	0.19	0.44
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE1	16	0.46	0.19	0.44
(1,617)	1:73:A:ALA:HB2	1:75:A:GLY:H	16	0.44	0.09	0.48
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	16	0.44	0.09	0.48
(1,617)	1:73:A:ALA:HB3	1:75:A:GLY:H	16	0.44	0.09	0.48
(2,623)	1:128:A:LYS:HE2	1:126:A:VAL:HG11	16	0.36	0.18	0.33
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	16	0.36	0.18	0.33
(2,623)	1:128:A:LYS:HE3	1:126:A:VAL:HG13	16	0.36	0.18	0.33
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG11	16	0.36	0.18	0.33
(2,623)	1:128:A:LYS:HE3	1:126:A:VAL:HG11	16	0.36	0.18	0.33
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG13	16	0.36	0.18	0.33
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	16	0.26	0.09	0.26
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB2	16	0.26	0.09	0.26
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB1	16	0.26	0.09	0.26
(2,1679)	2:1001:A:OLA:H172	2:1001:A:OLA:H181	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H71	1:36:A:ILE:HG21	16	0.26	0.13	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1679)	1:83:A:LEU:HD21	2:1001:A:OLA:H62	16	0.26	0.13	0.22
(2,1679)	1:94:A:LEU:HB3	1:94:A:LEU:HD21	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H41	2:1001:A:OLA:H181	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H172	2:1001:A:OLA:H183	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H71	1:36:A:ILE:HG23	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H61	1:36:A:ILE:HG21	16	0.26	0.13	0.22
(2,1679)	1:94:A:LEU:HB3	1:94:A:LEU:HD11	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H61	1:36:A:ILE:HG22	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H41	2:1001:A:OLA:H182	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H62	1:36:A:ILE:HG22	16	0.26	0.13	0.22
(2,1679)	2:1001:A:OLA:H62	1:36:A:ILE:HG21	16	0.26	0.13	0.22
(2,837)	1:58:A:MET:HE1	1:60:A:ASN:HD21	16	0.25	0.11	0.23
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	16	0.25	0.11	0.23
(2,837)	1:58:A:MET:HE3	1:60:A:ASN:HD21	16	0.25	0.11	0.23
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	16	0.25	0.1	0.22
(1,1171)	1:32:A:MET:HE3	1:33:A:ARG:H	16	0.25	0.1	0.22
(1,1171)	1:32:A:MET:HE2	1:33:A:ARG:H	16	0.25	0.1	0.22
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD3	16	0.2	0.03	0.21
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD2	16	0.2	0.03	0.21
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	16	0.2	0.03	0.21
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD3	16	0.2	0.03	0.21
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	16	0.17	0.03	0.16
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG11	16	0.17	0.03	0.16
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG13	16	0.17	0.03	0.16
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	15	2.09	0.39	2.13
(2,547)	1:100:A:LEU:HD12	1:94:A:LEU:HA	15	2.09	0.39	2.13
(2,547)	1:100:A:LEU:HD13	1:117:A:GLU:HA	15	2.09	0.39	2.13
(2,547)	1:100:A:LEU:HD11	1:94:A:LEU:HA	15	2.09	0.39	2.13
(1,796)	1:100:A:LEU:HD12	1:101:A:THR:H	15	1.78	0.2	1.76
(1,796)	1:100:A:LEU:HD13	1:101:A:THR:H	15	1.78	0.2	1.76
(1,796)	1:100:A:LEU:HD11	1:101:A:THR:H	15	1.78	0.2	1.76
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	15	1.72	0.39	1.69
(1,789)	1:100:A:LEU:HD23	1:3:A:LEU:HD11	15	1.72	0.39	1.69
(1,789)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	15	1.72	0.39	1.69
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	15	1.72	0.39	1.69
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD12	15	1.72	0.39	1.69
(1,789)	1:100:A:LEU:HD23	1:3:A:LEU:HD12	15	1.72	0.39	1.69
(1,797)	1:100:A:LEU:HD11	1:93:A:ASP:H	15	1.7	0.23	1.74
(1,797)	1:100:A:LEU:HD12	1:93:A:ASP:H	15	1.7	0.23	1.74
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	15	1.7	0.23	1.74
(1,2063)	1:100:A:LEU:HD12	1:101:A:THR:H	15	1.5	0.2	1.48
(1,2063)	1:100:A:LEU:HD13	1:101:A:THR:H	15	1.5	0.2	1.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2063)	1:100:A:LEU:HD11	1:101:A:THR:H	15	1.5	0.2	1.48
(1,1963)	1:100:A:LEU:HD11	1:93:A:ASP:H	15	1.39	0.23	1.43
(1,1963)	1:100:A:LEU:HD12	1:93:A:ASP:H	15	1.39	0.23	1.43
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	15	1.39	0.23	1.43
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD21	15	1.37	0.31	1.32
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	15	1.37	0.31	1.32
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD23	15	1.37	0.31	1.32
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	15	1.24	0.51	1.45
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD22	15	1.24	0.51	1.45
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD23	15	1.24	0.51	1.45
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	15	1.22	0.85	0.95
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD11	15	1.22	0.85	0.95
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD12	15	1.22	0.85	0.95
(2,161)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	15	1.2	0.17	1.25
(2,161)	1:13:A:LEU:HD21	1:140:A:TYR:HE2	15	1.2	0.17	1.25
(2,161)	1:13:A:LEU:HD22	1:139:A:TYR:HD1	15	1.2	0.17	1.25
(2,161)	1:13:A:LEU:HD21	1:140:A:TYR:HE1	15	1.2	0.17	1.25
(2,161)	1:13:A:LEU:HD23	1:140:A:TYR:HE1	15	1.2	0.17	1.25
(2,161)	1:13:A:LEU:HD23	1:140:A:TYR:HE2	15	1.2	0.17	1.25
(2,161)	1:13:A:LEU:HD23	1:139:A:TYR:HD1	15	1.2	0.17	1.25
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	15	1.18	0.28	1.17
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD12	15	1.18	0.28	1.17
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	15	1.18	0.28	1.17
(1,794)	1:100:A:LEU:HD13	1:100:A:LEU:HA	15	1.15	0.12	1.19
(1,794)	1:100:A:LEU:HD11	1:100:A:LEU:HA	15	1.15	0.12	1.19
(1,794)	1:100:A:LEU:HD12	1:100:A:LEU:HA	15	1.15	0.12	1.19
(2,1103)	1:87:A:GLN:H	1:107:A:VAL:HG13	15	1.06	0.38	1.15
(2,1103)	1:87:A:GLN:H	1:107:A:VAL:HG11	15	1.06	0.38	1.15
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB1	15	1.06	0.38	1.15
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	15	1.06	0.38	1.15
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB2	15	1.06	0.38	1.15
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD11	15	1.04	0.29	1.09
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD12	15	1.04	0.29	1.09
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD13	15	1.04	0.29	1.09
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB3	15	0.92	0.4	0.76
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB2	15	0.92	0.4	0.76
(2,49)	1:48:A:ALA:HB3	1:55:A:ARG:HD2	15	0.92	0.4	0.76
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB1	15	0.92	0.4	0.76
(2,49)	1:47:A:ASN:HB2	1:48:A:ALA:HB2	15	0.92	0.4	0.76
(2,49)	1:48:A:ALA:HB1	1:55:A:ARG:HD2	15	0.92	0.4	0.76
(2,49)	1:48:A:ALA:HB2	1:55:A:ARG:HD2	15	0.92	0.4	0.76
(2,49)	1:52:A:LYS:HE2	1:48:A:ALA:HB3	15	0.92	0.4	0.76

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,49)	1:52:A:LYS:HE3	1:48:A:ALA:HB3	15	0.92	0.4	0.76
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	15	0.91	0.49	0.82
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG13	15	0.91	0.03	0.91
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG12	15	0.91	0.03	0.91
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG11	15	0.91	0.03	0.91
(2,143)	1:11:A:PHE:HD2	1:10:A:THR:HG21	15	0.85	0.27	0.87
(2,143)	1:127:A:MET:HG3	1:140:A:TYR:HD2	15	0.85	0.27	0.87
(2,143)	1:42:A:THR:HG22	1:140:A:TYR:HD1	15	0.85	0.27	0.87
(2,143)	1:42:A:THR:HG21	1:140:A:TYR:HD1	15	0.85	0.27	0.87
(2,143)	1:11:A:PHE:HD2	1:10:A:THR:HG22	15	0.85	0.27	0.87
(2,143)	1:42:A:THR:HG23	1:140:A:TYR:HD1	15	0.85	0.27	0.87
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	15	0.82	0.35	0.59
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD11	15	0.82	0.35	0.59
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD13	15	0.82	0.35	0.59
(2,1037)	1:42:A:THR:H	1:41:A:VAL:HG22	15	0.82	0.06	0.82
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG22	15	0.82	0.06	0.82
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG21	15	0.82	0.06	0.82
(2,1037)	1:42:A:THR:H	1:41:A:VAL:HG21	15	0.82	0.06	0.82
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG23	15	0.82	0.06	0.82
(2,160)	1:13:A:LEU:HD21	1:41:A:VAL:H	15	0.67	0.32	0.64
(2,160)	1:13:A:LEU:HD22	1:140:A:TYR:HD2	15	0.67	0.32	0.64
(2,160)	1:13:A:LEU:HD23	1:41:A:VAL:H	15	0.67	0.32	0.64
(2,160)	1:13:A:LEU:HD22	1:41:A:VAL:H	15	0.67	0.32	0.64
(2,160)	1:13:A:LEU:HD23	1:140:A:TYR:HD1	15	0.67	0.32	0.64
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	15	0.66	0.12	0.67
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD11	15	0.66	0.12	0.67
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD12	15	0.66	0.12	0.67
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	15	0.65	0.17	0.68
(2,687)	1:141:A:LYS:HD2	1:141:A:LYS:HA	15	0.65	0.17	0.68
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	15	0.59	0.27	0.62
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG23	15	0.59	0.27	0.62
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG21	15	0.59	0.27	0.62
(2,494)	1:90:A:ILE:HD13	1:104:A:HIS:HB3	15	0.57	0.16	0.51
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	15	0.57	0.16	0.51
(2,494)	1:90:A:ILE:HD12	1:104:A:HIS:HB3	15	0.57	0.16	0.51
(2,533)	1:99:A:THR:HG23	1:96:A:ASP:HB2	15	0.55	0.18	0.52
(2,533)	1:95:A:LYS:HE2	1:99:A:THR:HG23	15	0.55	0.18	0.52
(2,533)	1:99:A:THR:HG22	1:95:A:LYS:HE3	15	0.55	0.18	0.52
(2,533)	1:99:A:THR:HG21	1:96:A:ASP:HB2	15	0.55	0.18	0.52
(2,533)	1:95:A:LYS:HE2	1:99:A:THR:HG21	15	0.55	0.18	0.52
(2,533)	1:99:A:THR:HG21	1:95:A:LYS:HE3	15	0.55	0.18	0.52
(2,533)	1:99:A:THR:HG22	1:96:A:ASP:HB2	15	0.55	0.18	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	15	0.54	0.2	0.54
(2,380)	1:65:A:LYS:HB2	2:1001:A:OLA:H10	15	0.54	0.2	0.54
(2,380)	1:65:A:LYS:HB2	2:1001:A:OLA:H9	15	0.54	0.2	0.54
(2,380)	2:1001:A:OLA:H9	1:64:A:LYS:HB3	15	0.54	0.2	0.54
(2,727)	1:3:A:LEU:HD21	1:7:A:PHE:HA	15	0.51	0.21	0.51
(2,727)	1:3:A:LEU:HD23	1:7:A:PHE:HA	15	0.51	0.21	0.51
(2,727)	1:3:A:LEU:HD22	1:7:A:PHE:HA	15	0.51	0.21	0.51
(2,727)	1:7:A:PHE:HA	1:125:A:LEU:HD11	15	0.51	0.21	0.51
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	15	0.49	0.14	0.47
(2,838)	1:127:A:MET:HE2	1:116:A:TYR:HE2	15	0.49	0.14	0.47
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE1	15	0.49	0.14	0.47
(2,838)	1:127:A:MET:HE2	1:116:A:TYR:HE1	15	0.49	0.14	0.47
(2,838)	1:127:A:MET:HE1	1:116:A:TYR:HE2	15	0.49	0.14	0.47
(2,838)	1:127:A:MET:HE2	1:60:A:ASN:HD21	15	0.49	0.14	0.47
(2,1079)	1:89:A:LYS:H	1:79:A:GLN:HB3	15	0.46	0.26	0.48
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	15	0.46	0.26	0.48
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HB2	15	0.46	0.26	0.48
(2,706)	1:41:A:VAL:HG22	1:62:A:THR:HG1	15	0.46	0.23	0.39
(2,706)	1:41:A:VAL:HG21	1:62:A:THR:HG1	15	0.46	0.23	0.39
(2,706)	1:41:A:VAL:HG23	1:62:A:THR:HG1	15	0.46	0.23	0.39
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD21	15	0.45	0.09	0.46
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	15	0.45	0.09	0.46
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD22	15	0.45	0.09	0.46
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	15	0.45	0.19	0.52
(2,1623)	2:1001:A:OLA:H81	1:36:A:ILE:HA	15	0.45	0.19	0.52
(2,675)	1:139:A:TYR:HA	1:139:A:TYR:HE2	15	0.34	0.14	0.33
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	15	0.34	0.14	0.33
(2,675)	1:126:A:VAL:HA	1:139:A:TYR:HE2	15	0.34	0.14	0.33
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	15	0.32	0.16	0.26
(2,155)	1:12:A:LYS:HE2	1:12:A:LYS:HA	15	0.32	0.16	0.26
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	15	0.25	0.11	0.24
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	15	0.25	0.11	0.24
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H131	15	0.25	0.11	0.24
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	15	0.19	0.03	0.2
(2,612)	1:125:A:LEU:HD21	1:125:A:LEU:HB3	15	0.18	0.03	0.19
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	15	0.18	0.03	0.19
(2,612)	1:125:A:LEU:HD22	1:125:A:LEU:HB3	15	0.18	0.03	0.19
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	15	0.17	0.05	0.15
(2,310)	1:38:A:LEU:HD21	1:38:A:LEU:HG	15	0.11	0.01	0.11
(2,310)	1:38:A:LEU:HD22	1:38:A:LEU:HG	15	0.11	0.01	0.11
(2,310)	1:38:A:LEU:HD23	1:38:A:LEU:HG	15	0.11	0.01	0.11
(2,310)	1:38:A:LEU:HB3	1:38:A:LEU:HD22	15	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	14	1.71	0.63	1.56
(2,308)	1:35:A:VAL:HA	1:38:A:LEU:HD13	14	1.71	0.63	1.56
(2,308)	1:35:A:VAL:HA	1:38:A:LEU:HD11	14	1.71	0.63	1.56
(2,308)	1:35:A:VAL:HA	1:38:A:LEU:HD12	14	1.71	0.63	1.56
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	14	1.3	0.31	1.27
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	14	1.13	0.95	0.78
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD12	14	1.13	0.95	0.78
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD13	14	1.13	0.95	0.78
(2,461)	1:86:A:THR:HG23	1:84:A:ASP:HB3	14	1.05	0.44	1.09
(2,461)	1:41:A:VAL:HG22	1:60:A:ASN:HB3	14	1.05	0.44	1.09
(2,461)	1:41:A:VAL:HG23	1:60:A:ASN:HB3	14	1.05	0.44	1.09
(2,461)	1:41:A:VAL:HG21	1:60:A:ASN:HB3	14	1.05	0.44	1.09
(2,461)	1:86:A:THR:HG21	1:84:A:ASP:HB3	14	1.05	0.44	1.09
(2,461)	1:86:A:THR:HG22	1:84:A:ASP:HB3	14	1.05	0.44	1.09
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG12	14	1.01	0.41	1.11
(2,624)	1:128:A:LYS:HD3	1:126:A:VAL:HG11	14	1.01	0.41	1.11
(2,624)	1:128:A:LYS:HD3	1:126:A:VAL:HG13	14	1.01	0.41	1.11
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG13	14	1.01	0.41	1.11
(2,624)	1:127:A:MET:HB3	1:126:A:VAL:HG11	14	1.01	0.41	1.11
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG11	14	1.01	0.41	1.11
(2,624)	1:127:A:MET:HB3	1:126:A:VAL:HG13	14	1.01	0.41	1.11
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	14	0.94	0.31	0.92
(2,486)	1:90:A:ILE:HG23	1:104:A:HIS:HB3	14	0.86	0.09	0.86
(2,486)	1:90:A:ILE:HG21	1:104:A:HIS:HB3	14	0.86	0.09	0.86
(2,486)	1:90:A:ILE:HG22	1:104:A:HIS:HB3	14	0.86	0.09	0.86
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE2	14	0.84	0.05	0.85
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE1	14	0.84	0.05	0.85
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE3	14	0.84	0.05	0.85
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	14	0.84	0.4	0.62
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	14	0.72	0.35	0.72
(2,139)	1:14:A:GLU:HG2	1:124:A:TYR:HD2	14	0.72	0.35	0.72
(2,760)	1:118:A:TYR:H	1:127:A:MET:HE2	14	0.69	0.33	0.65
(2,760)	1:127:A:MET:HE3	1:140:A:TYR:HH	14	0.69	0.33	0.65
(2,760)	1:127:A:MET:HE1	1:140:A:TYR:HH	14	0.69	0.33	0.65
(2,760)	1:127:A:MET:HE2	1:140:A:TYR:HH	14	0.69	0.33	0.65
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	14	0.65	0.35	0.82
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG12	14	0.65	0.35	0.82
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG11	14	0.65	0.35	0.82
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	14	0.64	0.51	0.46
(2,820)	1:41:A:VAL:HG21	1:43:A:LYS:HE2	14	0.64	0.51	0.46
(2,820)	1:41:A:VAL:HG22	1:43:A:LYS:HE2	14	0.64	0.51	0.46
(2,820)	1:41:A:VAL:HG23	1:43:A:LYS:HE2	14	0.64	0.51	0.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,144)	1:124:A:TYR:HD2	1:141:A:LYS:HG3	14	0.6	0.23	0.65
(2,144)	1:126:A:VAL:HG23	1:124:A:TYR:HD2	14	0.6	0.23	0.65
(2,144)	1:11:A:PHE:HD1	1:141:A:LYS:HG3	14	0.6	0.23	0.65
(2,144)	1:126:A:VAL:HG22	1:124:A:TYR:HD2	14	0.6	0.23	0.65
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	14	0.59	0.21	0.63
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	14	0.59	0.21	0.63
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	14	0.59	0.21	0.63
(2,568)	1:113:A:VAL:HG23	1:113:A:VAL:HA	14	0.59	0.2	0.68
(2,568)	1:113:A:VAL:HG22	1:113:A:VAL:HA	14	0.59	0.2	0.68
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG23	14	0.59	0.2	0.68
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG21	14	0.59	0.2	0.68
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG22	14	0.59	0.2	0.68
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD11	14	0.47	0.34	0.42
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD13	14	0.47	0.34	0.42
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD12	14	0.47	0.34	0.42
(2,694)	1:141:A:LYS:H	1:141:A:LYS:HE3	14	0.44	0.18	0.44
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	14	0.44	0.18	0.44
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE2	14	0.39	0.05	0.4
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE1	14	0.39	0.05	0.4
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE3	14	0.39	0.05	0.4
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	14	0.39	0.12	0.38
(2,1652)	1:32:A:MET:HE3	2:1001:A:OLA:H131	14	0.38	0.15	0.38
(2,1652)	1:32:A:MET:HE3	1:35:A:VAL:HG11	14	0.38	0.15	0.38
(2,1652)	1:32:A:MET:HE3	1:35:A:VAL:HG12	14	0.38	0.15	0.38
(2,1652)	1:32:A:MET:HE1	2:1001:A:OLA:H131	14	0.38	0.15	0.38
(2,1652)	1:32:A:MET:HE2	2:1001:A:OLA:H131	14	0.38	0.15	0.38
(2,1652)	2:1001:A:OLA:H142	1:32:A:MET:HE1	14	0.38	0.15	0.38
(2,1652)	1:32:A:MET:HE2	1:35:A:VAL:HG13	14	0.38	0.15	0.38
(2,1652)	2:1001:A:OLA:H142	1:32:A:MET:HE3	14	0.38	0.15	0.38
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	14	0.37	0.14	0.37
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	14	0.36	0.15	0.32
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG23	14	0.36	0.15	0.32
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG21	14	0.36	0.15	0.32
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	14	0.33	0.13	0.34
(1,2814)	2:1001:A:OLA:H182	1:19:A:PHE:HE1	14	0.33	0.13	0.34
(1,2814)	2:1001:A:OLA:H182	1:19:A:PHE:HE2	14	0.33	0.13	0.34
(1,2814)	2:1001:A:OLA:H183	1:19:A:PHE:HE1	14	0.33	0.13	0.34
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB3	14	0.32	0.1	0.32
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB2	14	0.32	0.1	0.32
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB1	14	0.32	0.1	0.32
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB1	14	0.23	0.07	0.24
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB3	14	0.23	0.07	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB2	14	0.23	0.07	0.24
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	14	0.17	0.04	0.16
(2,810)	1:52:A:LYS:HE2	1:50:A:SER:HB3	13	1.27	0.73	1.64
(2,810)	1:52:A:LYS:HE2	1:53:A:PRO:HD3	13	1.27	0.73	1.64
(2,810)	1:52:A:LYS:HE3	1:53:A:PRO:HD3	13	1.27	0.73	1.64
(2,810)	1:52:A:LYS:HE3	1:50:A:SER:HB3	13	1.27	0.73	1.64
(2,420)	1:106:A:LYS:HG2	1:105:A:ILE:HA	13	0.79	0.3	0.89
(2,420)	1:74:A:LEU:HD12	1:55:A:ARG:HA	13	0.79	0.3	0.89
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD11	13	0.79	0.3	0.89
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD12	13	0.79	0.3	0.89
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD13	13	0.79	0.3	0.89
(2,420)	1:41:A:VAL:HA	1:61:A:LEU:HD11	13	0.79	0.3	0.89
(2,1581)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	13	0.77	0.34	0.74
(2,1581)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	13	0.77	0.34	0.74
(2,1581)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	13	0.77	0.34	0.74
(2,1581)	2:1001:A:OLA:H81	1:36:A:ILE:HD13	13	0.77	0.34	0.74
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	13	0.71	0.33	0.72
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	13	0.67	0.23	0.73
(2,791)	1:131:A:TRP:HB2	1:131:A:TRP:HZ2	13	0.67	0.23	0.73
(2,718)	1:73:A:ALA:HB2	1:0:A:SER:HA	13	0.67	0.32	0.84
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	13	0.67	0.32	0.84
(2,718)	1:73:A:ALA:HB1	1:0:A:SER:HA	13	0.67	0.32	0.84
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD23	13	0.64	0.22	0.59
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD22	13	0.64	0.22	0.59
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD21	13	0.64	0.22	0.59
(2,751)	1:104:A:HIS:HE1	1:82:A:ALA:HB3	13	0.63	0.27	0.69
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD23	13	0.63	0.27	0.69
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD22	13	0.63	0.27	0.69
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD21	13	0.63	0.27	0.69
(2,751)	1:83:A:LEU:HD13	1:104:A:HIS:HE1	13	0.63	0.27	0.69
(2,751)	1:104:A:HIS:HE1	1:82:A:ALA:HB1	13	0.63	0.27	0.69
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG23	13	0.61	0.22	0.65
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG22	13	0.61	0.22	0.65
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG21	13	0.61	0.22	0.65
(2,716)	1:5:A:ASP:H	1:2:A:THR:HG21	13	0.61	0.22	0.65
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG22	13	0.53	0.34	0.52
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG23	13	0.53	0.34	0.52
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG21	13	0.53	0.34	0.52
(2,299)	1:37:A:LYS:HG3	1:38:A:LEU:HD21	13	0.53	0.34	0.52
(2,299)	1:37:A:LYS:HG3	1:38:A:LEU:HD23	13	0.53	0.34	0.52
(2,500)	1:90:A:ILE:HD13	1:88:A:HIS:H	13	0.49	0.26	0.45
(2,500)	1:90:A:ILE:HD12	1:88:A:HIS:H	13	0.49	0.26	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,500)	1:90:A:ILE:HD11	1:88:A:HIS:H	13	0.49	0.26	0.45
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	13	0.48	0.03	0.5
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD11	13	0.48	0.03	0.5
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	13	0.47	0.28	0.43
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	13	0.47	0.14	0.54
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD3	13	0.47	0.14	0.54
(2,62)	1:0:A:SER:HB3	1:2:A:THR:H	13	0.44	0.22	0.49
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	13	0.44	0.22	0.49
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	13	0.42	0.16	0.45
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB2	13	0.42	0.16	0.45
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB3	13	0.42	0.16	0.45
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG21	13	0.42	0.07	0.44
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	13	0.42	0.07	0.44
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG22	13	0.42	0.07	0.44
(1,2243)	1:23:A:LEU:HD23	1:37:A:LYS:H	13	0.4	0.13	0.43
(1,2243)	1:23:A:LEU:HD21	1:37:A:LYS:H	13	0.4	0.13	0.43
(1,2243)	1:23:A:LEU:HD22	1:37:A:LYS:H	13	0.4	0.13	0.43
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	13	0.4	0.19	0.34
(1,130)	1:3:A:LEU:HD11	1:7:A:PHE:HB3	13	0.4	0.19	0.34
(1,130)	1:3:A:LEU:HD13	1:7:A:PHE:HB3	13	0.4	0.19	0.34
(1,441)	1:38:A:LEU:HD23	1:38:A:LEU:HA	13	0.39	0.2	0.4
(1,441)	1:38:A:LEU:HD22	1:38:A:LEU:HA	13	0.39	0.2	0.4
(1,441)	1:38:A:LEU:HD21	1:38:A:LEU:HA	13	0.39	0.2	0.4
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD23	13	0.38	0.13	0.39
(2,116)	1:8:A:LEU:HD23	1:9:A:GLY:H	13	0.38	0.13	0.39
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD21	13	0.38	0.13	0.39
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD22	13	0.38	0.13	0.39
(2,116)	1:8:A:LEU:HD22	1:9:A:GLY:H	13	0.38	0.13	0.39
(2,785)	1:32:A:MET:HE3	2:1001:A:OLA:H131	13	0.38	0.14	0.37
(2,785)	1:32:A:MET:HE3	1:35:A:VAL:HG11	13	0.38	0.14	0.37
(2,785)	1:32:A:MET:HE3	1:35:A:VAL:HG12	13	0.38	0.14	0.37
(2,785)	1:32:A:MET:HE1	2:1001:A:OLA:H131	13	0.38	0.14	0.37
(2,785)	1:32:A:MET:HE2	2:1001:A:OLA:H131	13	0.38	0.14	0.37
(2,785)	1:32:A:MET:HE2	1:35:A:VAL:HG13	13	0.38	0.14	0.37
(2,785)	2:1001:A:OLA:H142	1:32:A:MET:HE3	13	0.38	0.14	0.37
(1,1168)	1:32:A:MET:HE3	1:35:A:VAL:H	13	0.31	0.17	0.24
(1,1168)	1:32:A:MET:HE1	1:35:A:VAL:H	13	0.31	0.17	0.24
(1,1168)	1:32:A:MET:HE2	1:35:A:VAL:H	13	0.31	0.17	0.24
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG22	13	0.3	0.13	0.29
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG22	13	0.3	0.13	0.29
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG21	13	0.3	0.13	0.29
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG23	13	0.3	0.13	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG23	13	0.3	0.13	0.29
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG21	13	0.3	0.13	0.29
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB3	13	0.29	0.1	0.28
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB2	13	0.29	0.1	0.28
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB1	13	0.29	0.1	0.28
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG12	13	0.27	0.04	0.27
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG13	13	0.27	0.04	0.27
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG11	13	0.27	0.04	0.27
(2,1636)	1:65:A:LYS:HG2	1:62:A:THR:HG1	13	0.27	0.11	0.27
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	13	0.27	0.11	0.27
(2,1636)	1:83:A:LEU:HB3	1:62:A:THR:HG1	13	0.27	0.11	0.27
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	13	0.26	0.1	0.25
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD12	13	0.21	0.07	0.19
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD13	13	0.21	0.07	0.19
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD11	13	0.21	0.07	0.19
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	13	0.14	0.06	0.11
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	13	0.13	0.01	0.12
(1,636)	1:61:A:LEU:HD22	1:66:A:ASP:HB2	12	1.72	1.42	1.1
(1,636)	1:61:A:LEU:HD21	1:66:A:ASP:HB2	12	1.72	1.42	1.1
(1,636)	1:61:A:LEU:HD23	1:66:A:ASP:HB2	12	1.72	1.42	1.1
(1,793)	1:100:A:LEU:HD13	1:118:A:TYR:HB3	12	1.13	1.08	0.3
(1,793)	1:100:A:LEU:HD11	1:118:A:TYR:HB3	12	1.13	1.08	0.3
(1,793)	1:100:A:LEU:HD12	1:118:A:TYR:HB3	12	1.13	1.08	0.3
(1,755)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	12	1.01	0.6	1.02
(1,755)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	12	1.01	0.6	1.02
(1,755)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	12	1.01	0.6	1.02
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD12	12	0.74	0.01	0.74
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD13	12	0.74	0.01	0.74
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD11	12	0.74	0.01	0.74
(2,534)	1:99:A:THR:HG22	1:95:A:LYS:HD3	12	0.62	0.39	0.5
(2,534)	1:119:A:ARG:HG2	1:99:A:THR:HG21	12	0.62	0.39	0.5
(2,534)	1:99:A:THR:HG23	1:95:A:LYS:HD3	12	0.62	0.39	0.5
(2,534)	1:99:A:THR:HG21	1:95:A:LYS:HD2	12	0.62	0.39	0.5
(2,534)	1:95:A:LYS:HB2	1:99:A:THR:HG23	12	0.62	0.39	0.5
(2,534)	1:99:A:THR:HG21	1:95:A:LYS:HD3	12	0.62	0.39	0.5
(2,534)	1:95:A:LYS:HB2	1:99:A:THR:HG21	12	0.62	0.39	0.5
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	12	0.62	0.46	0.62
(2,459)	1:86:A:THR:HB	1:107:A:VAL:HB	12	0.62	0.46	0.62
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG21	12	0.62	0.39	0.52
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG23	12	0.62	0.39	0.52
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG22	12	0.62	0.39	0.52
(2,376)	1:40:A:GLY:HA3	1:62:A:THR:HG21	12	0.62	0.39	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,376)	1:40:A:GLY:HA3	1:62:A:THR:HG22	12	0.62	0.39	0.52
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	12	0.61	0.32	0.52
(2,1637)	1:64:A:LYS:HG2	1:62:A:THR:HG1	12	0.61	0.32	0.52
(2,1637)	2:1001:A:OLA:H71	1:62:A:THR:HG1	12	0.61	0.32	0.52
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG11	12	0.6	0.2	0.62
(2,1579)	1:41:A:VAL:HG13	2:1001:A:OLA:H21	12	0.6	0.2	0.62
(2,1579)	1:41:A:VAL:HG12	2:1001:A:OLA:H21	12	0.6	0.2	0.62
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG12	12	0.6	0.2	0.62
(2,1579)	1:41:A:VAL:HG11	2:1001:A:OLA:H21	12	0.6	0.2	0.62
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG13	12	0.6	0.2	0.62
(2,7)	1:31:A:ILE:HD12	1:34:A:GLN:HB2	12	0.6	0.1	0.58
(2,7)	1:31:A:ILE:HD13	1:34:A:GLN:HB2	12	0.6	0.1	0.58
(2,7)	1:31:A:ILE:HD11	1:34:A:GLN:HB2	12	0.6	0.1	0.58
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG22	12	0.52	0.06	0.54
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG21	12	0.52	0.06	0.54
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG23	12	0.52	0.06	0.54
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD12	12	0.5	0.36	0.44
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD13	12	0.5	0.36	0.44
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD21	12	0.5	0.36	0.44
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD22	12	0.5	0.36	0.44
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD11	12	0.5	0.36	0.44
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	12	0.46	0.15	0.51
(1,1111)	1:58:A:MET:HE1	1:43:A:LYS:HE2	12	0.43	0.09	0.46
(1,1111)	1:58:A:MET:HE3	1:43:A:LYS:HE2	12	0.43	0.09	0.46
(1,1111)	1:58:A:MET:HE2	1:43:A:LYS:HE2	12	0.43	0.09	0.46
(1,13)	1:31:A:ILE:HD12	1:31:A:ILE:H	12	0.42	0.02	0.42
(1,13)	1:31:A:ILE:HD13	1:31:A:ILE:H	12	0.42	0.02	0.42
(1,13)	1:31:A:ILE:HD11	1:31:A:ILE:H	12	0.42	0.02	0.42
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	12	0.41	0.1	0.4
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG23	12	0.41	0.1	0.4
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	12	0.41	0.1	0.4
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD21	12	0.4	0.25	0.33
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD22	12	0.4	0.25	0.33
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	12	0.4	0.25	0.33
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD12	12	0.4	0.25	0.33
(2,501)	1:90:A:ILE:HD13	1:80:A:ASP:H	12	0.39	0.2	0.38
(2,501)	1:90:A:ILE:HD11	1:80:A:ASP:H	12	0.39	0.2	0.38
(2,501)	1:90:A:ILE:HD12	1:80:A:ASP:H	12	0.39	0.2	0.38
(2,263)	1:30:A:TRP:HA	1:30:A:TRP:HE3	12	0.26	0.11	0.19
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	12	0.26	0.11	0.19
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG23	12	0.26	0.11	0.22
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG21	12	0.26	0.11	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG22	12	0.26	0.11	0.22
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	12	0.2	0.04	0.21
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	12	0.2	0.06	0.19
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	12	0.19	0.1	0.14
(1,1036)	1:124:A:TYR:HE1	1:141:A:LYS:HD2	12	0.19	0.1	0.14
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	12	0.17	0.04	0.16
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG22	12	0.16	0.02	0.16
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG21	12	0.16	0.02	0.16
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG23	12	0.16	0.02	0.16
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD11	12	0.13	0.01	0.13
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	12	0.13	0.01	0.13
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD13	12	0.13	0.01	0.13
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	12	0.11	0.01	0.11
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	12	0.11	0.01	0.11
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	11	1.5	0.22	1.59
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD21	11	1.24	0.4	1.18
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD22	11	1.24	0.4	1.18
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD23	11	1.24	0.4	1.18
(2,1394)	1:143:A:GLN:H	1:141:A:LYS:HD3	11	1.09	0.49	1.37
(2,1394)	1:143:A:GLN:H	1:12:A:LYS:HG3	11	1.09	0.49	1.37
(2,414)	1:73:A:ALA:HB3	1:76:A:GLU:HG2	11	0.81	0.15	0.76
(2,414)	1:73:A:ALA:HB2	1:76:A:GLU:HG2	11	0.81	0.15	0.76
(2,414)	1:73:A:ALA:HB1	1:76:A:GLU:HG2	11	0.81	0.15	0.76
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	11	0.79	0.09	0.81
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	11	0.77	0.39	0.63
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB2	11	0.76	0.4	0.71
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB3	11	0.76	0.4	0.71
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB1	11	0.76	0.4	0.71
(2,844)	1:107:A:VAL:H	1:82:A:ALA:HB3	11	0.76	0.4	0.71
(2,844)	1:87:A:GLN:HE22	1:82:A:ALA:HB2	11	0.76	0.4	0.71
(2,544)	1:100:A:LEU:HD21	1:58:A:MET:HG3	11	0.75	0.55	0.45
(2,544)	1:100:A:LEU:HD21	1:94:A:LEU:HB2	11	0.75	0.55	0.45
(2,544)	1:100:A:LEU:HD22	1:94:A:LEU:HB2	11	0.75	0.55	0.45
(2,544)	1:8:A:LEU:HG	1:100:A:LEU:HD21	11	0.75	0.55	0.45
(2,544)	1:100:A:LEU:HD23	1:58:A:MET:HG3	11	0.75	0.55	0.45
(2,544)	1:100:A:LEU:HD23	1:94:A:LEU:HB2	11	0.75	0.55	0.45
(2,1112)	1:143:A:GLN:HE21	1:142:A:LYS:HG2	11	0.61	0.33	0.37
(2,1112)	1:143:A:GLN:HE21	1:61:A:LEU:HD11	11	0.61	0.33	0.37
(2,1112)	1:143:A:GLN:HE21	1:141:A:LYS:HG3	11	0.61	0.33	0.37
(2,1112)	1:143:A:GLN:HE21	1:61:A:LEU:HD23	11	0.61	0.33	0.37
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	11	0.59	0.24	0.52
(2,1306)	1:49:A:ALA:HB2	1:72:A:TRP:H	11	0.59	0.24	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,400)	1:83:A:LEU:HD11	1:65:A:LYS:HG2	11	0.58	0.33	0.59
(2,400)	1:65:A:LYS:HG2	1:83:A:LEU:HD21	11	0.58	0.33	0.59
(2,400)	1:83:A:LEU:HD12	1:65:A:LYS:HG2	11	0.58	0.33	0.59
(2,400)	1:83:A:LEU:HD13	1:65:A:LYS:HG2	11	0.58	0.33	0.59
(2,783)	1:127:A:MET:HE3	1:140:A:TYR:HE2	11	0.56	0.15	0.59
(2,783)	1:127:A:MET:HE1	1:140:A:TYR:HE2	11	0.56	0.15	0.59
(2,783)	1:127:A:MET:HE2	1:140:A:TYR:HE2	11	0.56	0.15	0.59
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	11	0.53	0.24	0.57
(2,446)	1:83:A:LEU:HD12	1:60:A:ASN:HD21	11	0.49	0.22	0.45
(2,446)	1:83:A:LEU:HD13	1:60:A:ASN:HD21	11	0.49	0.22	0.45
(2,446)	1:83:A:LEU:HD11	1:60:A:ASN:HD21	11	0.49	0.22	0.45
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG12	11	0.48	0.28	0.4
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG11	11	0.48	0.28	0.4
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG13	11	0.48	0.28	0.4
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	11	0.45	0.2	0.49
(2,52)	1:49:A:ALA:HB1	1:50:A:SER:HB3	11	0.45	0.2	0.49
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	11	0.43	0.17	0.51
(2,171)	1:15:A:ARG:HD3	1:16:A:ASP:H	11	0.43	0.17	0.51
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	11	0.36	0.15	0.33
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	11	0.35	0.43	0.17
(2,498)	1:90:A:ILE:HD13	1:69:A:HIS:HD2	11	0.35	0.25	0.25
(2,498)	1:90:A:ILE:HD12	1:78:A:PHE:HD2	11	0.35	0.25	0.25
(2,498)	1:90:A:ILE:HD11	1:78:A:PHE:HD2	11	0.35	0.25	0.25
(2,498)	1:90:A:ILE:HD13	1:78:A:PHE:HD2	11	0.35	0.25	0.25
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	11	0.32	0.12	0.34
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	11	0.29	0.11	0.28
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG22	11	0.29	0.12	0.25
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG21	11	0.29	0.12	0.25
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG23	11	0.29	0.12	0.25
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	11	0.24	0.06	0.25
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	11	0.23	0.07	0.25
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG11	11	0.22	0.08	0.21
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG13	11	0.22	0.08	0.21
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD2	11	0.21	0.07	0.21
(2,213)	1:23:A:LEU:HD22	1:19:A:PHE:HD2	11	0.21	0.07	0.21
(2,213)	1:23:A:LEU:HD21	1:19:A:PHE:HD2	11	0.21	0.07	0.21
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD1	11	0.21	0.07	0.21
(1,1249)	1:3:A:LEU:HD22	1:3:A:LEU:H	11	0.19	0.06	0.18
(1,1249)	1:3:A:LEU:HD21	1:3:A:LEU:H	11	0.19	0.06	0.18
(1,1249)	1:3:A:LEU:HD23	1:3:A:LEU:H	11	0.19	0.06	0.18
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD11	11	0.18	0.05	0.21
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD12	11	0.18	0.05	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD13	11	0.18	0.05	0.21
(2,1671)	1:24:A:LYS:HB3	1:24:A:LYS:HG2	11	0.15	0.02	0.16
(2,1671)	2:1001:A:OLA:H82	2:1001:A:OLA:H71	11	0.15	0.02	0.16
(2,1671)	2:1001:A:OLA:H41	2:1001:A:OLA:H21	11	0.15	0.02	0.16
(2,1671)	2:1001:A:OLA:H81	2:1001:A:OLA:H62	11	0.15	0.02	0.16
(2,1671)	2:1001:A:OLA:H82	2:1001:A:OLA:H61	11	0.15	0.02	0.16
(2,1671)	2:1001:A:OLA:H41	2:1001:A:OLA:H22	11	0.15	0.02	0.16
(2,1671)	2:1001:A:OLA:H42	2:1001:A:OLA:H22	11	0.15	0.02	0.16
(2,1671)	2:1001:A:OLA:H122	2:1001:A:OLA:H111	11	0.15	0.02	0.16
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	11	0.15	0.02	0.15
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	10	0.97	0.17	0.96
(2,125)	1:65:A:LYS:HE3	1:67:A:THR:HG22	10	0.66	0.28	0.62
(2,125)	1:65:A:LYS:HE3	1:67:A:THR:HG23	10	0.66	0.28	0.62
(2,125)	1:35:A:VAL:HG13	1:64:A:LYS:HE3	10	0.66	0.28	0.62
(2,125)	1:35:A:VAL:HG12	1:64:A:LYS:HE3	10	0.66	0.28	0.62
(2,125)	1:35:A:VAL:HG11	1:64:A:LYS:HE3	10	0.66	0.28	0.62
(2,125)	1:65:A:LYS:HE3	1:67:A:THR:HG21	10	0.66	0.28	0.62
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	10	0.58	0.47	0.34
(2,591)	1:118:A:TYR:HA	1:127:A:MET:HG2	10	0.58	0.47	0.34
(2,591)	1:118:A:TYR:HA	1:128:A:LYS:HB3	10	0.58	0.47	0.34
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	10	0.56	0.22	0.6
(2,1466)	1:98:A:ASN:H	1:95:A:LYS:HD3	10	0.56	0.22	0.6
(2,819)	1:36:A:ILE:HG22	2:1001:A:OLA:H82	10	0.54	0.22	0.51
(2,819)	1:36:A:ILE:HG23	2:1001:A:OLA:H82	10	0.54	0.22	0.51
(2,819)	1:36:A:ILE:HG21	2:1001:A:OLA:H82	10	0.54	0.22	0.51
(2,819)	2:1001:A:OLA:H81	1:36:A:ILE:HG21	10	0.54	0.22	0.51
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG13	10	0.53	0.29	0.43
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG12	10	0.53	0.29	0.43
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG11	10	0.53	0.29	0.43
(1,2489)	1:13:A:LEU:HD21	1:17:A:GLU:H	10	0.53	0.37	0.43
(1,2489)	1:13:A:LEU:HD22	1:17:A:GLU:H	10	0.53	0.37	0.43
(1,2489)	1:13:A:LEU:HD23	1:17:A:GLU:H	10	0.53	0.37	0.43
(1,2813)	1:127:A:MET:HE3	1:118:A:TYR:HH	10	0.53	0.45	0.34
(1,2813)	1:127:A:MET:HE1	1:118:A:TYR:HH	10	0.53	0.45	0.34
(1,2813)	1:127:A:MET:HE2	1:118:A:TYR:HH	10	0.53	0.45	0.34
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG12	10	0.5	0.19	0.45
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG13	10	0.5	0.19	0.45
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG11	10	0.5	0.19	0.45
(2,621)	1:139:A:TYR:HD2	1:126:A:VAL:HG12	10	0.5	0.19	0.45
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	10	0.5	0.19	0.58
(2,1117)	1:95:A:LYS:HD3	1:99:A:THR:H	10	0.5	0.19	0.58
(1,1112)	1:58:A:MET:HE3	1:43:A:LYS:HE3	10	0.5	0.17	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1112)	1:58:A:MET:HE1	1:43:A:LYS:HE3	10	0.5	0.17	0.52
(1,1112)	1:58:A:MET:HE2	1:43:A:LYS:HE3	10	0.5	0.17	0.52
(2,684)	1:13:A:LEU:HD21	1:140:A:TYR:HE2	10	0.49	0.32	0.35
(2,684)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	10	0.49	0.32	0.35
(2,684)	1:125:A:LEU:HD13	1:140:A:TYR:HE2	10	0.49	0.32	0.35
(2,684)	1:125:A:LEU:HD11	1:140:A:TYR:HE2	10	0.49	0.32	0.35
(2,684)	1:13:A:LEU:HD21	1:140:A:TYR:HE1	10	0.49	0.32	0.35
(2,684)	1:125:A:LEU:HD12	1:140:A:TYR:HE2	10	0.49	0.32	0.35
(2,65)	1:1:A:LYS:HG2	1:1:A:LYS:HE3	10	0.49	0.28	0.47
(2,65)	1:12:A:LYS:HE2	1:12:A:LYS:HG3	10	0.49	0.28	0.47
(2,65)	1:12:A:LYS:HE3	1:12:A:LYS:HG3	10	0.49	0.28	0.47
(2,350)	1:52:A:LYS:H	1:52:A:LYS:HD2	10	0.46	0.16	0.42
(2,350)	1:33:A:ARG:HG2	1:34:A:GLN:H	10	0.46	0.16	0.42
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB1	10	0.44	0.2	0.4
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB2	10	0.44	0.2	0.4
(2,1267)	1:80:A:ASP:H	1:107:A:VAL:HG13	10	0.44	0.2	0.4
(2,1267)	1:80:A:ASP:H	1:107:A:VAL:HG11	10	0.44	0.2	0.4
(2,1267)	1:80:A:ASP:H	1:107:A:VAL:HG12	10	0.44	0.2	0.4
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB3	10	0.44	0.2	0.4
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	10	0.43	0.17	0.4
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD2	10	0.43	0.17	0.4
(2,843)	1:17:A:GLU:HG3	1:139:A:TYR:HD1	10	0.43	0.17	0.4
(2,1540)	1:119:A:ARG:HG2	1:100:A:LEU:H	10	0.42	0.14	0.39
(2,1540)	1:94:A:LEU:HG	1:100:A:LEU:H	10	0.42	0.14	0.39
(2,1614)	1:58:A:MET:HE3	1:60:A:ASN:H	10	0.42	0.15	0.44
(2,1614)	1:58:A:MET:HE1	1:60:A:ASN:H	10	0.42	0.15	0.44
(2,1614)	1:64:A:LYS:H	2:1001:A:OLA:H81	10	0.42	0.15	0.44
(2,1614)	1:106:A:LYS:HB2	1:111:A:THR:H	10	0.42	0.15	0.44
(2,1614)	1:58:A:MET:HE2	1:60:A:ASN:H	10	0.42	0.15	0.44
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD12	10	0.41	0.23	0.33
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD13	10	0.41	0.23	0.33
(2,205)	1:23:A:LEU:HD11	1:37:A:LYS:HE3	10	0.41	0.23	0.33
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD11	10	0.41	0.23	0.33
(2,205)	1:23:A:LEU:HD12	1:37:A:LYS:HE3	10	0.41	0.23	0.33
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD11	10	0.4	0.23	0.36
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD12	10	0.4	0.23	0.36
(2,1175)	1:83:A:LEU:HD23	1:64:A:LYS:H	10	0.4	0.23	0.36
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD13	10	0.4	0.23	0.36
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	10	0.4	0.09	0.38
(2,692)	1:142:A:LYS:H	1:141:A:LYS:HD2	10	0.4	0.09	0.38
(2,412)	1:73:A:ALA:HB3	1:55:A:ARG:H	10	0.38	0.15	0.4
(2,412)	1:73:A:ALA:HB1	1:55:A:ARG:H	10	0.38	0.15	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,412)	1:73:A:ALA:HB2	1:55:A:ARG:H	10	0.38	0.15	0.4
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	10	0.37	0.35	0.27
(2,789)	1:26:A:ARG:HD3	1:131:A:TRP:HZ3	10	0.37	0.21	0.28
(2,789)	1:26:A:ARG:HD2	1:131:A:TRP:HZ3	10	0.37	0.21	0.28
(2,789)	1:114:A:GLU:HB3	1:131:A:TRP:HZ3	10	0.37	0.21	0.28
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	10	0.32	0.12	0.36
(1,137)	1:3:A:LEU:HD21	1:7:A:PHE:HB3	10	0.32	0.15	0.32
(1,137)	1:3:A:LEU:HD22	1:7:A:PHE:HB3	10	0.32	0.15	0.32
(1,137)	1:3:A:LEU:HD23	1:7:A:PHE:HB3	10	0.32	0.15	0.32
(2,1487)	1:67:A:THR:HG22	1:65:A:LYS:H	10	0.32	0.17	0.3
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG13	10	0.32	0.17	0.3
(2,1487)	1:67:A:THR:HG23	1:65:A:LYS:H	10	0.32	0.17	0.3
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG11	10	0.32	0.17	0.3
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG12	10	0.32	0.17	0.3
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	10	0.31	0.23	0.25
(2,778)	1:119:A:ARG:HD3	1:99:A:THR:HA	10	0.31	0.23	0.25
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	10	0.28	0.23	0.23
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG13	10	0.28	0.15	0.26
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG12	10	0.28	0.15	0.26
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG11	10	0.28	0.15	0.26
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	10	0.26	0.01	0.26
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG21	10	0.26	0.07	0.28
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG23	10	0.26	0.07	0.28
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG22	10	0.26	0.07	0.28
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	10	0.25	0.09	0.24
(2,688)	1:141:A:LYS:HD3	1:143:A:GLN:HA	10	0.25	0.09	0.24
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD12	10	0.24	0.09	0.22
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD11	10	0.24	0.09	0.22
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD13	10	0.24	0.09	0.22
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	10	0.23	0.0	0.23
(2,1471)	1:101:A:THR:HG22	1:93:A:ASP:H	10	0.23	0.1	0.2
(2,1471)	1:101:A:THR:HG23	1:93:A:ASP:H	10	0.23	0.1	0.2
(2,1471)	1:101:A:THR:HG21	1:93:A:ASP:H	10	0.23	0.1	0.2
(2,1471)	1:102:A:GLU:HG3	1:93:A:ASP:H	10	0.23	0.1	0.2
(1,616)	1:73:A:ALA:HB3	1:76:A:GLU:H	10	0.22	0.06	0.24
(1,616)	1:73:A:ALA:HB2	1:76:A:GLU:H	10	0.22	0.06	0.24
(1,616)	1:73:A:ALA:HB1	1:76:A:GLU:H	10	0.22	0.06	0.24
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	10	0.21	0.01	0.22
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	10	0.17	0.04	0.19
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	10	0.17	0.04	0.17
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD11	10	0.17	0.04	0.17
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD13	10	0.17	0.04	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	10	0.16	0.05	0.16
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD11	10	0.16	0.05	0.16
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD12	10	0.16	0.05	0.16
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	10	0.15	0.04	0.14
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG11	10	0.11	0.01	0.11
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG13	10	0.11	0.01	0.11
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	10	0.11	0.01	0.11
(2,274)	1:61:A:LEU:HD22	1:66:A:ASP:HB3	9	1.89	1.21	1.68
(2,274)	1:61:A:LEU:HD21	1:66:A:ASP:HB3	9	1.89	1.21	1.68
(2,274)	1:61:A:LEU:HD23	1:66:A:ASP:HB3	9	1.89	1.21	1.68
(2,274)	1:83:A:LEU:HD23	1:66:A:ASP:HB3	9	1.89	1.21	1.68
(2,274)	1:83:A:LEU:HD21	1:66:A:ASP:HB3	9	1.89	1.21	1.68
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	9	1.17	0.42	1.19
(2,419)	1:74:A:LEU:HD11	1:56:A:TYR:HD1	9	1.11	0.6	0.74
(2,419)	1:74:A:LEU:HD13	1:56:A:TYR:HD1	9	1.11	0.6	0.74
(2,419)	1:74:A:LEU:HD11	1:7:A:PHE:HD2	9	1.11	0.6	0.74
(2,1594)	2:1001:A:OLA:H32	1:13:A:LEU:HD13	9	1.09	0.33	1.13
(2,1594)	2:1001:A:OLA:H31	1:41:A:VAL:HG12	9	1.09	0.33	1.13
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG13	9	1.09	0.33	1.13
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG12	9	1.09	0.33	1.13
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG11	9	1.09	0.33	1.13
(2,1594)	2:1001:A:OLA:H32	2:1001:A:OLA:H131	9	1.09	0.33	1.13
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HG23	9	0.9	0.48	0.82
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HG22	9	0.9	0.48	0.82
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HG21	9	0.9	0.48	0.82
(2,393)	1:35:A:VAL:HG23	1:64:A:LYS:HE3	9	0.9	0.48	0.82
(2,393)	1:89:A:LYS:HE2	1:105:A:ILE:HG21	9	0.9	0.48	0.82
(2,393)	1:105:A:ILE:HD12	1:89:A:LYS:HE2	9	0.9	0.48	0.82
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HD11	9	0.9	0.48	0.82
(1,187)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	9	0.84	0.46	1.06
(1,187)	1:8:A:LEU:HD12	1:47:A:ASN:HD22	9	0.84	0.46	1.06
(1,187)	1:8:A:LEU:HD13	1:47:A:ASN:HD22	9	0.84	0.46	1.06
(1,2326)	1:74:A:LEU:HD13	1:2:A:THR:H	9	0.82	0.82	0.31
(1,2326)	1:74:A:LEU:HD11	1:2:A:THR:H	9	0.82	0.82	0.31
(1,2326)	1:74:A:LEU:HD12	1:2:A:THR:H	9	0.82	0.82	0.31
(2,409)	1:70:A:LYS:HB3	1:71:A:ASP:HB2	9	0.8	0.22	0.81
(2,409)	1:52:A:LYS:HD3	1:71:A:ASP:HB2	9	0.8	0.22	0.81
(2,409)	1:52:A:LYS:HB3	1:71:A:ASP:HB2	9	0.8	0.22	0.81
(2,571)	1:106:A:LYS:HB3	1:109:A:ASP:HB2	9	0.65	0.27	0.64
(2,571)	1:140:A:TYR:HB2	1:127:A:MET:HB2	9	0.65	0.27	0.64
(1,792)	1:100:A:LEU:HD11	1:118:A:TYR:HD2	9	0.64	0.21	0.71
(1,792)	1:100:A:LEU:HD12	1:118:A:TYR:HD2	9	0.64	0.21	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,792)	1:100:A:LEU:HD13	1:118:A:TYR:HD2	9	0.64	0.21	0.71
(2,26)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	9	0.57	0.32	0.53
(2,26)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	9	0.57	0.32	0.53
(2,26)	1:4:A:PRO:HG3	1:94:A:LEU:HD23	9	0.57	0.32	0.53
(2,26)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	9	0.57	0.32	0.53
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	9	0.55	0.11	0.57
(2,635)	1:130:A:SER:HB3	1:128:A:LYS:HD2	9	0.51	0.21	0.46
(2,635)	1:128:A:LYS:HD3	1:130:A:SER:HB3	9	0.51	0.21	0.46
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	9	0.48	0.21	0.57
(2,1583)	1:41:A:VAL:HG23	2:1001:A:OLA:H22	9	0.44	0.24	0.46
(2,1583)	2:1001:A:OLA:H161	2:1001:A:OLA:H22	9	0.44	0.24	0.46
(2,1583)	2:1001:A:OLA:H161	2:1001:A:OLA:H21	9	0.44	0.24	0.46
(2,1583)	1:41:A:VAL:HG21	2:1001:A:OLA:H21	9	0.44	0.24	0.46
(2,1583)	2:1001:A:OLA:H22	1:127:A:MET:HG3	9	0.44	0.24	0.46
(2,1583)	1:41:A:VAL:HG23	2:1001:A:OLA:H21	9	0.44	0.24	0.46
(2,811)	1:89:A:LYS:H	1:89:A:LYS:HE2	9	0.42	0.12	0.47
(2,811)	1:89:A:LYS:HE3	1:89:A:LYS:H	9	0.42	0.12	0.47
(1,1104)	1:58:A:MET:HE1	1:118:A:TYR:HE1	9	0.41	0.14	0.46
(1,1104)	1:58:A:MET:HE2	1:118:A:TYR:HE1	9	0.41	0.14	0.46
(1,1104)	1:58:A:MET:HE3	1:118:A:TYR:HE2	9	0.41	0.14	0.46
(1,1104)	1:58:A:MET:HE3	1:118:A:TYR:HE1	9	0.41	0.14	0.46
(2,301)	1:37:A:LYS:H	1:37:A:LYS:HE3	9	0.37	0.29	0.28
(2,301)	1:24:A:LYS:H	1:24:A:LYS:HE2	9	0.37	0.29	0.28
(2,301)	1:24:A:LYS:H	1:24:A:LYS:HE3	9	0.37	0.29	0.28
(2,301)	1:95:A:LYS:H	1:95:A:LYS:HE2	9	0.37	0.29	0.28
(2,158)	1:15:A:ARG:HA	1:13:A:LEU:HB3	9	0.35	0.14	0.3
(2,158)	1:41:A:VAL:HA	1:13:A:LEU:HB3	9	0.35	0.14	0.3
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	9	0.34	0.2	0.28
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE2	9	0.34	0.2	0.28
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	9	0.32	0.17	0.29
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE1	9	0.32	0.17	0.29
(2,433)	1:85:A:SER:H	1:81:A:GLU:HG2	9	0.31	0.14	0.31
(2,433)	1:81:A:GLU:HG2	1:81:A:GLU:H	9	0.31	0.14	0.31
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	9	0.28	0.14	0.33
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB3	9	0.26	0.09	0.33
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB2	9	0.26	0.09	0.33
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB1	9	0.26	0.09	0.33
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	9	0.26	0.01	0.27
(2,482)	1:90:A:ILE:HG21	1:78:A:PHE:HD1	9	0.26	0.1	0.25
(2,482)	1:90:A:ILE:HG22	1:78:A:PHE:HD1	9	0.26	0.1	0.25
(2,482)	1:90:A:ILE:HG23	1:78:A:PHE:HD1	9	0.26	0.1	0.25
(2,482)	1:69:A:HIS:HD2	1:90:A:ILE:HG21	9	0.26	0.1	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,482)	1:69:A:HIS:HD2	1:90:A:ILE:HG23	9	0.26	0.1	0.25
(2,1168)	1:128:A:LYS:HE3	1:135:A:SER:H	9	0.26	0.11	0.22
(2,1168)	1:56:A:TYR:H	1:55:A:ARG:HD2	9	0.26	0.11	0.22
(2,1168)	1:128:A:LYS:HE2	1:135:A:SER:H	9	0.26	0.11	0.22
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	9	0.25	0.19	0.16
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD13	9	0.2	0.07	0.2
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD21	9	0.2	0.07	0.2
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD23	9	0.2	0.07	0.2
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD22	9	0.2	0.07	0.2
(2,1018)	1:68:A:HIS:H	1:61:A:LEU:HD22	9	0.2	0.07	0.2
(2,1018)	1:68:A:HIS:H	1:61:A:LEU:HD21	9	0.2	0.07	0.2
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB3	9	0.19	0.04	0.21
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB2	9	0.19	0.04	0.21
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	9	0.15	0.04	0.14
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	9	0.12	0.03	0.12
(2,66)	1:12:A:LYS:HG3	1:141:A:LYS:HG3	8	1.28	0.83	1.28
(2,66)	1:1:A:LYS:HG2	1:74:A:LEU:HD21	8	1.28	0.83	1.28
(2,66)	1:1:A:LYS:HG2	1:74:A:LEU:HD22	8	1.28	0.83	1.28
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG23	8	0.98	0.51	0.89
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG22	8	0.98	0.51	0.89
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG21	8	0.98	0.51	0.89
(2,618)	1:125:A:LEU:HD22	1:100:A:LEU:H	8	0.94	0.85	0.45
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD23	8	0.94	0.85	0.45
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD21	8	0.94	0.85	0.45
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD22	8	0.94	0.85	0.45
(2,162)	1:16:A:ASP:HA	1:13:A:LEU:HD21	8	0.76	0.6	0.44
(2,162)	1:13:A:LEU:HD22	1:140:A:TYR:HA	8	0.76	0.6	0.44
(2,162)	1:13:A:LEU:HD23	1:140:A:TYR:HA	8	0.76	0.6	0.44
(2,162)	1:13:A:LEU:HD21	1:140:A:TYR:HA	8	0.76	0.6	0.44
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD22	8	0.65	0.28	0.78
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD23	8	0.65	0.28	0.78
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD21	8	0.65	0.28	0.78
(2,1488)	1:81:A:GLU:H	1:78:A:PHE:HE2	8	0.64	0.24	0.72
(2,1488)	1:81:A:GLU:H	1:87:A:GLN:HE21	8	0.64	0.24	0.72
(2,1596)	1:83:A:LEU:HD21	2:1001:A:OLA:H32	8	0.62	0.28	0.66
(2,1596)	1:83:A:LEU:HD23	2:1001:A:OLA:H32	8	0.62	0.28	0.66
(2,1596)	2:1001:A:OLA:H31	2:1001:A:OLA:H181	8	0.62	0.28	0.66
(2,1596)	2:1001:A:OLA:H31	2:1001:A:OLA:H182	8	0.62	0.28	0.66
(2,1596)	2:1001:A:OLA:H32	1:83:A:LEU:HD12	8	0.62	0.28	0.66
(2,413)	1:73:A:ALA:HB2	1:54:A:ASP:HB3	8	0.58	0.34	0.56
(2,413)	1:73:A:ALA:HB3	1:55:A:ARG:HD2	8	0.58	0.34	0.56
(2,413)	1:73:A:ALA:HB3	1:54:A:ASP:HB3	8	0.58	0.34	0.56

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,413)	1:73:A:ALA:HB2	1:55:A:ARG:HD2	8	0.58	0.34	0.56
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB3	8	0.56	0.12	0.55
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB1	8	0.56	0.12	0.55
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB2	8	0.56	0.12	0.55
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD23	8	0.53	0.16	0.58
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD22	8	0.53	0.16	0.58
(2,697)	1:65:A:LYS:HE2	1:83:A:LEU:HA	8	0.5	0.36	0.4
(2,697)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	8	0.5	0.36	0.4
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	8	0.49	0.17	0.52
(1,785)	1:100:A:LEU:HD22	1:45:A:PHE:HE2	8	0.46	0.19	0.44
(1,785)	1:100:A:LEU:HD23	1:45:A:PHE:HE2	8	0.46	0.19	0.44
(1,785)	1:100:A:LEU:HD21	1:45:A:PHE:HE2	8	0.46	0.19	0.44
(2,1360)	1:52:A:LYS:HG2	1:52:A:LYS:H	8	0.46	0.13	0.5
(2,1360)	1:52:A:LYS:H	1:52:A:LYS:HG3	8	0.46	0.13	0.5
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	8	0.45	0.17	0.48
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	8	0.45	0.28	0.35
(2,1098)	1:132:A:LYS:HD3	1:131:A:TRP:HE1	8	0.42	0.25	0.36
(2,1098)	1:132:A:LYS:HB3	1:131:A:TRP:HE1	8	0.42	0.25	0.36
(2,1098)	1:132:A:LYS:HD2	1:131:A:TRP:HE1	8	0.42	0.25	0.36
(2,349)	1:52:A:LYS:HG2	1:52:A:LYS:H	8	0.41	0.13	0.46
(2,349)	1:52:A:LYS:H	1:52:A:LYS:HG3	8	0.41	0.13	0.46
(1,1223)	1:127:A:MET:HE3	1:116:A:TYR:HD2	8	0.37	0.11	0.38
(1,1223)	1:127:A:MET:HE3	1:116:A:TYR:HD1	8	0.37	0.11	0.38
(1,1223)	1:127:A:MET:HE2	1:116:A:TYR:HD1	8	0.37	0.11	0.38
(1,1223)	1:127:A:MET:HE1	1:116:A:TYR:HD2	8	0.37	0.11	0.38
(2,120)	1:8:A:LEU:HD11	1:7:A:PHE:H	8	0.37	0.16	0.42
(2,120)	1:8:A:LEU:HD12	1:7:A:PHE:H	8	0.37	0.16	0.42
(2,120)	1:8:A:LEU:HD13	1:47:A:ASN:HD21	8	0.37	0.16	0.42
(2,120)	1:8:A:LEU:HD11	1:47:A:ASN:HD21	8	0.37	0.16	0.42
(2,120)	1:8:A:LEU:HD13	1:7:A:PHE:H	8	0.37	0.16	0.42
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD12	8	0.35	0.2	0.36
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD13	8	0.35	0.2	0.36
(2,421)	1:2:A:THR:HA	1:74:A:LEU:HD13	8	0.35	0.2	0.36
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD11	8	0.35	0.2	0.36
(2,421)	1:2:A:THR:HA	1:74:A:LEU:HD12	8	0.35	0.2	0.36
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	8	0.34	0.07	0.32
(2,1660)	2:1001:A:OLA:H81	1:36:A:ILE:HA	8	0.34	0.07	0.32
(2,541)	1:100:A:LEU:HD22	1:118:A:TYR:HB2	8	0.34	0.11	0.36
(2,541)	1:100:A:LEU:HD23	1:118:A:TYR:HB2	8	0.34	0.11	0.36
(2,541)	1:100:A:LEU:HD21	1:118:A:TYR:HB2	8	0.34	0.11	0.36
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	8	0.33	0.1	0.35
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	8	0.32	0.01	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1222)	1:127:A:MET:HE1	1:118:A:TYR:HD1	8	0.31	0.11	0.28
(1,1222)	1:127:A:MET:HE2	1:118:A:TYR:HD1	8	0.31	0.11	0.28
(1,1222)	1:127:A:MET:HE3	1:118:A:TYR:HD1	8	0.31	0.11	0.28
(1,2809)	2:1001:A:OLA:H183	1:36:A:ILE:HD12	8	0.28	0.15	0.2
(1,2809)	2:1001:A:OLA:H183	1:36:A:ILE:HD13	8	0.28	0.15	0.2
(1,2809)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	8	0.28	0.15	0.2
(1,2809)	2:1001:A:OLA:H181	1:36:A:ILE:HD12	8	0.28	0.15	0.2
(1,2809)	2:1001:A:OLA:H182	1:36:A:ILE:HD13	8	0.28	0.15	0.2
(1,2836)	2:1001:A:OLA:H183	1:36:A:ILE:HD12	8	0.28	0.15	0.2
(1,2836)	2:1001:A:OLA:H183	1:36:A:ILE:HD13	8	0.28	0.15	0.2
(1,2836)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	8	0.28	0.15	0.2
(1,2836)	2:1001:A:OLA:H181	1:36:A:ILE:HD12	8	0.28	0.15	0.2
(1,2836)	2:1001:A:OLA:H182	1:36:A:ILE:HD13	8	0.28	0.15	0.2
(1,752)	1:94:A:LEU:HD11	1:7:A:PHE:HD2	8	0.26	0.05	0.26
(1,752)	1:94:A:LEU:HD13	1:7:A:PHE:HD2	8	0.26	0.05	0.26
(1,752)	1:94:A:LEU:HD12	1:7:A:PHE:HD2	8	0.26	0.05	0.26
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	8	0.26	0.15	0.22
(2,632)	1:128:A:LYS:HB3	1:128:A:LYS:HE2	8	0.25	0.05	0.24
(2,632)	1:128:A:LYS:HE3	1:128:A:LYS:HB3	8	0.25	0.05	0.24
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	8	0.25	0.03	0.24
(1,1981)	1:8:A:LEU:HD22	1:47:A:ASN:H	8	0.25	0.03	0.24
(2,1325)	1:130:A:SER:H	1:128:A:LYS:HG2	8	0.24	0.1	0.28
(2,1325)	1:129:A:MET:HE1	1:130:A:SER:H	8	0.24	0.1	0.28
(2,1325)	1:129:A:MET:HE2	1:130:A:SER:H	8	0.24	0.1	0.28
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG23	8	0.24	0.07	0.22
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG22	8	0.24	0.07	0.22
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG21	8	0.24	0.07	0.22
(2,1553)	1:136:A:THR:H	1:129:A:MET:HE1	8	0.22	0.08	0.2
(2,1553)	1:136:A:THR:H	1:129:A:MET:HE2	8	0.22	0.08	0.2
(2,1553)	1:136:A:THR:H	1:128:A:LYS:HG2	8	0.22	0.08	0.2
(2,1332)	1:75:A:GLY:H	1:74:A:LEU:HD23	8	0.22	0.07	0.2
(2,1332)	1:75:A:GLY:H	1:74:A:LEU:HD22	8	0.22	0.07	0.2
(2,1332)	1:75:A:GLY:H	1:91:A:THR:HG22	8	0.22	0.07	0.2
(2,1332)	1:75:A:GLY:H	1:91:A:THR:HG23	8	0.22	0.07	0.2
(2,1332)	1:75:A:GLY:H	1:74:A:LEU:HD21	8	0.22	0.07	0.2
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	8	0.21	0.04	0.22
(2,880)	1:128:A:LYS:HE2	1:128:A:LYS:HB2	8	0.2	0.07	0.17
(2,880)	1:128:A:LYS:HE3	1:128:A:LYS:HB2	8	0.2	0.07	0.17
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	7	1.26	0.12	1.28
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	7	1.2	0.23	1.16
(1,1240)	1:125:A:LEU:HD21	1:120:A:ARG:HD2	7	0.84	0.71	0.47
(1,1240)	1:125:A:LEU:HD22	1:120:A:ARG:HD2	7	0.84	0.71	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1240)	1:125:A:LEU:HD23	1:120:A:ARG:HD2	7	0.84	0.71	0.47
(1,1982)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	7	0.82	0.38	0.89
(1,1982)	1:8:A:LEU:HD12	1:47:A:ASN:HD22	7	0.82	0.38	0.89
(1,1982)	1:8:A:LEU:HD13	1:47:A:ASN:HD22	7	0.82	0.38	0.89
(2,331)	1:44:A:LYS:HE3	1:44:A:LYS:HA	7	0.49	0.2	0.44
(2,331)	1:44:A:LYS:HA	1:11:A:PHE:HB2	7	0.49	0.2	0.44
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD12	7	0.47	0.15	0.39
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD11	7	0.47	0.15	0.39
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD13	7	0.47	0.15	0.39
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	7	0.46	0.32	0.33
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD11	7	0.46	0.29	0.42
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD22	7	0.46	0.29	0.42
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD12	7	0.46	0.29	0.42
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD23	7	0.46	0.29	0.42
(1,628)	1:74:A:LEU:HD11	1:74:A:LEU:H	7	0.42	0.14	0.45
(1,628)	1:74:A:LEU:HD13	1:74:A:LEU:H	7	0.42	0.14	0.45
(2,154)	1:13:A:LEU:H	1:12:A:LYS:HE3	7	0.42	0.21	0.34
(2,154)	1:12:A:LYS:HE2	1:13:A:LEU:H	7	0.42	0.21	0.34
(2,374)	2:1001:A:OLA:H81	1:62:A:THR:HG23	7	0.41	0.18	0.41
(2,374)	1:62:A:THR:HG22	1:83:A:LEU:HG	7	0.41	0.18	0.41
(2,374)	1:62:A:THR:HG22	2:1001:A:OLA:H82	7	0.41	0.18	0.41
(2,374)	2:1001:A:OLA:H81	1:62:A:THR:HG22	7	0.41	0.18	0.41
(2,1232)	1:65:A:LYS:HB3	1:85:A:SER:H	7	0.4	0.21	0.36
(2,1232)	1:85:A:SER:H	1:81:A:GLU:HB2	7	0.4	0.21	0.36
(2,1232)	1:85:A:SER:H	1:81:A:GLU:HB3	7	0.4	0.21	0.36
(2,1232)	1:85:A:SER:H	1:81:A:GLU:HG2	7	0.4	0.21	0.36
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG21	7	0.4	0.18	0.33
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG22	7	0.4	0.18	0.33
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG23	7	0.4	0.18	0.33
(2,1461)	1:136:A:THR:H	1:128:A:LYS:HB3	7	0.4	0.17	0.44
(2,1461)	1:136:A:THR:H	1:127:A:MET:HG2	7	0.4	0.17	0.44
(2,378)	1:83:A:LEU:HD12	1:62:A:THR:HG21	7	0.36	0.24	0.18
(2,378)	1:62:A:THR:HG23	1:83:A:LEU:HD21	7	0.36	0.24	0.18
(2,378)	1:83:A:LEU:HD12	1:62:A:THR:HG22	7	0.36	0.24	0.18
(2,378)	1:83:A:LEU:HD11	1:62:A:THR:HG21	7	0.36	0.24	0.18
(2,378)	1:62:A:THR:HG21	1:83:A:LEU:HD23	7	0.36	0.24	0.18
(2,378)	1:83:A:LEU:HD13	1:62:A:THR:HG22	7	0.36	0.24	0.18
(2,1544)	1:134:A:VAL:HG13	1:21:A:GLU:H	7	0.32	0.22	0.23
(2,1544)	1:134:A:VAL:HG11	1:21:A:GLU:H	7	0.32	0.22	0.23
(2,1544)	1:134:A:VAL:HG12	1:21:A:GLU:H	7	0.32	0.22	0.23
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HG2	7	0.32	0.22	0.2
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HB2	7	0.32	0.22	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HB3	7	0.32	0.22	0.2
(2,456)	1:85:A:SER:HA	1:65:A:LYS:HB3	7	0.32	0.22	0.2
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	7	0.29	0.19	0.19
(1,729)	1:90:A:ILE:HD11	1:78:A:PHE:HZ	7	0.29	0.05	0.28
(1,729)	1:90:A:ILE:HD12	1:78:A:PHE:HZ	7	0.29	0.05	0.28
(1,729)	1:90:A:ILE:HD13	1:78:A:PHE:HZ	7	0.29	0.05	0.28
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB2	7	0.28	0.11	0.24
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB1	7	0.28	0.11	0.24
(2,596)	1:100:A:LEU:HG	1:118:A:TYR:HD2	7	0.26	0.07	0.27
(2,596)	1:118:A:TYR:HD1	1:125:A:LEU:HG	7	0.26	0.07	0.27
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG11	7	0.24	0.09	0.22
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG13	7	0.24	0.09	0.22
(1,1456)	1:103:A:THR:HG21	1:104:A:HIS:H	7	0.22	0.09	0.23
(1,1456)	1:103:A:THR:HG22	1:104:A:HIS:H	7	0.22	0.09	0.23
(2,1619)	2:1001:A:OLA:H142	1:84:A:ASP:HB3	7	0.21	0.06	0.21
(2,1619)	2:1001:A:OLA:H141	1:84:A:ASP:HB3	7	0.21	0.06	0.21
(2,1619)	1:84:A:ASP:HB3	2:1001:A:OLA:H131	7	0.21	0.06	0.21
(1,310)	1:25:A:ALA:HB3	1:134:A:VAL:HB	7	0.21	0.06	0.22
(1,310)	1:25:A:ALA:HB1	1:134:A:VAL:HB	7	0.21	0.06	0.22
(1,2839)	2:1001:A:OLA:H182	1:19:A:PHE:HE1	7	0.2	0.05	0.2
(1,2839)	2:1001:A:OLA:H182	1:19:A:PHE:HE2	7	0.2	0.05	0.2
(1,2839)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	7	0.2	0.05	0.2
(1,2839)	2:1001:A:OLA:H183	1:19:A:PHE:HE1	7	0.2	0.05	0.2
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	7	0.19	0.04	0.2
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD13	7	0.17	0.04	0.18
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD12	7	0.17	0.04	0.18
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD11	7	0.17	0.04	0.18
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	7	0.12	0.01	0.13
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	7	0.12	0.02	0.12
(2,262)	1:30:A:TRP:HA	1:33:A:ARG:HG3	6	0.98	0.37	1.14
(2,262)	1:30:A:TRP:HA	1:34:A:GLN:HB2	6	0.98	0.37	1.14
(2,1330)	1:79:A:GLN:H	1:89:A:LYS:HB3	6	0.95	0.22	0.99
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD22	6	0.88	0.75	0.42
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD21	6	0.88	0.75	0.42
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD23	6	0.88	0.75	0.42
(1,114)	1:50:A:SER:HB3	1:52:A:LYS:HB2	6	0.88	0.3	0.91
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD11	6	0.86	0.36	0.74
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD23	6	0.86	0.36	0.74
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD13	6	0.86	0.36	0.74
(2,826)	1:59:A:GLU:HB3	1:61:A:LEU:HD13	6	0.86	0.36	0.74
(2,85)	1:125:A:LEU:HD13	1:118:A:TYR:HE1	6	0.73	0.75	0.27
(2,85)	1:125:A:LEU:HD12	1:118:A:TYR:HE1	6	0.73	0.75	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,85)	1:11:A:PHE:HD2	1:125:A:LEU:HD11	6	0.73	0.75	0.27
(2,85)	1:125:A:LEU:HD11	1:118:A:TYR:HE1	6	0.73	0.75	0.27
(2,85)	1:125:A:LEU:HD13	1:140:A:TYR:HD2	6	0.73	0.75	0.27
(2,85)	1:125:A:LEU:HD11	1:140:A:TYR:HD2	6	0.73	0.75	0.27
(2,320)	1:67:A:THR:HG21	1:60:A:ASN:HD21	6	0.71	0.11	0.72
(2,320)	1:67:A:THR:HG22	1:60:A:ASN:HD21	6	0.71	0.11	0.72
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD13	6	0.7	0.66	0.44
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD12	6	0.7	0.66	0.44
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD11	6	0.7	0.66	0.44
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD13	6	0.69	0.66	0.43
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD12	6	0.69	0.66	0.43
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD11	6	0.69	0.66	0.43
(2,555)	1:89:A:LYS:HE3	1:105:A:ILE:HG21	6	0.6	0.23	0.66
(2,555)	1:89:A:LYS:HE3	1:105:A:ILE:HG23	6	0.6	0.23	0.66
(2,555)	1:88:A:HIS:HB2	1:105:A:ILE:HG21	6	0.6	0.23	0.66
(2,555)	1:89:A:LYS:HE2	1:105:A:ILE:HG22	6	0.6	0.23	0.66
(2,555)	1:89:A:LYS:HE2	1:105:A:ILE:HG21	6	0.6	0.23	0.66
(2,61)	1:73:A:ALA:HB2	1:0:A:SER:HB3	6	0.58	0.33	0.5
(2,61)	1:73:A:ALA:HB3	1:0:A:SER:HB3	6	0.58	0.33	0.5
(2,61)	1:0:A:SER:HB3	1:1:A:LYS:HG2	6	0.58	0.33	0.5
(2,61)	1:73:A:ALA:HB1	1:0:A:SER:HB3	6	0.58	0.33	0.5
(1,2826)	1:127:A:MET:HE3	1:118:A:TYR:HH	6	0.54	0.48	0.34
(1,2826)	1:127:A:MET:HE1	1:118:A:TYR:HH	6	0.54	0.48	0.34
(1,111)	1:48:A:ALA:HB1	1:71:A:ASP:HB2	6	0.54	0.14	0.56
(1,111)	1:48:A:ALA:HB2	1:71:A:ASP:HB2	6	0.54	0.14	0.56
(1,111)	1:48:A:ALA:HB3	1:71:A:ASP:HB2	6	0.54	0.14	0.56
(2,527)	1:96:A:ASP:H	1:95:A:LYS:HD3	6	0.52	0.24	0.53
(2,527)	1:95:A:LYS:H	1:95:A:LYS:HD2	6	0.52	0.24	0.53
(2,527)	1:95:A:LYS:H	1:95:A:LYS:HD3	6	0.52	0.24	0.53
(2,779)	1:120:A:ARG:HA	1:119:A:ARG:HD2	6	0.49	0.2	0.48
(2,779)	1:119:A:ARG:HA	1:119:A:ARG:HD2	6	0.49	0.2	0.48
(2,1511)	1:61:A:LEU:HB2	1:67:A:THR:H	6	0.46	0.11	0.44
(1,1762)	1:8:A:LEU:HD13	1:47:A:ASN:HD21	6	0.46	0.21	0.49
(1,1762)	1:8:A:LEU:HD11	1:47:A:ASN:HD21	6	0.46	0.21	0.49
(1,1762)	1:8:A:LEU:HD12	1:47:A:ASN:HD21	6	0.46	0.21	0.49
(2,535)	1:117:A:GLU:HB2	1:99:A:THR:HG21	6	0.43	0.33	0.32
(2,535)	1:99:A:THR:HG22	1:95:A:LYS:HB3	6	0.43	0.33	0.32
(2,535)	1:99:A:THR:HG23	1:95:A:LYS:HB3	6	0.43	0.33	0.32
(2,535)	1:99:A:THR:HG21	1:95:A:LYS:HB3	6	0.43	0.33	0.32
(2,183)	1:24:A:LYS:HE2	1:21:A:GLU:HA	6	0.43	0.25	0.35
(2,183)	1:21:A:GLU:HA	1:24:A:LYS:HE3	6	0.43	0.25	0.35
(2,1019)	1:33:A:ARG:H	1:33:A:ARG:HG3	6	0.41	0.05	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,653)	1:132:A:LYS:HG3	1:132:A:LYS:HE3	6	0.4	0.02	0.41
(2,653)	1:132:A:LYS:HG2	1:132:A:LYS:HE3	6	0.4	0.02	0.41
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD13	6	0.4	0.2	0.4
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD12	6	0.4	0.2	0.4
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD11	6	0.4	0.2	0.4
(2,1279)	1:80:A:ASP:H	1:89:A:LYS:HB3	6	0.39	0.07	0.4
(1,2841)	1:36:A:ILE:HD12	2:1001:A:OLA:H10	6	0.38	0.12	0.4
(1,2841)	1:36:A:ILE:HD11	2:1001:A:OLA:H10	6	0.38	0.12	0.4
(2,447)	1:84:A:ASP:HA	2:1001:A:OLA:H82	6	0.38	0.2	0.36
(2,447)	1:84:A:ASP:HA	1:65:A:LYS:HD2	6	0.38	0.2	0.36
(2,447)	1:84:A:ASP:HA	2:1001:A:OLA:H112	6	0.38	0.2	0.36
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD22	6	0.36	0.16	0.31
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD21	6	0.36	0.16	0.31
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD23	6	0.36	0.16	0.31
(2,925)	1:65:A:LYS:HG3	1:67:A:THR:H	6	0.34	0.11	0.36
(2,925)	1:67:A:THR:H	1:44:A:LYS:HG2	6	0.34	0.11	0.36
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB2	6	0.34	0.15	0.32
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB3	6	0.34	0.15	0.32
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB1	6	0.34	0.15	0.32
(2,121)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	6	0.34	0.21	0.29
(2,121)	1:142:A:LYS:HE2	1:9:A:GLY:HA2	6	0.34	0.21	0.29
(2,487)	1:90:A:ILE:HG21	1:92:A:PHE:HB2	6	0.34	0.12	0.36
(2,487)	1:90:A:ILE:HG23	1:92:A:PHE:HB2	6	0.34	0.12	0.36
(2,487)	1:90:A:ILE:HG22	1:92:A:PHE:HB2	6	0.34	0.12	0.36
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD12	6	0.33	0.21	0.22
(2,1155)	1:60:A:ASN:H	1:61:A:LEU:HD21	6	0.33	0.21	0.22
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD11	6	0.33	0.21	0.22
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD23	6	0.33	0.21	0.22
(2,677)	1:139:A:TYR:HE2	1:121:A:ASP:HB3	6	0.33	0.1	0.31
(2,677)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	6	0.33	0.1	0.31
(2,247)	1:26:A:ARG:HD3	1:26:A:ARG:H	6	0.33	0.14	0.26
(2,247)	1:26:A:ARG:HD2	1:131:A:TRP:HE3	6	0.33	0.14	0.26
(2,247)	1:26:A:ARG:HD2	1:26:A:ARG:H	6	0.33	0.14	0.26
(2,247)	1:26:A:ARG:HD3	1:131:A:TRP:HE3	6	0.33	0.14	0.26
(1,100)	1:48:A:ALA:HB3	1:50:A:SER:H	6	0.32	0.12	0.31
(1,100)	1:48:A:ALA:HB1	1:50:A:SER:H	6	0.32	0.12	0.31
(1,100)	1:48:A:ALA:HB2	1:50:A:SER:H	6	0.32	0.12	0.31
(2,418)	1:106:A:LYS:HG2	1:107:A:VAL:H	6	0.3	0.22	0.18
(2,495)	1:90:A:ILE:HD12	1:82:A:ALA:HA	6	0.29	0.14	0.28
(2,495)	1:90:A:ILE:HD11	1:90:A:ILE:HA	6	0.29	0.14	0.28
(2,495)	1:90:A:ILE:HD13	1:82:A:ALA:HA	6	0.29	0.14	0.28
(2,495)	1:90:A:ILE:HD11	1:82:A:ALA:HA	6	0.29	0.14	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,564)	1:88:A:HIS:HB2	1:107:A:VAL:HA	6	0.28	0.13	0.27
(2,564)	1:107:A:VAL:HA	1:89:A:LYS:HE2	6	0.28	0.13	0.27
(2,488)	1:90:A:ILE:HG23	1:102:A:GLU:HB2	6	0.28	0.17	0.24
(2,488)	1:102:A:GLU:HB3	1:90:A:ILE:HG22	6	0.28	0.17	0.24
(2,488)	1:102:A:GLU:HB3	1:90:A:ILE:HG21	6	0.28	0.17	0.24
(2,683)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	6	0.27	0.07	0.25
(2,683)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	6	0.27	0.07	0.25
(2,683)	1:41:A:VAL:HG22	1:140:A:TYR:HE1	6	0.27	0.07	0.25
(2,928)	1:90:A:ILE:H	1:89:A:LYS:HE3	6	0.25	0.15	0.22
(2,928)	1:89:A:LYS:HE2	1:90:A:ILE:H	6	0.25	0.15	0.22
(2,928)	1:104:A:HIS:HB3	1:90:A:ILE:H	6	0.25	0.15	0.22
(2,928)	1:88:A:HIS:HB2	1:90:A:ILE:H	6	0.25	0.15	0.22
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD12	6	0.25	0.05	0.24
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD11	6	0.25	0.05	0.24
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD13	6	0.25	0.05	0.24
(1,17)	1:31:A:ILE:HD11	1:31:A:ILE:HA	6	0.2	0.05	0.2
(1,17)	1:31:A:ILE:HD13	1:31:A:ILE:HA	6	0.2	0.05	0.2
(1,2413)	1:23:A:LEU:HD22	1:33:A:ARG:H	6	0.17	0.04	0.16
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD12	6	0.16	0.03	0.15
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD11	6	0.16	0.03	0.15
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD13	6	0.16	0.03	0.15
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG21	6	0.16	0.04	0.15
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG22	6	0.16	0.04	0.15
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG23	6	0.16	0.04	0.15
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG23	6	0.14	0.02	0.14
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG22	6	0.14	0.02	0.14
(1,839)	1:108:A:ASP:HA	1:108:A:ASP:HB3	6	0.13	0.01	0.13
(2,1074)	1:95:A:LYS:HB2	1:96:A:ASP:H	6	0.13	0.03	0.11
(2,567)	1:88:A:HIS:HB2	1:107:A:VAL:HG11	5	2.05	0.91	2.38
(2,567)	1:88:A:HIS:HB2	1:107:A:VAL:HG13	5	2.05	0.91	2.38
(2,567)	1:88:A:HIS:HB3	1:107:A:VAL:HG13	5	2.05	0.91	2.38
(1,1621)	1:61:A:LEU:HD22	1:61:A:LEU:HA	5	1.6	0.02	1.6
(1,1621)	1:61:A:LEU:HD23	1:61:A:LEU:HA	5	1.6	0.02	1.6
(1,1621)	1:61:A:LEU:HD21	1:61:A:LEU:HA	5	1.6	0.02	1.6
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG13	5	1.4	0.31	1.44
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG11	5	1.4	0.31	1.44
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG12	5	1.4	0.31	1.44
(1,868)	1:113:A:VAL:HG22	1:113:A:VAL:H	5	1.14	0.15	1.16
(1,868)	1:113:A:VAL:HG23	1:113:A:VAL:H	5	1.14	0.15	1.16
(1,868)	1:113:A:VAL:HG21	1:113:A:VAL:H	5	1.14	0.15	1.16
(2,377)	1:41:A:VAL:HG11	1:62:A:THR:HG21	5	0.94	0.08	0.93
(2,377)	1:41:A:VAL:HG13	1:62:A:THR:HG23	5	0.94	0.08	0.93

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,377)	1:41:A:VAL:HG12	1:62:A:THR:HG23	5	0.94	0.08	0.93
(2,377)	1:41:A:VAL:HG13	1:62:A:THR:HG21	5	0.94	0.08	0.93
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD23	5	0.91	0.35	0.84
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD21	5	0.91	0.35	0.84
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD22	5	0.91	0.35	0.84
(2,316)	1:41:A:VAL:HG22	1:41:A:VAL:H	5	0.87	0.08	0.85
(2,316)	1:41:A:VAL:HG23	1:41:A:VAL:H	5	0.87	0.08	0.85
(2,316)	1:41:A:VAL:HG21	1:41:A:VAL:H	5	0.87	0.08	0.85
(2,1640)	2:1001:A:OLA:H31	1:140:A:TYR:HH	5	0.8	0.42	0.88
(2,1640)	1:140:A:TYR:HH	2:1001:A:OLA:H32	5	0.8	0.42	0.88
(2,1640)	1:140:A:TYR:HH	1:62:A:THR:HG22	5	0.8	0.42	0.88
(2,1640)	1:127:A:MET:HE2	1:140:A:TYR:HH	5	0.8	0.42	0.88
(2,1283)	1:127:A:MET:HE3	1:127:A:MET:H	5	0.79	0.07	0.77
(2,1283)	1:127:A:MET:HE2	1:127:A:MET:H	5	0.79	0.07	0.77
(2,1283)	1:127:A:MET:HE1	1:127:A:MET:H	5	0.79	0.07	0.77
(2,604)	1:124:A:TYR:HE2	1:14:A:GLU:HG2	5	0.77	0.22	0.89
(2,604)	1:124:A:TYR:HE2	1:139:A:TYR:HB2	5	0.77	0.22	0.89
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG11	5	0.74	0.07	0.77
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG12	5	0.74	0.07	0.77
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG13	5	0.74	0.07	0.77
(2,834)	1:68:A:HIS:HE1	1:49:A:ALA:HB1	5	0.59	0.35	0.49
(2,834)	1:68:A:HIS:HE1	1:49:A:ALA:HB3	5	0.59	0.35	0.49
(2,834)	1:68:A:HIS:HE1	1:70:A:LYS:HD2	5	0.59	0.35	0.49
(2,834)	1:68:A:HIS:HE1	1:49:A:ALA:HB2	5	0.59	0.35	0.49
(2,545)	1:100:A:LEU:HD21	1:94:A:LEU:HD23	5	0.51	0.24	0.65
(2,545)	1:100:A:LEU:HD22	1:94:A:LEU:HD21	5	0.51	0.24	0.65
(2,545)	1:100:A:LEU:HD22	1:94:A:LEU:HD22	5	0.51	0.24	0.65
(2,545)	1:100:A:LEU:HD22	1:94:A:LEU:HD23	5	0.51	0.24	0.65
(2,518)	1:96:A:ASP:H	1:94:A:LEU:HD11	5	0.5	0.25	0.38
(2,518)	1:95:A:LYS:H	1:94:A:LEU:HD13	5	0.5	0.25	0.38
(2,518)	1:95:A:LYS:H	1:94:A:LEU:HD11	5	0.5	0.25	0.38
(2,518)	1:95:A:LYS:H	1:94:A:LEU:HD12	5	0.5	0.25	0.38
(2,132)	1:85:A:SER:H	1:65:A:LYS:HE2	5	0.5	0.16	0.48
(2,132)	1:10:A:THR:H	1:142:A:LYS:HE3	5	0.5	0.16	0.48
(2,410)	1:71:A:ASP:HB3	1:55:A:ARG:HB3	5	0.46	0.1	0.43
(2,410)	1:71:A:ASP:HB3	1:48:A:ALA:HB2	5	0.46	0.1	0.43
(2,410)	1:71:A:ASP:HB3	1:48:A:ALA:HB3	5	0.46	0.1	0.43
(2,410)	1:70:A:LYS:HG2	1:71:A:ASP:HB3	5	0.46	0.1	0.43
(2,326)	1:140:A:TYR:HE2	1:43:A:LYS:HE3	5	0.45	0.23	0.4
(2,326)	1:45:A:PHE:HE1	1:43:A:LYS:HE3	5	0.45	0.23	0.4
(2,698)	1:142:A:LYS:HG2	1:142:A:LYS:HE3	5	0.38	0.26	0.17
(2,1480)	1:46:A:ARG:HG3	1:71:A:ASP:H	5	0.38	0.12	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1480)	1:71:A:ASP:H	1:55:A:ARG:HG3	5	0.38	0.12	0.4
(2,1480)	1:49:A:ALA:HB2	1:71:A:ASP:H	5	0.38	0.12	0.4
(1,925)	1:125:A:LEU:HD21	1:7:A:PHE:HA	5	0.36	0.08	0.35
(1,925)	1:125:A:LEU:HD22	1:7:A:PHE:HA	5	0.36	0.08	0.35
(2,603)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	5	0.35	0.09	0.32
(2,603)	1:124:A:TYR:HE2	1:141:A:LYS:HE2	5	0.35	0.09	0.32
(2,849)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	5	0.35	0.09	0.32
(2,849)	1:124:A:TYR:HE2	1:141:A:LYS:HE2	5	0.35	0.09	0.32
(2,122)	1:9:A:GLY:HA3	1:142:A:LYS:HE3	5	0.34	0.17	0.36
(2,122)	1:9:A:GLY:HA3	1:142:A:LYS:HE2	5	0.34	0.17	0.36
(1,2314)	1:81:A:GLU:H	1:87:A:GLN:HE21	5	0.33	0.07	0.36
(2,1411)	1:13:A:LEU:H	1:143:A:GLN:HE22	5	0.33	0.14	0.24
(2,511)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	5	0.32	0.12	0.34
(2,511)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	5	0.32	0.12	0.34
(2,1075)	1:94:A:LEU:HD21	1:93:A:ASP:H	5	0.28	0.14	0.25
(2,1075)	1:94:A:LEU:HD23	1:93:A:ASP:H	5	0.28	0.14	0.25
(2,1075)	1:93:A:ASP:H	1:74:A:LEU:HD21	5	0.28	0.14	0.25
(2,1075)	1:94:A:LEU:HD22	1:93:A:ASP:H	5	0.28	0.14	0.25
(2,23)	1:34:A:GLN:HG3	1:34:A:GLN:H	5	0.27	0.09	0.27
(2,23)	1:34:A:GLN:HG3	1:30:A:TRP:HZ2	5	0.27	0.09	0.27
(1,952)	1:129:A:MET:HB2	1:136:A:THR:HG23	5	0.27	0.15	0.23
(1,952)	1:129:A:MET:HB2	1:136:A:THR:HG22	5	0.27	0.15	0.23
(2,580)	1:111:A:THR:HG22	1:110:A:PRO:HG2	5	0.27	0.07	0.25
(2,580)	1:111:A:THR:HG21	1:110:A:PRO:HG2	5	0.27	0.07	0.25
(2,580)	1:111:A:THR:HG23	1:110:A:PRO:HG2	5	0.27	0.07	0.25
(2,33)	1:52:A:LYS:HG2	1:53:A:PRO:HD3	5	0.26	0.06	0.29
(2,33)	1:52:A:LYS:HG3	1:53:A:PRO:HD3	5	0.26	0.06	0.29
(2,878)	1:132:A:LYS:HG3	1:132:A:LYS:H	5	0.26	0.03	0.26
(2,1102)	1:58:A:MET:H	1:70:A:LYS:HG2	5	0.26	0.07	0.23
(2,759)	1:32:A:MET:HE1	2:1001:A:OLA:H121	5	0.25	0.03	0.24
(2,759)	1:32:A:MET:HE3	2:1001:A:OLA:H121	5	0.25	0.03	0.24
(2,759)	1:32:A:MET:HE2	2:1001:A:OLA:H121	5	0.25	0.03	0.24
(1,1106)	1:58:A:MET:HE2	1:45:A:PHE:HE1	5	0.24	0.13	0.2
(1,1106)	1:58:A:MET:HE3	1:45:A:PHE:HE1	5	0.24	0.13	0.2
(2,1653)	1:32:A:MET:HE1	2:1001:A:OLA:H121	5	0.23	0.03	0.22
(2,1653)	1:32:A:MET:HE3	2:1001:A:OLA:H121	5	0.23	0.03	0.22
(2,1653)	1:32:A:MET:HE2	2:1001:A:OLA:H121	5	0.23	0.03	0.22
(1,843)	1:108:A:ASP:HB2	1:108:A:ASP:H	5	0.22	0.01	0.23
(2,803)	1:-2:A:HIS:HB2	1:1:A:LYS:HA	5	0.21	0.05	0.21
(2,803)	1:1:A:LYS:HA	1:-2:A:HIS:HB3	5	0.21	0.05	0.21
(2,803)	1:-5:A:HIS:HA	1:-2:A:HIS:HB2	5	0.21	0.05	0.21
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG23	5	0.2	0.09	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG21	5	0.2	0.09	0.17
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG22	5	0.2	0.09	0.17
(2,990)	1:132:A:LYS:HG3	1:132:A:LYS:H	5	0.2	0.03	0.19
(1,1603)	1:86:A:THR:HG21	1:86:A:THR:H	5	0.19	0.06	0.22
(1,1603)	1:86:A:THR:HG23	1:86:A:THR:H	5	0.19	0.06	0.22
(1,1603)	1:86:A:THR:HG22	1:86:A:THR:H	5	0.19	0.06	0.22
(1,2331)	1:60:A:ASN:HB3	1:67:A:THR:H	5	0.19	0.08	0.18
(2,53)	1:33:A:ARG:HD3	1:30:A:TRP:HA	5	0.18	0.06	0.16
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE1	5	0.18	0.05	0.15
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE3	5	0.18	0.05	0.15
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE2	5	0.18	0.05	0.15
(1,2000)	1:8:A:LEU:HD22	1:47:A:ASN:HD21	5	0.17	0.03	0.15
(1,2000)	1:8:A:LEU:HD21	1:47:A:ASN:HD21	5	0.17	0.03	0.15
(1,2000)	1:8:A:LEU:HD23	1:47:A:ASN:HD21	5	0.17	0.03	0.15
(2,150)	1:12:A:LYS:HA	1:12:A:LYS:HG2	5	0.17	0.0	0.17
(2,313)	1:129:A:MET:HE1	1:22:A:TYR:HD1	5	0.16	0.07	0.12
(2,313)	1:129:A:MET:HE2	1:22:A:TYR:HD1	5	0.16	0.07	0.12
(2,313)	1:129:A:MET:HE3	1:22:A:TYR:HD1	5	0.16	0.07	0.12
(1,1037)	1:124:A:TYR:HE2	1:141:A:LYS:HD3	5	0.14	0.02	0.14
(1,1643)	1:19:A:PHE:H	1:19:A:PHE:HD1	5	0.14	0.03	0.13
(2,403)	1:66:A:ASP:HA	1:61:A:LEU:HD22	4	2.39	0.22	2.33
(2,403)	1:66:A:ASP:HA	1:83:A:LEU:HD21	4	2.39	0.22	2.33
(1,675)	1:101:A:THR:H	1:94:A:LEU:HD23	4	1.98	1.08	2.56
(1,675)	1:101:A:THR:H	1:94:A:LEU:HD21	4	1.98	1.08	2.56
(2,1441)	1:34:A:GLN:HE22	1:38:A:LEU:HD23	4	1.74	0.4	1.93
(2,1441)	1:35:A:VAL:HG22	1:34:A:GLN:HE22	4	1.74	0.4	1.93
(2,1441)	1:38:A:LEU:HD11	1:34:A:GLN:HE22	4	1.74	0.4	1.93
(2,1441)	1:35:A:VAL:HG23	1:34:A:GLN:HE22	4	1.74	0.4	1.93
(2,615)	1:125:A:LEU:HD21	1:120:A:ARG:HA	4	1.61	1.33	1.66
(1,835)	1:89:A:LYS:H	1:107:A:VAL:HG11	4	1.53	0.18	1.6
(1,1617)	1:107:A:VAL:H	1:107:A:VAL:HG12	4	1.41	0.06	1.44
(1,1617)	1:107:A:VAL:H	1:107:A:VAL:HG11	4	1.41	0.06	1.44
(1,1925)	1:107:A:VAL:HG21	1:79:A:GLN:HE22	4	1.37	0.91	1.46
(1,1925)	1:107:A:VAL:HG23	1:79:A:GLN:HE22	4	1.37	0.91	1.46
(1,76)	1:96:A:ASP:HB3	1:97:A:PRO:HG2	4	1.33	0.02	1.33
(1,1890)	1:89:A:LYS:H	1:107:A:VAL:HG11	4	1.22	0.18	1.28
(1,836)	1:88:A:HIS:HA	1:107:A:VAL:HG13	4	1.19	0.05	1.19
(1,836)	1:88:A:HIS:HA	1:107:A:VAL:HG11	4	1.19	0.05	1.19
(2,426)	1:13:A:LEU:HD21	1:15:A:ARG:HB2	4	1.14	0.7	1.14
(2,426)	1:15:A:ARG:HB3	1:13:A:LEU:HD21	4	1.14	0.7	1.14
(1,218)	1:13:A:LEU:HD21	1:139:A:TYR:H	4	1.06	0.44	1.18
(1,227)	1:41:A:VAL:H	1:13:A:LEU:HD11	4	0.99	0.5	1.03

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,227)	1:41:A:VAL:H	1:13:A:LEU:HD12	4	0.99	0.5	1.03
(2,1144)	1:105:A:ILE:H	1:113:A:VAL:HB	4	0.96	0.47	0.92
(2,1144)	1:105:A:ILE:H	1:110:A:PRO:HB2	4	0.96	0.47	0.92
(2,691)	1:141:A:LYS:HD2	1:141:A:LYS:H	4	0.95	0.02	0.96
(1,442)	1:38:A:LEU:HD23	1:38:A:LEU:HB2	4	0.94	0.03	0.95
(1,442)	1:38:A:LEU:HD22	1:38:A:LEU:HB2	4	0.94	0.03	0.95
(2,1645)	1:127:A:MET:HE2	1:140:A:TYR:HH	4	0.93	0.28	1.0
(2,1645)	1:140:A:TYR:HH	1:62:A:THR:HG22	4	0.93	0.28	1.0
(2,1645)	2:1001:A:OLA:H31	1:140:A:TYR:HH	4	0.93	0.28	1.0
(2,1645)	1:140:A:TYR:HH	2:1001:A:OLA:H32	4	0.93	0.28	1.0
(1,1092)	1:44:A:LYS:HA	1:10:A:THR:HG21	4	0.92	0.03	0.92
(1,1092)	1:44:A:LYS:HA	1:10:A:THR:HG22	4	0.92	0.03	0.92
(1,1092)	1:44:A:LYS:HA	1:10:A:THR:HG23	4	0.92	0.03	0.92
(2,590)	1:117:A:GLU:HG2	1:115:A:THR:HG22	4	0.91	0.01	0.92
(2,590)	1:117:A:GLU:HG2	1:101:A:THR:HG23	4	0.91	0.01	0.92
(2,590)	1:117:A:GLU:HG2	1:101:A:THR:HG21	4	0.91	0.01	0.92
(2,570)	1:87:A:GLN:HA	1:107:A:VAL:HG21	4	0.91	0.56	0.93
(2,570)	1:108:A:ASP:HA	1:107:A:VAL:HG22	4	0.91	0.56	0.93
(2,570)	1:87:A:GLN:HA	1:82:A:ALA:HB1	4	0.91	0.56	0.93
(1,2138)	1:107:A:VAL:H	1:107:A:VAL:HG12	4	0.84	0.07	0.88
(1,2138)	1:107:A:VAL:H	1:107:A:VAL:HG11	4	0.84	0.07	0.88
(2,1641)	1:127:A:MET:HE2	1:140:A:TYR:HH	4	0.82	0.28	0.89
(2,1641)	1:140:A:TYR:HH	1:62:A:THR:HG22	4	0.82	0.28	0.89
(2,1641)	2:1001:A:OLA:H31	1:140:A:TYR:HH	4	0.82	0.28	0.89
(2,1641)	1:140:A:TYR:HH	2:1001:A:OLA:H32	4	0.82	0.28	0.89
(1,591)	1:70:A:LYS:HE3	1:70:A:LYS:HB3	4	0.78	0.16	0.84
(2,1439)	1:13:A:LEU:H	1:143:A:GLN:HE21	4	0.76	0.16	0.82
(2,415)	1:0:A:SER:HB2	1:73:A:ALA:HB2	4	0.72	0.09	0.71
(2,415)	1:73:A:ALA:HB3	1:0:A:SER:HB3	4	0.72	0.09	0.71
(2,415)	1:0:A:SER:HB2	1:73:A:ALA:HB1	4	0.72	0.09	0.71
(2,415)	1:0:A:SER:HB2	1:73:A:ALA:HB3	4	0.72	0.09	0.71
(2,86)	1:125:A:LEU:HD11	1:45:A:PHE:HE1	4	0.72	0.53	0.53
(2,86)	1:125:A:LEU:HD13	1:45:A:PHE:HE1	4	0.72	0.53	0.53
(2,123)	1:10:A:THR:HB	1:143:A:GLN:HB2	4	0.67	0.01	0.67
(2,1216)	1:34:A:GLN:HE22	1:33:A:ARG:HG2	4	0.67	0.24	0.66
(2,1216)	1:36:A:ILE:HB	1:34:A:GLN:HE22	4	0.67	0.24	0.66
(2,680)	1:140:A:TYR:HE2	1:43:A:LYS:HG2	4	0.58	0.56	0.32
(2,680)	1:140:A:TYR:HE2	2:1001:A:OLA:H22	4	0.58	0.56	0.32
(2,680)	1:140:A:TYR:HE1	1:43:A:LYS:HG2	4	0.58	0.56	0.32
(2,1658)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	4	0.54	0.27	0.54
(2,1658)	1:19:A:PHE:HE1	2:1001:A:OLA:H21	4	0.54	0.27	0.54
(2,478)	1:88:A:HIS:HB2	1:90:A:ILE:HG13	4	0.52	0.13	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1601)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	4	0.52	0.22	0.49
(2,1601)	2:1001:A:OLA:H22	2:1001:A:OLA:H182	4	0.52	0.22	0.49
(2,1601)	2:1001:A:OLA:H22	2:1001:A:OLA:H183	4	0.52	0.22	0.49
(2,1125)	1:118:A:TYR:H	1:95:A:LYS:HD3	4	0.51	0.22	0.53
(2,1125)	1:118:A:TYR:H	1:95:A:LYS:HB2	4	0.51	0.22	0.53
(2,1125)	1:118:A:TYR:H	1:127:A:MET:HB3	4	0.51	0.22	0.53
(2,1125)	1:118:A:TYR:H	1:119:A:ARG:HG2	4	0.51	0.22	0.53
(2,1139)	1:100:A:LEU:H	1:119:A:ARG:HB3	4	0.5	0.11	0.52
(2,1139)	1:100:A:LEU:H	1:119:A:ARG:HG3	4	0.5	0.11	0.52
(1,743)	1:93:A:ASP:HB2	1:91:A:THR:HG21	4	0.5	0.18	0.46
(1,743)	1:93:A:ASP:HB2	1:91:A:THR:HG22	4	0.5	0.18	0.46
(1,743)	1:93:A:ASP:HB2	1:91:A:THR:HG23	4	0.5	0.18	0.46
(2,1305)	1:116:A:TYR:H	1:127:A:MET:HG2	4	0.48	0.46	0.28
(2,757)	1:58:A:MET:HE3	1:43:A:LYS:HD2	4	0.48	0.36	0.33
(2,757)	1:58:A:MET:HE2	1:43:A:LYS:HD2	4	0.48	0.36	0.33
(2,757)	1:58:A:MET:HE3	1:43:A:LYS:HB3	4	0.48	0.36	0.33
(2,780)	1:37:A:LYS:HD2	1:34:A:GLN:HE22	4	0.47	0.15	0.46
(2,780)	1:109:A:ASP:H	1:106:A:LYS:HD2	4	0.47	0.15	0.46
(2,1593)	1:84:A:ASP:HA	2:1001:A:OLA:H112	4	0.47	0.13	0.45
(1,2463)	1:111:A:THR:HG21	1:113:A:VAL:H	4	0.47	0.21	0.47
(1,2463)	1:111:A:THR:HG23	1:113:A:VAL:H	4	0.47	0.21	0.47
(2,835)	1:37:A:LYS:HA	1:37:A:LYS:HE2	4	0.46	0.32	0.36
(2,835)	1:20:A:ASP:HA	1:37:A:LYS:HE2	4	0.46	0.32	0.36
(1,195)	1:11:A:PHE:H	1:10:A:THR:HG21	4	0.44	0.02	0.44
(1,195)	1:11:A:PHE:H	1:10:A:THR:HG22	4	0.44	0.02	0.44
(1,195)	1:11:A:PHE:H	1:10:A:THR:HG23	4	0.44	0.02	0.44
(2,84)	1:3:A:LEU:HD22	1:7:A:PHE:H	4	0.43	0.31	0.26
(2,84)	1:3:A:LEU:HD21	1:7:A:PHE:H	4	0.43	0.31	0.26
(2,556)	1:89:A:LYS:HE3	1:105:A:ILE:HD13	4	0.42	0.04	0.43
(2,556)	1:89:A:LYS:HE3	1:105:A:ILE:HD11	4	0.42	0.04	0.43
(2,556)	1:105:A:ILE:HD12	1:89:A:LYS:HE2	4	0.42	0.04	0.43
(1,1097)	1:136:A:THR:HG22	1:129:A:MET:HB3	4	0.41	0.03	0.42
(1,1097)	1:136:A:THR:HG21	1:129:A:MET:HB3	4	0.41	0.03	0.42
(2,904)	1:106:A:LYS:H	1:106:A:LYS:HE2	4	0.39	0.3	0.28
(2,904)	1:106:A:LYS:H	1:109:A:ASP:HB3	4	0.39	0.3	0.28
(2,286)	2:1001:A:OLA:H71	1:36:A:ILE:HG21	4	0.37	0.36	0.2
(2,286)	2:1001:A:OLA:H41	1:36:A:ILE:HG23	4	0.37	0.36	0.2
(2,286)	2:1001:A:OLA:H172	1:36:A:ILE:HG21	4	0.37	0.36	0.2
(2,286)	2:1001:A:OLA:H61	1:36:A:ILE:HG23	4	0.37	0.36	0.2
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD13	4	0.37	0.15	0.41
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD11	4	0.37	0.15	0.41
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD23	4	0.37	0.15	0.41

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD12	4	0.37	0.15	0.41
(2,1006)	1:81:A:GLU:H	1:87:A:GLN:HE22	4	0.37	0.13	0.38
(2,1006)	1:81:A:GLU:H	1:69:A:HIS:HE1	4	0.37	0.13	0.38
(2,1495)	1:13:A:LEU:H	1:42:A:THR:HG22	4	0.36	0.17	0.34
(2,1495)	1:13:A:LEU:H	1:42:A:THR:HG21	4	0.36	0.17	0.34
(1,120)	1:1:A:LYS:HG3	1:1:A:LYS:HA	4	0.36	0.15	0.4
(2,526)	1:95:A:LYS:HG2	1:99:A:THR:HB	4	0.36	0.18	0.34
(2,526)	1:13:A:LEU:HA	1:12:A:LYS:HG3	4	0.36	0.18	0.34
(2,652)	1:132:A:LYS:HG2	1:132:A:LYS:HE2	4	0.33	0.01	0.32
(2,1396)	1:63:A:THR:HG22	1:41:A:VAL:H	4	0.32	0.18	0.32
(2,1396)	1:63:A:THR:HG21	1:41:A:VAL:H	4	0.32	0.18	0.32
(2,1396)	1:62:A:THR:HG23	1:41:A:VAL:H	4	0.32	0.18	0.32
(2,1396)	1:62:A:THR:HG21	1:41:A:VAL:H	4	0.32	0.18	0.32
(2,1577)	1:83:A:LEU:HD13	2:1001:A:OLA:H72	4	0.32	0.22	0.3
(2,1577)	2:1001:A:OLA:H72	1:36:A:ILE:HG22	4	0.32	0.22	0.3
(1,2029)	1:114:A:GLU:H	1:103:A:THR:HG23	4	0.31	0.16	0.25
(1,2029)	1:114:A:GLU:H	1:103:A:THR:HG21	4	0.31	0.16	0.25
(2,448)	1:84:A:ASP:HA	2:1001:A:OLA:H121	4	0.31	0.13	0.34
(2,448)	2:1001:A:OLA:H151	1:84:A:ASP:HA	4	0.31	0.13	0.34
(2,1061)	1:118:A:TYR:HD1	1:128:A:LYS:H	4	0.3	0.15	0.29
(2,1061)	1:118:A:TYR:HD2	1:128:A:LYS:H	4	0.3	0.15	0.29
(2,250)	1:26:A:ARG:HD2	1:131:A:TRP:HD1	4	0.29	0.19	0.22
(2,1610)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	4	0.28	0.16	0.18
(2,1610)	1:19:A:PHE:HZ	2:1001:A:OLA:H21	4	0.28	0.16	0.18
(2,1659)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	4	0.27	0.16	0.18
(2,1659)	1:19:A:PHE:HZ	2:1001:A:OLA:H21	4	0.27	0.16	0.18
(1,193)	1:10:A:THR:HA	1:10:A:THR:HG21	4	0.26	0.02	0.26
(1,193)	1:10:A:THR:HA	1:10:A:THR:HG22	4	0.26	0.02	0.26
(1,193)	1:10:A:THR:HA	1:10:A:THR:HG23	4	0.26	0.02	0.26
(1,620)	1:73:A:ALA:HB1	1:76:A:GLU:HB3	4	0.26	0.12	0.26
(1,620)	1:73:A:ALA:HB3	1:76:A:GLU:HB3	4	0.26	0.12	0.26
(1,620)	1:73:A:ALA:HB2	1:76:A:GLU:HB3	4	0.26	0.12	0.26
(2,76)	1:3:A:LEU:HD12	1:45:A:PHE:HB2	4	0.26	0.16	0.22
(2,888)	1:59:A:GLU:HG2	1:68:A:HIS:HD2	4	0.25	0.04	0.24
(2,888)	1:59:A:GLU:HG3	1:68:A:HIS:HD2	4	0.25	0.04	0.24
(2,1580)	1:129:A:MET:HE1	2:1001:A:OLA:H181	4	0.25	0.1	0.23
(2,1580)	2:1001:A:OLA:H32	2:1001:A:OLA:H183	4	0.25	0.1	0.23
(2,1580)	1:129:A:MET:HE3	2:1001:A:OLA:H182	4	0.25	0.1	0.23
(1,954)	1:129:A:MET:HG3	1:116:A:TYR:HD2	4	0.25	0.18	0.16
(1,954)	1:129:A:MET:HG3	1:116:A:TYR:HD1	4	0.25	0.18	0.16
(2,1478)	1:45:A:PHE:HD1	1:11:A:PHE:H	4	0.25	0.08	0.28
(1,1183)	1:35:A:VAL:HB	1:32:A:MET:HE3	4	0.24	0.15	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1183)	1:35:A:VAL:HB	1:32:A:MET:HE2	4	0.24	0.15	0.18
(1,1183)	1:35:A:VAL:HB	1:32:A:MET:HE1	4	0.24	0.15	0.18
(2,720)	1:14:A:GLU:H	1:124:A:TYR:HE2	4	0.24	0.06	0.26
(2,720)	1:124:A:TYR:HE2	1:141:A:LYS:H	4	0.24	0.06	0.26
(2,1568)	2:1001:A:OLA:H82	2:1001:A:OLA:H181	4	0.23	0.11	0.21
(2,1568)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	4	0.23	0.11	0.21
(2,1568)	2:1001:A:OLA:H82	2:1001:A:OLA:H183	4	0.23	0.11	0.21
(2,1651)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	4	0.23	0.11	0.2
(2,1651)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	4	0.23	0.11	0.2
(1,678)	1:60:A:ASN:HB3	1:83:A:LEU:HD21	4	0.23	0.02	0.23
(1,678)	1:60:A:ASN:HB3	1:83:A:LEU:HD23	4	0.23	0.02	0.23
(2,1080)	1:102:A:GLU:H	1:92:A:PHE:HD2	4	0.22	0.05	0.22
(1,1461)	1:55:A:ARG:HG2	1:56:A:TYR:H	4	0.22	0.11	0.19
(2,1315)	1:105:A:ILE:HG13	1:113:A:VAL:H	4	0.22	0.13	0.16
(2,1665)	1:22:A:TYR:HD1	2:1001:A:OLA:H182	4	0.22	0.09	0.2
(2,1665)	1:22:A:TYR:HD2	1:26:A:ARG:HG2	4	0.22	0.09	0.2
(2,1665)	1:22:A:TYR:HD1	2:1001:A:OLA:H181	4	0.22	0.09	0.2
(1,191)	1:10:A:THR:HB	1:143:A:GLN:H	4	0.2	0.06	0.2
(3,43)	1:55:A:ARG:H	1:53:A:PRO:O	4	0.2	0.06	0.19
(1,1148)	1:37:A:LYS:H	1:36:A:ILE:HG21	4	0.19	0.09	0.15
(1,1148)	1:37:A:LYS:H	1:36:A:ILE:HG22	4	0.19	0.09	0.15
(1,1148)	1:37:A:LYS:H	1:36:A:ILE:HG23	4	0.19	0.09	0.15
(2,1647)	1:36:A:ILE:HD13	2:1001:A:OLA:H131	4	0.18	0.04	0.17
(2,1647)	1:36:A:ILE:HD11	2:1001:A:OLA:H131	4	0.18	0.04	0.17
(2,930)	1:134:A:VAL:H	1:132:A:LYS:HB3	4	0.18	0.04	0.17
(2,930)	1:134:A:VAL:H	1:25:A:ALA:HB1	4	0.18	0.04	0.17
(2,930)	1:134:A:VAL:H	1:25:A:ALA:HB3	4	0.18	0.04	0.17
(2,661)	1:128:A:LYS:HE3	1:135:A:SER:HB2	4	0.17	0.05	0.18
(2,661)	1:128:A:LYS:HE2	1:135:A:SER:HB2	4	0.17	0.05	0.18
(2,1644)	2:1001:A:OLA:H82	2:1001:A:OLA:H9	4	0.17	0.04	0.18
(2,1644)	2:1001:A:OLA:H10	2:1001:A:OLA:H111	4	0.17	0.04	0.18
(2,402)	1:66:A:ASP:HA	1:62:A:THR:HG22	4	0.17	0.06	0.14
(2,402)	1:66:A:ASP:HA	1:62:A:THR:HG21	4	0.17	0.06	0.14
(2,212)	1:23:A:LEU:HD23	1:26:A:ARG:H	4	0.16	0.04	0.15
(2,212)	1:23:A:LEU:HD22	1:26:A:ARG:H	4	0.16	0.04	0.15
(1,968)	1:130:A:SER:HB2	1:131:A:TRP:H	4	0.16	0.05	0.14
(2,622)	1:127:A:MET:HA	1:126:A:VAL:HG11	4	0.15	0.02	0.16
(2,622)	1:127:A:MET:HA	1:126:A:VAL:HG13	4	0.15	0.02	0.16
(3,89)	1:117:A:GLU:H	1:128:A:LYS:O	4	0.15	0.03	0.14
(2,231)	1:25:A:ALA:HB1	1:134:A:VAL:HG21	4	0.15	0.04	0.13
(2,231)	1:25:A:ALA:HB2	1:134:A:VAL:HG22	4	0.15	0.04	0.13
(2,231)	1:25:A:ALA:HB1	1:134:A:VAL:HG23	4	0.15	0.04	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,231)	1:25:A:ALA:HB2	1:134:A:VAL:HG23	4	0.15	0.04	0.13
(2,743)	1:104:A:HIS:HD2	1:102:A:GLU:HG3	4	0.14	0.04	0.13
(2,743)	1:104:A:HIS:HD2	1:105:A:ILE:HG13	4	0.14	0.04	0.13
(2,130)	1:11:A:PHE:HA	1:142:A:LYS:HG2	4	0.14	0.03	0.12
(1,81)	1:97:A:PRO:HD2	1:96:A:ASP:HB3	4	0.12	0.01	0.12
(3,67)	1:89:A:LYS:H	1:105:A:ILE:O	4	0.12	0.02	0.11
(3,33)	1:23:A:LEU:H	1:20:A:ASP:O	4	0.11	0.0	0.11
(1,70)	1:97:A:PRO:HA	1:94:A:LEU:HD13	3	2.46	0.22	2.43
(1,70)	1:97:A:PRO:HA	1:94:A:LEU:HD12	3	2.46	0.22	2.43
(1,70)	1:97:A:PRO:HA	1:94:A:LEU:HD11	3	2.46	0.22	2.43
(1,217)	1:14:A:GLU:H	1:13:A:LEU:HD21	3	1.93	0.11	1.97
(1,2663)	1:14:A:GLU:H	1:13:A:LEU:HD21	3	1.6	0.11	1.64
(1,630)	1:74:A:LEU:HD13	1:3:A:LEU:H	3	1.55	0.56	1.78
(1,630)	1:74:A:LEU:HD12	1:3:A:LEU:H	3	1.55	0.56	1.78
(1,221)	1:13:A:LEU:HD22	1:14:A:GLU:HA	3	1.43	0.11	1.49
(1,219)	1:13:A:LEU:HD21	1:15:A:ARG:H	3	1.36	0.25	1.2
(1,2189)	1:13:A:LEU:HD21	1:15:A:ARG:H	3	1.3	0.25	1.14
(2,536)	1:99:A:THR:HG23	1:117:A:GLU:HB3	3	1.21	0.38	0.99
(2,536)	1:99:A:THR:HG22	1:117:A:GLU:HB3	3	1.21	0.38	0.99
(1,1387)	1:94:A:LEU:HA	1:94:A:LEU:HD21	3	1.14	0.04	1.17
(1,1387)	1:94:A:LEU:HA	1:94:A:LEU:HD22	3	1.14	0.04	1.17
(1,1531)	1:70:A:LYS:HG2	1:68:A:HIS:HD2	3	1.12	0.5	1.17
(1,2390)	1:74:A:LEU:HD13	1:3:A:LEU:H	3	1.07	0.56	1.3
(1,2390)	1:74:A:LEU:HD12	1:3:A:LEU:H	3	1.07	0.56	1.3
(2,714)	1:127:A:MET:H	1:125:A:LEU:HD12	3	1.02	0.08	1.02
(2,714)	1:127:A:MET:H	1:125:A:LEU:HD13	3	1.02	0.08	1.02
(2,714)	1:127:A:MET:H	1:125:A:LEU:HD11	3	1.02	0.08	1.02
(1,2797)	1:116:A:TYR:HD1	1:118:A:TYR:HH	3	0.9	0.8	0.53
(1,2797)	1:116:A:TYR:HD2	1:118:A:TYR:HH	3	0.9	0.8	0.53
(2,1469)	1:52:A:LYS:HE2	1:52:A:LYS:H	3	0.82	0.09	0.86
(2,1469)	1:52:A:LYS:HE3	1:52:A:LYS:H	3	0.82	0.09	0.86
(1,2182)	1:99:A:THR:H	1:94:A:LEU:HD13	3	0.78	0.3	0.58
(1,2182)	1:99:A:THR:H	1:94:A:LEU:HD12	3	0.78	0.3	0.58
(1,2182)	1:99:A:THR:H	1:94:A:LEU:HD11	3	0.78	0.3	0.58
(2,442)	1:83:A:LEU:H	1:83:A:LEU:HD23	3	0.74	0.33	0.94
(2,442)	1:83:A:LEU:H	1:83:A:LEU:HD21	3	0.74	0.33	0.94
(1,220)	1:13:A:LEU:HD23	1:13:A:LEU:HA	3	0.72	0.02	0.72
(2,311)	1:38:A:LEU:HA	1:38:A:LEU:HD12	3	0.67	0.48	0.6
(2,311)	1:67:A:THR:HG1	1:83:A:LEU:HD23	3	0.67	0.48	0.6
(2,1537)	1:41:A:VAL:H	1:41:A:VAL:HG13	3	0.62	0.22	0.76
(2,1537)	1:41:A:VAL:H	1:13:A:LEU:HD11	3	0.62	0.22	0.76
(2,1627)	1:83:A:LEU:HB2	1:84:A:ASP:HB3	3	0.61	0.2	0.71

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1627)	2:1001:A:OLA:H122	1:84:A:ASP:HB3	3	0.61	0.2	0.71
(2,1627)	2:1001:A:OLA:H151	1:84:A:ASP:HB3	3	0.61	0.2	0.71
(1,1330)	1:126:A:VAL:H	1:125:A:LEU:HD12	3	0.59	0.04	0.57
(1,1330)	1:126:A:VAL:H	1:125:A:LEU:HD13	3	0.59	0.04	0.57
(1,1330)	1:126:A:VAL:H	1:125:A:LEU:HD11	3	0.59	0.04	0.57
(2,523)	1:128:A:LYS:HG2	1:129:A:MET:H	3	0.58	0.06	0.57
(2,523)	1:95:A:LYS:HG2	1:96:A:ASP:H	3	0.58	0.06	0.57
(1,2123)	1:82:A:ALA:H	1:81:A:GLU:HG3	3	0.57	0.33	0.45
(2,860)	1:64:A:LYS:HB2	2:1001:A:OLA:H9	3	0.52	0.27	0.6
(2,860)	1:64:A:LYS:HB2	2:1001:A:OLA:H10	3	0.52	0.27	0.6
(2,388)	1:63:A:THR:HB	1:64:A:LYS:HD2	3	0.51	0.14	0.58
(2,388)	1:65:A:LYS:HA	1:64:A:LYS:HD2	3	0.51	0.14	0.58
(2,388)	1:63:A:THR:HB	1:64:A:LYS:HD3	3	0.51	0.14	0.58
(2,1626)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	3	0.51	0.23	0.61
(1,2559)	1:85:A:SER:H	1:65:A:LYS:HE2	3	0.5	0.18	0.63
(1,212)	1:13:A:LEU:HD23	1:13:A:LEU:HA	3	0.48	0.02	0.48
(1,1278)	1:113:A:VAL:H	1:113:A:VAL:HG13	3	0.46	0.29	0.34
(1,1278)	1:113:A:VAL:H	1:113:A:VAL:HG12	3	0.46	0.29	0.34
(1,1173)	1:125:A:LEU:HD21	1:120:A:ARG:HD3	3	0.46	0.24	0.36
(1,1173)	1:125:A:LEU:HD23	1:120:A:ARG:HD3	3	0.46	0.24	0.36
(1,1193)	1:114:A:GLU:HG3	1:131:A:TRP:HE3	3	0.44	0.06	0.41
(1,1262)	1:100:A:LEU:HD22	1:101:A:THR:H	3	0.43	0.13	0.51
(1,1262)	1:100:A:LEU:HD23	1:101:A:THR:H	3	0.43	0.13	0.51
(1,1262)	1:100:A:LEU:HD21	1:101:A:THR:H	3	0.43	0.13	0.51
(2,1635)	2:1001:A:OLA:H81	1:62:A:THR:HG1	3	0.39	0.26	0.25
(2,1635)	1:83:A:LEU:HG	1:62:A:THR:HG1	3	0.39	0.26	0.25
(2,441)	1:141:A:LYS:H	1:141:A:LYS:HG3	3	0.36	0.17	0.3
(2,1602)	2:1001:A:OLA:H111	1:65:A:LYS:HB3	3	0.35	0.17	0.47
(2,1602)	1:32:A:MET:HE1	2:1001:A:OLA:H111	3	0.35	0.17	0.47
(2,1602)	1:32:A:MET:HE2	2:1001:A:OLA:H111	3	0.35	0.17	0.47
(2,1599)	1:61:A:LEU:HD11	1:44:A:LYS:HG2	3	0.35	0.2	0.34
(2,1599)	1:94:A:LEU:HD11	1:100:A:LEU:HB3	3	0.35	0.2	0.34
(2,936)	1:67:A:THR:H	1:83:A:LEU:HD13	3	0.34	0.16	0.37
(1,2828)	2:1001:A:OLA:H10	1:32:A:MET:HE1	3	0.33	0.04	0.3
(1,2828)	2:1001:A:OLA:H10	1:32:A:MET:HE3	3	0.33	0.04	0.3
(2,1243)	1:134:A:VAL:H	1:135:A:SER:HB3	3	0.32	0.09	0.26
(2,1243)	1:134:A:VAL:H	1:130:A:SER:HB2	3	0.32	0.09	0.26
(2,1664)	1:102:A:GLU:HG3	1:118:A:TYR:HE2	3	0.32	0.17	0.21
(2,1664)	1:88:A:HIS:HD2	1:86:A:THR:HG22	3	0.32	0.17	0.21
(1,719)	1:90:A:ILE:HG23	1:104:A:HIS:HD2	3	0.31	0.2	0.21
(1,719)	1:90:A:ILE:HG21	1:104:A:HIS:HD2	3	0.31	0.2	0.21
(1,719)	1:90:A:ILE:HG22	1:104:A:HIS:HD2	3	0.31	0.2	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,814)	1:60:A:ASN:HD21	1:83:A:LEU:HD21	3	0.31	0.08	0.3
(2,814)	1:60:A:ASN:HD21	1:83:A:LEU:HD23	3	0.31	0.08	0.3
(2,1613)	1:102:A:GLU:HG3	1:118:A:TYR:HE2	3	0.3	0.04	0.31
(2,367)	1:83:A:LEU:H	1:83:A:LEU:HD13	3	0.28	0.19	0.17
(2,367)	1:61:A:LEU:H	1:61:A:LEU:HD11	3	0.28	0.19	0.17
(1,1259)	1:125:A:LEU:HA	1:125:A:LEU:HD12	3	0.28	0.05	0.3
(1,1259)	1:125:A:LEU:HA	1:125:A:LEU:HD13	3	0.28	0.05	0.3
(1,1259)	1:125:A:LEU:HA	1:125:A:LEU:HD11	3	0.28	0.05	0.3
(2,249)	1:26:A:ARG:HD2	1:131:A:TRP:HZ2	3	0.27	0.02	0.28
(2,3)	1:89:A:LYS:H	1:105:A:ILE:HG21	3	0.25	0.07	0.3
(2,3)	1:89:A:LYS:H	1:105:A:ILE:HG23	3	0.25	0.07	0.3
(2,967)	1:88:A:HIS:H	1:82:A:ALA:HB1	3	0.25	0.07	0.29
(2,967)	1:88:A:HIS:H	1:82:A:ALA:HB3	3	0.25	0.07	0.29
(1,2548)	1:112:A:ASP:H	1:106:A:LYS:HD2	3	0.25	0.16	0.13
(2,808)	1:78:A:PHE:H	1:77:A:GLU:HG2	3	0.24	0.1	0.24
(1,449)	1:61:A:LEU:HB2	1:42:A:THR:HB	3	0.23	0.05	0.2
(2,1157)	1:26:A:ARG:HD3	1:26:A:ARG:H	3	0.22	0.16	0.11
(2,1157)	1:26:A:ARG:HD2	1:26:A:ARG:H	3	0.22	0.16	0.11
(2,297)	1:37:A:LYS:HG3	1:19:A:PHE:HD2	3	0.22	0.11	0.18
(2,674)	1:16:A:ASP:HA	1:139:A:TYR:HE1	3	0.21	0.08	0.18
(2,1040)	1:34:A:GLN:HE21	1:35:A:VAL:HG22	3	0.21	0.1	0.17
(2,1040)	1:34:A:GLN:HE21	1:35:A:VAL:HG21	3	0.21	0.1	0.17
(2,1040)	1:34:A:GLN:HE21	1:35:A:VAL:HG23	3	0.21	0.1	0.17
(1,1480)	1:119:A:ARG:HA	1:119:A:ARG:HG2	3	0.2	0.02	0.19
(2,1193)	1:42:A:THR:HG23	1:61:A:LEU:H	3	0.2	0.06	0.2
(2,1193)	1:42:A:THR:HG22	1:61:A:LEU:H	3	0.2	0.06	0.2
(2,1193)	1:42:A:THR:HG21	1:61:A:LEU:H	3	0.2	0.06	0.2
(2,894)	1:64:A:LYS:HG3	1:64:A:LYS:H	3	0.2	0.08	0.16
(3,65)	1:88:A:HIS:H	1:80:A:ASP:O	3	0.19	0.05	0.16
(2,633)	1:128:A:LYS:H	1:128:A:LYS:HD2	3	0.19	0.02	0.2
(2,633)	1:128:A:LYS:HD3	1:128:A:LYS:H	3	0.19	0.02	0.2
(2,1203)	1:112:A:ASP:H	1:106:A:LYS:HB3	3	0.19	0.09	0.14
(2,1442)	1:64:A:LYS:HG3	1:64:A:LYS:H	3	0.19	0.09	0.15
(1,1194)	1:139:A:TYR:HE2	1:126:A:VAL:HG23	3	0.18	0.05	0.17
(1,1194)	1:139:A:TYR:HE2	1:126:A:VAL:HG21	3	0.18	0.05	0.17
(1,1228)	1:139:A:TYR:HE2	1:126:A:VAL:HG23	3	0.18	0.05	0.17
(1,1228)	1:139:A:TYR:HE2	1:126:A:VAL:HG21	3	0.18	0.05	0.17
(1,228)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	3	0.18	0.0	0.18
(1,228)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	3	0.18	0.0	0.18
(1,2694)	1:28:A:TYR:H	1:28:A:TYR:HE1	3	0.17	0.01	0.17
(2,405)	1:66:A:ASP:HA	1:61:A:LEU:HB2	3	0.17	0.04	0.16
(2,457)	1:86:A:THR:HB	1:87:A:GLN:HG2	3	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,524)	1:95:A:LYS:H	1:95:A:LYS:HG3	3	0.16	0.06	0.14
(2,946)	1:56:A:TYR:H	1:55:A:ARG:HG3	3	0.16	0.0	0.16
(1,571)	1:65:A:LYS:HD3	1:66:A:ASP:H	3	0.15	0.01	0.14
(1,2429)	1:65:A:LYS:HA	1:66:A:ASP:H	3	0.14	0.01	0.14
(1,2737)	1:86:A:THR:HG21	1:86:A:THR:H	3	0.13	0.02	0.12
(1,2737)	1:86:A:THR:HG22	1:86:A:THR:H	3	0.13	0.02	0.12
(2,239)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	3	0.13	0.01	0.13
(1,369)	1:32:A:MET:H	1:32:A:MET:HG3	3	0.11	0.01	0.11
(1,2768)	1:120:A:ARG:H	1:125:A:LEU:HD22	2	2.37	0.0	2.37
(1,2129)	1:121:A:ASP:H	1:125:A:LEU:HD21	2	2.29	0.05	2.29
(2,57)	1:40:A:GLY:HA2	1:13:A:LEU:HD11	2	1.71	0.24	1.71
(2,57)	1:41:A:VAL:HG12	1:40:A:GLY:HA2	2	1.71	0.24	1.71
(1,927)	1:125:A:LEU:HD22	1:119:A:ARG:H	2	1.65	0.04	1.65
(1,1264)	1:125:A:LEU:HD22	1:126:A:VAL:H	2	1.65	0.05	1.65
(1,1264)	1:125:A:LEU:HD23	1:126:A:VAL:H	2	1.65	0.05	1.65
(2,362)	1:61:A:LEU:HD22	1:61:A:LEU:HA	2	1.31	0.02	1.31
(2,362)	1:61:A:LEU:HD23	1:61:A:LEU:HA	2	1.31	0.02	1.31
(1,2640)	1:125:A:LEU:HD22	1:126:A:VAL:H	2	1.26	0.05	1.26
(1,2640)	1:125:A:LEU:HD23	1:126:A:VAL:H	2	1.26	0.05	1.26
(1,921)	1:125:A:LEU:HD21	1:125:A:LEU:HA	2	1.23	0.01	1.23
(1,229)	1:140:A:TYR:HE1	1:13:A:LEU:HD12	2	1.22	0.11	1.22
(1,229)	1:140:A:TYR:HE1	1:13:A:LEU:HD11	2	1.22	0.11	1.22
(2,1301)	1:13:A:LEU:HD23	1:141:A:LYS:H	2	1.04	0.65	1.04
(2,1301)	1:125:A:LEU:HD13	1:141:A:LYS:H	2	1.04	0.65	1.04
(1,2819)	1:116:A:TYR:HD1	1:118:A:TYR:HH	2	1.0	0.74	1.0
(1,2819)	1:116:A:TYR:HD2	1:118:A:TYR:HH	2	1.0	0.74	1.0
(2,919)	1:125:A:LEU:HD22	1:100:A:LEU:H	2	0.99	0.03	0.99
(2,801)	1:41:A:VAL:HG12	2:1001:A:OLA:H72	2	0.93	0.22	0.93
(2,801)	1:39:A:ALA:HB2	1:41:A:VAL:HG12	2	0.93	0.22	0.93
(1,914)	1:124:A:TYR:HE2	1:141:A:LYS:HB3	2	0.92	0.2	0.92
(1,1172)	1:125:A:LEU:HD21	1:120:A:ARG:HD2	2	0.9	0.09	0.9
(2,1561)	1:66:A:ASP:H	1:65:A:LYS:HD2	2	0.78	0.02	0.78
(2,423)	1:3:A:LEU:HD23	1:74:A:LEU:HD13	2	0.76	0.24	0.76
(1,2520)	1:143:A:GLN:HE22	1:12:A:LYS:HB2	2	0.75	0.27	0.75
(1,1277)	1:127:A:MET:HE3	1:118:A:TYR:HH	2	0.73	0.37	0.73
(1,1216)	1:70:A:LYS:HG2	1:68:A:HIS:HD2	2	0.72	0.27	0.72
(2,1656)	1:19:A:PHE:HZ	2:1001:A:OLA:H172	2	0.72	0.03	0.72
(1,570)	1:66:A:ASP:H	1:65:A:LYS:HD2	2	0.72	0.02	0.72
(2,184)	1:21:A:GLU:HA	1:24:A:LYS:HD3	2	0.7	0.14	0.7
(2,184)	1:24:A:LYS:HD2	1:21:A:GLU:HA	2	0.7	0.14	0.7
(2,1590)	2:1001:A:OLA:H31	1:19:A:PHE:HE1	2	0.69	0.27	0.69
(2,1590)	2:1001:A:OLA:H32	1:116:A:TYR:HD2	2	0.69	0.27	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1608)	1:19:A:PHE:HZ	2:1001:A:OLA:H172	2	0.67	0.03	0.67
(1,1217)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	2	0.64	0.26	0.64
(1,1245)	1:11:A:PHE:H	1:44:A:LYS:HG2	2	0.64	0.17	0.64
(2,1473)	1:6:A:LYS:H	1:6:A:LYS:HE2	2	0.61	0.07	0.61
(2,1473)	1:6:A:LYS:HE3	1:6:A:LYS:H	2	0.61	0.07	0.61
(1,1034)	1:124:A:TYR:HE2	1:141:A:LYS:HB3	2	0.6	0.2	0.6
(1,1955)	1:125:A:LEU:HD22	1:119:A:ARG:H	2	0.6	0.04	0.6
(2,906)	1:41:A:VAL:HG12	1:40:A:GLY:H	2	0.56	0.01	0.56
(2,628)	1:116:A:TYR:HB3	1:127:A:MET:HG3	2	0.56	0.39	0.56
(2,1560)	1:11:A:PHE:H	1:44:A:LYS:HG3	2	0.56	0.26	0.56
(1,754)	1:94:A:LEU:HD11	1:100:A:LEU:HA	2	0.55	0.03	0.55
(1,599)	1:70:A:LYS:HD2	1:70:A:LYS:HE3	2	0.52	0.02	0.52
(1,1517)	1:80:A:ASP:H	1:79:A:GLN:HG3	2	0.48	0.0	0.48
(1,1459)	1:55:A:ARG:H	1:55:A:ARG:HD3	2	0.44	0.1	0.44
(1,97)	1:52:A:LYS:H	1:48:A:ALA:HB3	2	0.44	0.08	0.44
(2,821)	1:14:A:GLU:HB2	1:141:A:LYS:HG3	2	0.43	0.11	0.43
(1,753)	1:94:A:LEU:HD11	1:94:A:LEU:HA	2	0.42	0.04	0.42
(2,1459)	1:10:A:THR:HG22	1:45:A:PHE:H	2	0.41	0.02	0.41
(2,1459)	1:10:A:THR:HG23	1:45:A:PHE:H	2	0.41	0.02	0.41
(1,2325)	1:90:A:ILE:H	1:77:A:GLU:HG2	2	0.4	0.16	0.4
(1,173)	1:56:A:TYR:HD2	1:8:A:LEU:HD21	2	0.38	0.1	0.38
(2,1397)	1:113:A:VAL:HG13	1:112:A:ASP:H	2	0.38	0.09	0.38
(2,1397)	1:112:A:ASP:H	1:105:A:ILE:HG21	2	0.38	0.09	0.38
(2,1555)	1:96:A:ASP:H	1:94:A:LEU:HD21	2	0.37	0.11	0.37
(2,1555)	1:96:A:ASP:H	1:94:A:LEU:HD22	2	0.37	0.11	0.37
(2,665)	1:136:A:THR:HG21	1:19:A:PHE:HE1	2	0.36	0.02	0.36
(1,703)	1:24:A:LYS:HG2	1:21:A:GLU:HA	2	0.34	0.08	0.34
(1,426)	1:37:A:LYS:HG3	1:37:A:LYS:H	2	0.32	0.01	0.32
(2,91)	1:125:A:LEU:HB3	1:125:A:LEU:HD11	2	0.32	0.02	0.32
(2,372)	1:62:A:THR:HG23	1:42:A:THR:H	2	0.32	0.04	0.32
(2,569)	1:108:A:ASP:H	1:107:A:VAL:HG21	2	0.3	0.2	0.3
(2,569)	1:114:A:GLU:H	1:113:A:VAL:HG23	2	0.3	0.2	0.3
(2,224)	1:36:A:ILE:HG13	1:37:A:LYS:H	2	0.3	0.01	0.3
(2,169)	1:15:A:ARG:HD2	1:139:A:TYR:HD1	2	0.29	0.16	0.29
(2,605)	1:14:A:GLU:HB3	1:124:A:TYR:HE2	2	0.28	0.13	0.28
(2,802)	1:62:A:THR:HA	1:41:A:VAL:HG13	2	0.28	0.12	0.28
(2,1564)	2:1001:A:OLA:H81	1:83:A:LEU:HD11	2	0.28	0.14	0.28
(2,1564)	2:1001:A:OLA:H81	1:36:A:ILE:HG21	2	0.28	0.14	0.28
(1,101)	1:49:A:ALA:H	1:48:A:ALA:HB2	2	0.26	0.14	0.26
(1,375)	1:36:A:ILE:HD13	1:32:A:MET:HG3	2	0.26	0.12	0.26
(1,375)	1:36:A:ILE:HD12	1:32:A:MET:HG3	2	0.26	0.12	0.26
(1,1972)	1:21:A:GLU:H	1:21:A:GLU:HG2	2	0.25	0.04	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,752)	1:69:A:HIS:HE1	1:67:A:THR:HG21	2	0.25	0.14	0.25
(2,979)	1:132:A:LYS:HG3	1:131:A:TRP:HE1	2	0.25	0.05	0.25
(2,979)	1:132:A:LYS:HG2	1:131:A:TRP:HE1	2	0.25	0.05	0.25
(2,893)	1:64:A:LYS:HG3	2:1001:A:OLA:H10	2	0.24	0.06	0.24
(2,893)	1:64:A:LYS:HG3	2:1001:A:OLA:H9	2	0.24	0.06	0.24
(1,2040)	1:48:A:ALA:HB2	1:50:A:SER:H	2	0.24	0.08	0.24
(1,2040)	1:48:A:ALA:HB3	1:50:A:SER:H	2	0.24	0.08	0.24
(1,132)	1:72:A:TRP:HZ3	1:3:A:LEU:HD11	2	0.22	0.12	0.22
(1,132)	1:72:A:TRP:HZ3	1:3:A:LEU:HD12	2	0.22	0.12	0.22
(1,2059)	1:143:A:GLN:H	1:142:A:LYS:HG2	2	0.22	0.1	0.22
(2,1520)	1:126:A:VAL:HG21	1:119:A:ARG:H	2	0.22	0.01	0.22
(1,466)	1:44:A:LYS:HE3	1:44:A:LYS:HB3	2	0.21	0.02	0.21
(1,772)	1:118:A:TYR:H	1:99:A:THR:HG21	2	0.21	0.07	0.21
(1,772)	1:118:A:TYR:H	1:99:A:THR:HG22	2	0.21	0.07	0.21
(2,319)	1:61:A:LEU:HD23	1:42:A:THR:HB	2	0.21	0.01	0.21
(2,319)	1:42:A:THR:HB	1:61:A:LEU:HD11	2	0.21	0.01	0.21
(2,917)	1:86:A:THR:H	1:82:A:ALA:HB2	2	0.21	0.02	0.21
(2,917)	1:86:A:THR:H	1:82:A:ALA:HB3	2	0.21	0.02	0.21
(2,1432)	1:34:A:GLN:HE22	1:35:A:VAL:H	2	0.2	0.03	0.2
(2,1432)	1:30:A:TRP:HH2	1:34:A:GLN:HE22	2	0.2	0.03	0.2
(1,2041)	1:52:A:LYS:H	1:48:A:ALA:HB3	2	0.2	0.08	0.2
(2,660)	1:128:A:LYS:HE3	1:135:A:SER:HB3	2	0.2	0.07	0.2
(2,660)	1:135:A:SER:HB3	1:128:A:LYS:HE2	2	0.2	0.07	0.2
(1,2590)	1:6:A:LYS:HG2	1:7:A:PHE:H	2	0.2	0.05	0.2
(2,395)	1:85:A:SER:HA	1:65:A:LYS:HE3	2	0.2	0.02	0.2
(1,2497)	1:78:A:PHE:H	1:77:A:GLU:HG2	2	0.19	0.06	0.19
(2,1017)	1:8:A:LEU:HD12	1:9:A:GLY:H	2	0.18	0.06	0.18
(2,1017)	1:8:A:LEU:HD11	1:9:A:GLY:H	2	0.18	0.06	0.18
(1,932)	1:137:A:SER:HA	1:126:A:VAL:HG13	2	0.18	0.06	0.18
(1,932)	1:137:A:SER:HA	1:126:A:VAL:HG11	2	0.18	0.06	0.18
(1,2132)	1:69:A:HIS:H	1:68:A:HIS:HD2	2	0.18	0.06	0.18
(2,219)	1:23:A:LEU:HD22	1:36:A:ILE:HB	2	0.18	0.08	0.18
(2,219)	1:23:A:LEU:HD23	1:36:A:ILE:HB	2	0.18	0.08	0.18
(2,1222)	1:118:A:TYR:HD1	1:119:A:ARG:H	2	0.18	0.06	0.18
(2,1617)	1:36:A:ILE:HA	2:1001:A:OLA:H71	2	0.18	0.06	0.18
(2,839)	1:129:A:MET:HE2	1:19:A:PHE:HE1	2	0.16	0.02	0.16
(2,1674)	1:120:A:ARG:HB2	1:120:A:ARG:HG3	2	0.16	0.05	0.16
(2,1674)	1:129:A:MET:HE2	2:1001:A:OLA:H181	2	0.16	0.05	0.16
(1,2300)	1:90:A:ILE:HD11	1:90:A:ILE:H	2	0.16	0.04	0.16
(1,2300)	1:90:A:ILE:HD13	1:90:A:ILE:H	2	0.16	0.04	0.16
(2,611)	1:125:A:LEU:HD22	1:7:A:PHE:HD1	2	0.15	0.03	0.15
(2,611)	1:125:A:LEU:HD22	1:118:A:TYR:HD1	2	0.15	0.03	0.15

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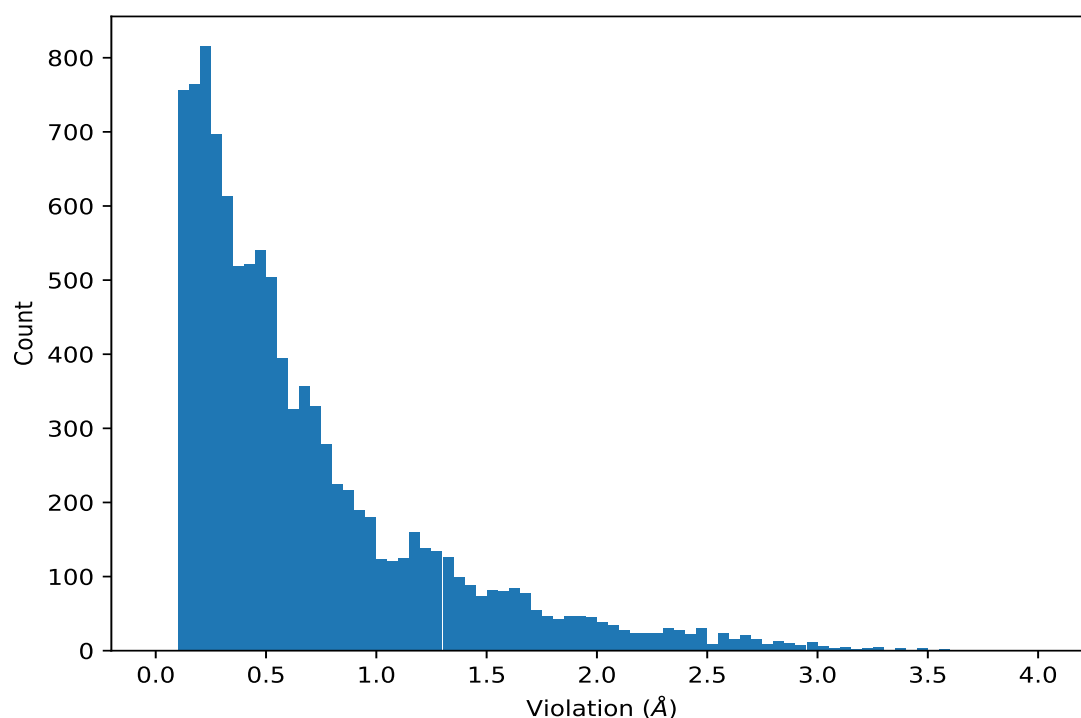
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1675)	2:1001:A:OLA:H172	2:1001:A:OLA:H183	2	0.15	0.02	0.15
(2,1675)	1:94:A:LEU:HB3	1:94:A:LEU:HD21	2	0.15	0.02	0.15
(1,82)	1:96:A:ASP:HB3	1:97:A:PRO:HD3	2	0.14	0.03	0.14
(1,2403)	1:98:A:ASN:HB3	1:98:A:ASN:H	2	0.14	0.03	0.14
(2,792)	1:131:A:TRP:HB2	1:131:A:TRP:HZ3	2	0.14	0.0	0.14
(2,1221)	1:89:A:LYS:HB3	1:78:A:PHE:H	2	0.14	0.0	0.14
(2,1259)	1:120:A:ARG:H	1:7:A:PHE:HD1	2	0.14	0.02	0.14
(2,1634)	1:22:A:TYR:HD1	2:1001:A:OLA:H183	2	0.14	0.03	0.14
(2,1634)	1:22:A:TYR:HD1	2:1001:A:OLA:H181	2	0.14	0.03	0.14
(3,23)	1:114:A:GLU:H	1:104:A:HIS:O	2	0.14	0.0	0.14
(2,1456)	1:95:A:LYS:HB2	1:93:A:ASP:H	2	0.14	0.01	0.14
(1,2766)	1:111:A:THR:HG23	1:112:A:ASP:H	2	0.13	0.01	0.13
(1,2766)	1:111:A:THR:HG21	1:112:A:ASP:H	2	0.13	0.01	0.13
(1,1483)	1:14:A:GLU:HA	1:14:A:GLU:HG2	2	0.12	0.02	0.12
(2,701)	1:143:A:GLN:HG3	1:11:A:PHE:HA	2	0.12	0.01	0.12
(2,1031)	1:109:A:ASP:H	1:110:A:PRO:HB3	2	0.12	0.02	0.12
(1,398)	1:35:A:VAL:HA	1:35:A:VAL:HG12	2	0.12	0.0	0.12
(1,597)	1:70:A:LYS:HD2	1:70:A:LYS:HE3	2	0.12	0.01	0.12
(1,993)	1:135:A:SER:H	1:135:A:SER:HB2	2	0.12	0.01	0.12
(2,1162)	1:67:A:THR:HG23	1:85:A:SER:H	2	0.12	0.01	0.12
(2,1162)	1:86:A:THR:HG22	1:85:A:SER:H	2	0.12	0.01	0.12
(2,203)	1:23:A:LEU:HD13	1:19:A:PHE:HE2	2	0.12	0.02	0.12
(2,203)	1:23:A:LEU:HD12	1:19:A:PHE:HE2	2	0.12	0.02	0.12
(1,1688)	1:143:A:GLN:HA	1:143:A:GLN:HE22	2	0.11	0.0	0.11
(2,1419)	1:42:A:THR:HG23	1:43:A:LYS:H	2	0.11	0.01	0.11
(2,1419)	1:42:A:THR:HG22	1:43:A:LYS:H	2	0.11	0.01	0.11

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)
(2,274)	1:61:A:LEU:HD23	1:66:A:ASP:HB3	4	4.02
(2,274)	1:83:A:LEU:HD23	1:66:A:ASP:HB3	19	3.76
(1,756)	1:94:A:LEU:HD11	1:3:A:LEU:HD13	15	3.7
(1,636)	1:61:A:LEU:HD23	1:66:A:ASP:HB2	20	3.6
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD12	12	3.58
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD13	6	3.56
(1,636)	1:61:A:LEU:HD23	1:66:A:ASP:HB2	4	3.5
(1,636)	1:61:A:LEU:HD21	1:66:A:ASP:HB2	19	3.48
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD13	9	3.47
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	5	3.46
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG13	12	3.41
(2,88)	1:3:A:LEU:HD23	1:45:A:PHE:HA	1	3.37
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD13	6	3.37
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG11	11	3.35
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD11	4	3.31
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD12	15	3.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	8	3.27
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD12	12	3.27
(1,636)	1:61:A:LEU:HD22	1:66:A:ASP:HB2	1	3.27
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD11	2	3.27
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	19	3.23
(2,89)	1:3:A:LEU:HD22	1:9:A:GLY:H	1	3.22
(1,430)	1:23:A:LEU:HD22	1:37:A:LYS:HG2	15	3.22
(2,463)	1:90:A:ILE:HG13	1:87:A:GLN:HB3	1	3.2
(1,2818)	1:83:A:LEU:HD22	1:62:A:THR:HG1	2	3.19
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	12	3.19
(2,465)	1:87:A:GLN:HG2	1:107:A:VAL:HG13	1	3.13
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD12	17	3.13
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	8	3.13
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	7	3.12
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD13	5	3.1
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD13	15	3.09
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	1	3.08
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	19	3.08
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	5	3.08
(1,2799)	1:83:A:LEU:HD22	1:62:A:THR:HG1	2	3.04
(2,89)	1:125:A:LEU:HD13	1:139:A:TYR:H	13	3.03
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	5	3.03
(1,2818)	1:83:A:LEU:HD22	1:62:A:THR:HG1	12	3.02
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	19	3.01
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	15	3.0
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG13	9	2.99
(2,615)	1:125:A:LEU:HD21	1:120:A:ARG:HA	5	2.98
(2,465)	1:87:A:GLN:HG2	1:107:A:VAL:HG11	2	2.97
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	8	2.97
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	1	2.97
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	7	2.97
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	19	2.97
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD21	16	2.96
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB3	13	2.96
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	5	2.96
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	6	2.95
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB3	6	2.93
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	1	2.93
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	11	2.93
(2,308)	1:35:A:VAL:HA	1:38:A:LEU:HD12	17	2.92
(1,756)	1:94:A:LEU:HD11	1:3:A:LEU:HD11	1	2.91
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD12	12	2.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,66)	1:12:A:LYS:HG3	1:141:A:LYS:HG3	2	2.9
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD13	1	2.89
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	20	2.89
(2,615)	1:125:A:LEU:HD21	1:120:A:ARG:HA	1	2.88
(2,72)	1:3:A:LEU:HD12	1:58:A:MET:HG2	20	2.87
(1,2799)	1:83:A:LEU:HD22	1:62:A:THR:HG1	12	2.87
(1,636)	1:61:A:LEU:HD22	1:66:A:ASP:HB2	2	2.87
(1,756)	1:94:A:LEU:HD11	1:3:A:LEU:HD11	4	2.86
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG11	10	2.85
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	4	2.85
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	9	2.85
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	9	2.84
(1,2818)	1:83:A:LEU:HD22	1:62:A:THR:HG1	17	2.84
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	1	2.84
(2,89)	1:3:A:LEU:HD21	1:46:A:ARG:H	3	2.83
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H131	5	2.82
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD23	8	2.82
(2,88)	1:3:A:LEU:HD21	1:45:A:PHE:HA	5	2.82
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD11	19	2.82
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD11	14	2.82
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	2	2.81
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD13	9	2.81
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	5	2.81
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD13	18	2.8
(2,89)	1:125:A:LEU:HD11	1:139:A:TYR:H	11	2.78
(1,2818)	1:83:A:LEU:HD23	1:62:A:THR:HG1	13	2.78
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	1	2.78
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG21	6	2.77
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	14	2.77
(2,403)	1:66:A:ASP:HA	1:61:A:LEU:HD22	1	2.75
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD13	9	2.75
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	16	2.75
(1,70)	1:97:A:PRO:HA	1:94:A:LEU:HD13	17	2.75
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG21	1	2.74
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H161	8	2.73
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG23	12	2.73
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD11	16	2.73
(1,429)	1:23:A:LEU:HD22	1:37:A:LYS:HG3	3	2.73
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	12	2.72
(2,89)	1:125:A:LEU:HD12	1:139:A:TYR:H	2	2.72
(1,2818)	1:83:A:LEU:HD23	1:62:A:THR:HG1	14	2.72
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	10	2.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H131	11	2.71
(2,89)	1:125:A:LEU:HD13	1:139:A:TYR:H	20	2.71
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	19	2.71
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	20	2.71
(2,567)	1:88:A:HIS:HB3	1:107:A:VAL:HG13	20	2.7
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG22	10	2.7
(1,675)	1:101:A:THR:H	1:94:A:LEU:HD21	10	2.7
(2,547)	1:100:A:LEU:HD13	1:117:A:GLU:HA	7	2.69
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG22	2	2.69
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	10	2.69
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	6	2.69
(1,2799)	1:83:A:LEU:HD22	1:62:A:THR:HG1	17	2.69
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	6	2.68
(2,89)	1:125:A:LEU:HD11	1:9:A:GLY:H	5	2.68
(2,89)	1:125:A:LEU:HD12	1:139:A:TYR:H	12	2.68
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	1	2.68
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD11	3	2.68
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD11	8	2.68
(2,567)	1:88:A:HIS:HB3	1:107:A:VAL:HG13	17	2.67
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG22	17	2.67
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD23	5	2.67
(1,675)	1:101:A:THR:H	1:94:A:LEU:HD23	17	2.67
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	16	2.67
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD23	1	2.66
(2,89)	1:3:A:LEU:HD21	1:46:A:ARG:H	18	2.66
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H161	19	2.65
(1,2326)	1:74:A:LEU:HD12	1:2:A:THR:H	5	2.65
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	20	2.65
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG23	11	2.64
(2,89)	1:125:A:LEU:HD12	1:139:A:TYR:H	7	2.64
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	17	2.64
(2,89)	1:3:A:LEU:HD23	1:46:A:ARG:H	19	2.63
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD11	4	2.63
(1,2799)	1:83:A:LEU:HD23	1:62:A:THR:HG1	13	2.63
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	3	2.63
(2,489)	1:58:A:MET:HE1	1:90:A:ILE:HG22	8	2.62
(2,89)	1:125:A:LEU:HD12	1:139:A:TYR:H	9	2.62
(1,2818)	1:83:A:LEU:HD22	1:62:A:THR:HG1	9	2.62
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG22	19	2.61
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	10	2.61
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	2	2.6
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD12	13	2.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	2	2.6
(2,493)	1:90:A:ILE:HD11	1:114:A:GLU:HB3	13	2.59
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	7	2.59
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	2	2.59
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	3	2.59
(2,1649)	1:23:A:LEU:HD12	2:1001:A:OLA:H161	16	2.58
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H131	18	2.58
(2,547)	1:100:A:LEU:HD11	1:94:A:LEU:HA	17	2.58
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	17	2.58
(2,89)	1:3:A:LEU:HD22	1:46:A:ARG:H	10	2.58
(1,2799)	1:83:A:LEU:HD23	1:62:A:THR:HG1	14	2.58
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD22	10	2.58
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	9	2.58
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	14	2.58
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H131	2	2.57
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H161	4	2.57
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H161	12	2.57
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	5	2.57
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	5	2.57
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD12	16	2.57
(1,2818)	1:83:A:LEU:HD23	1:62:A:THR:HG1	18	2.57
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB1	17	2.56
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	1	2.56
(1,756)	1:94:A:LEU:HD11	1:3:A:LEU:HD13	18	2.55
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB1	18	2.54
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	6	2.54
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG23	7	2.53
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	16	2.53
(2,1376)	1:59:A:GLU:H	1:83:A:LEU:HD11	19	2.52
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	8	2.52
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	1	2.52
(2,89)	1:125:A:LEU:HD12	1:139:A:TYR:H	16	2.5
(1,429)	1:23:A:LEU:HD22	1:37:A:LYS:HG3	19	2.5
(2,465)	1:87:A:GLN:HG2	1:107:A:VAL:HG13	18	2.49
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	15	2.49
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	15	2.49
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD11	2	2.49
(2,1649)	1:23:A:LEU:HD12	2:1001:A:OLA:H131	14	2.48
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD22	1	2.48
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD12	2	2.48
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD11	1	2.48
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	7	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,793)	1:100:A:LEU:HD13	1:118:A:TYR:HB3	13	2.48
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD22	3	2.47
(2,734)	1:58:A:MET:HE1	1:100:A:LEU:HD21	8	2.47
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD22	18	2.47
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD12	20	2.47
(1,2799)	1:83:A:LEU:HD22	1:62:A:THR:HG1	9	2.47
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	12	2.47
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	12	2.47
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	5	2.46
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	8	2.46
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	14	2.46
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	19	2.46
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	11	2.46
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	13	2.46
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	15	2.46
(1,128)	1:100:A:LEU:HD23	1:3:A:LEU:HD12	17	2.46
(2,81)	1:3:A:LEU:HD22	1:45:A:PHE:HB2	9	2.45
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	20	2.45
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD13	13	2.45
(1,675)	1:101:A:THR:H	1:94:A:LEU:HD23	7	2.45
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	9	2.45
(1,128)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	14	2.45
(2,81)	1:3:A:LEU:HD23	1:2:A:THR:HB	2	2.44
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD21	12	2.44
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD22	14	2.44
(2,1376)	1:59:A:GLU:H	1:83:A:LEU:HD13	4	2.43
(2,493)	1:90:A:ILE:HD11	1:81:A:GLU:HB3	4	2.43
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD22	9	2.43
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	18	2.43
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD11	14	2.43
(1,70)	1:97:A:PRO:HA	1:94:A:LEU:HD12	10	2.43
(2,618)	1:125:A:LEU:HD22	1:100:A:LEU:H	1	2.42
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB2	8	2.42
(1,2799)	1:83:A:LEU:HD23	1:62:A:THR:HG1	18	2.42
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	6	2.42
(1,793)	1:100:A:LEU:HD13	1:118:A:TYR:HB3	1	2.42
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD11	5	2.42
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	1	2.42
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	14	2.41
(2,1649)	1:23:A:LEU:HD13	2:1001:A:OLA:H131	1	2.4
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD13	16	2.4
(1,2818)	1:83:A:LEU:HD23	1:62:A:THR:HG1	10	2.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	7	2.4
(1,793)	1:100:A:LEU:HD12	1:118:A:TYR:HB3	6	2.4
(2,540)	1:7:A:PHE:HA	1:100:A:LEU:HD23	14	2.39
(2,89)	1:3:A:LEU:HD21	1:46:A:ARG:H	6	2.39
(2,89)	1:125:A:LEU:HD11	1:139:A:TYR:H	15	2.39
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD12	20	2.39
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD13	9	2.39
(1,1925)	1:107:A:VAL:HG21	1:79:A:GLN:HE22	12	2.39
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD22	12	2.39
(2,567)	1:88:A:HIS:HB3	1:107:A:VAL:HG13	16	2.38
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG23	14	2.38
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD13	11	2.38
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	10	2.38
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	11	2.38
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	11	2.37
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	9	2.37
(2,79)	1:3:A:LEU:HD12	1:55:A:ARG:HA	6	2.37
(1,2768)	1:120:A:ARG:H	1:125:A:LEU:HD22	1	2.37
(1,2768)	1:120:A:ARG:H	1:125:A:LEU:HD22	5	2.37
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	4	2.37
(1,793)	1:100:A:LEU:HD13	1:118:A:TYR:HB3	9	2.37
(2,618)	1:125:A:LEU:HD22	1:100:A:LEU:H	5	2.36
(2,81)	1:3:A:LEU:HD22	1:2:A:THR:HB	11	2.36
(2,72)	1:3:A:LEU:HD12	1:58:A:MET:HG2	12	2.36
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD12	12	2.36
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG22	20	2.35
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	15	2.35
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD11	19	2.35
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	11	2.35
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	5	2.35
(2,1376)	1:59:A:GLU:H	1:83:A:LEU:HD22	2	2.34
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	3	2.34
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	5	2.34
(2,72)	1:3:A:LEU:HD11	1:58:A:MET:HG2	10	2.34
(1,2129)	1:121:A:ASP:H	1:125:A:LEU:HD21	5	2.34
(1,789)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	14	2.34
(1,789)	1:100:A:LEU:HD23	1:3:A:LEU:HD12	17	2.34
(2,1376)	1:59:A:GLU:H	1:83:A:LEU:HD11	20	2.33
(2,403)	1:66:A:ASP:HA	1:61:A:LEU:HD22	2	2.33
(2,403)	1:66:A:ASP:HA	1:83:A:LEU:HD21	4	2.33
(2,81)	1:125:A:LEU:HD12	1:45:A:PHE:HB2	10	2.33
(2,81)	1:3:A:LEU:HD22	1:45:A:PHE:HB2	19	2.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	7	2.33
(1,793)	1:100:A:LEU:HD13	1:118:A:TYR:HB3	4	2.33
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG12	8	2.32
(2,493)	1:90:A:ILE:HD13	1:81:A:GLU:HB3	15	2.32
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD13	6	2.32
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	11	2.32
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	3	2.32
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD23	15	2.31
(2,493)	1:90:A:ILE:HD11	1:79:A:GLN:HB3	12	2.31
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	2	2.31
(2,89)	1:3:A:LEU:HD23	1:46:A:ARG:H	8	2.31
(2,553)	1:132:A:LYS:HE2	1:134:A:VAL:HG23	8	2.3
(2,547)	1:100:A:LEU:HD12	1:94:A:LEU:HA	8	2.3
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD13	7	2.3
(2,81)	1:3:A:LEU:HD22	1:45:A:PHE:HB2	1	2.3
(2,81)	1:125:A:LEU:HD13	1:13:A:LEU:HA	16	2.3
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	2	2.3
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	18	2.3
(2,493)	1:90:A:ILE:HD11	1:79:A:GLN:HG3	9	2.29
(2,419)	1:74:A:LEU:HD11	1:56:A:TYR:HD1	2	2.29
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD21	7	2.28
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD22	17	2.28
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB3	15	2.28
(2,81)	1:125:A:LEU:HD13	1:13:A:LEU:HA	13	2.28
(2,79)	1:3:A:LEU:HD12	1:55:A:ARG:HA	15	2.28
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	3	2.27
(2,493)	1:90:A:ILE:HD12	1:79:A:GLN:HB3	10	2.27
(2,72)	1:3:A:LEU:HD13	1:58:A:MET:HG2	18	2.27
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	1	2.27
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	15	2.27
(2,1649)	1:23:A:LEU:HD12	2:1001:A:OLA:H161	9	2.26
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD11	5	2.26
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG22	3	2.25
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG22	19	2.25
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	12	2.25
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	18	2.25
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD22	10	2.25
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD13	11	2.25
(1,2799)	1:83:A:LEU:HD23	1:62:A:THR:HG1	10	2.25
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	13	2.25
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	19	2.25
(2,567)	1:88:A:HIS:HB2	1:107:A:VAL:HG11	1	2.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG23	1	2.24
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	15	2.24
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	1	2.24
(2,72)	1:3:A:LEU:HD11	1:58:A:MET:HG2	2	2.24
(1,2129)	1:121:A:ASP:H	1:125:A:LEU:HD21	1	2.24
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	7	2.24
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	6	2.23
(2,308)	1:35:A:VAL:HA	1:38:A:LEU:HD13	5	2.23
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	8	2.22
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	16	2.22
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	6	2.22
(2,734)	1:58:A:MET:HE1	1:100:A:LEU:HD22	20	2.21
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG21	17	2.21
(2,489)	1:58:A:MET:HE1	1:90:A:ILE:HG21	3	2.21
(2,274)	1:61:A:LEU:HD22	1:66:A:ASP:HB3	1	2.21
(2,72)	1:3:A:LEU:HD11	1:58:A:MET:HG2	19	2.21
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD13	5	2.21
(1,70)	1:97:A:PRO:HA	1:94:A:LEU:HD11	7	2.21
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	11	2.2
(2,820)	1:41:A:VAL:HG21	1:43:A:LYS:HE2	14	2.2
(2,81)	1:125:A:LEU:HD11	1:13:A:LEU:HA	3	2.2
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	2	2.2
(2,278)	1:35:A:VAL:HG23	2:1001:A:OLA:H10	6	2.19
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	11	2.19
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD13	13	2.19
(2,72)	1:3:A:LEU:HD11	1:58:A:MET:HG2	8	2.19
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	2	2.18
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD12	12	2.18
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD11	16	2.18
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD12	20	2.18
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	2	2.17
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	4	2.16
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD11	3	2.16
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD13	12	2.16
(2,81)	1:125:A:LEU:HD11	1:13:A:LEU:HA	20	2.16
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD13	18	2.16
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD22	3	2.16
(2,493)	1:90:A:ILE:HD13	1:79:A:GLN:HG3	3	2.15
(2,403)	1:66:A:ASP:HA	1:83:A:LEU:HD21	19	2.15
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	18	2.15
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD11	7	2.15
(2,81)	1:3:A:LEU:HD23	1:45:A:PHE:HB2	8	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD12	12	2.15
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	3	2.15
(1,128)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	16	2.15
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG11	6	2.14
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG11	16	2.14
(2,810)	1:52:A:LYS:HE2	1:53:A:PRO:HD3	9	2.14
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD23	10	2.14
(2,553)	1:131:A:TRP:HB2	1:134:A:VAL:HG22	6	2.14
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD13	11	2.14
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	17	2.14
(2,734)	1:58:A:MET:HE1	1:100:A:LEU:HD21	12	2.13
(2,547)	1:100:A:LEU:HD11	1:94:A:LEU:HA	10	2.13
(2,274)	1:61:A:LEU:HD22	1:66:A:ASP:HB3	2	2.13
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	18	2.13
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	3	2.13
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD21	18	2.12
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	6	2.12
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	2	2.12
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	4	2.12
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	9	2.12
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB1	7	2.11
(2,426)	1:15:A:ARG:HB3	1:13:A:LEU:HD21	9	2.11
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	4	2.11
(1,2810)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	12	2.11
(1,797)	1:100:A:LEU:HD11	1:93:A:ASP:H	19	2.11
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	7	2.1
(2,493)	1:90:A:ILE:HD13	1:79:A:GLN:HG3	18	2.1
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD11	10	2.1
(1,1925)	1:107:A:VAL:HG23	1:79:A:GLN:HE22	10	2.1
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	20	2.1
(2,493)	1:90:A:ILE:HD11	1:114:A:GLU:HB3	14	2.09
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD23	8	2.09
(2,81)	1:3:A:LEU:HD22	1:45:A:PHE:HB2	12	2.09
(2,78)	1:94:A:LEU:HA	1:3:A:LEU:HD11	4	2.09
(1,796)	1:100:A:LEU:HD12	1:101:A:THR:H	11	2.09
(1,630)	1:74:A:LEU:HD13	1:3:A:LEU:H	2	2.09
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	17	2.09
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	18	2.08
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB2	3	2.08
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB1	20	2.08
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	3	2.08
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	4	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2810)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	10	2.08
(1,796)	1:100:A:LEU:HD12	1:101:A:THR:H	2	2.08
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD21	16	2.08
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	6	2.07
(1,2810)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	19	2.07
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	1	2.07
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	7	2.07
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	9	2.07
(1,284)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	8	2.07
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	8	2.07
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	17	2.07
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	6	2.06
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD21	17	2.06
(2,391)	1:35:A:VAL:HG21	1:64:A:LYS:HD2	11	2.06
(2,81)	1:125:A:LEU:HD13	1:13:A:LEU:HA	7	2.06
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	11	2.06
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	5	2.06
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	11	2.05
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	2	2.05
(1,2810)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	1	2.05
(1,2077)	1:23:A:LEU:HD13	1:26:A:ARG:H	12	2.05
(1,430)	1:23:A:LEU:HD22	1:37:A:LYS:HG2	12	2.05
(1,2829)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	12	2.04
(1,789)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	16	2.04
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	13	2.04
(1,217)	1:14:A:GLU:H	1:13:A:LEU:HD21	9	2.04
(2,1441)	1:35:A:VAL:HG23	1:34:A:GLN:HE22	14	2.03
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD23	5	2.03
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	20	2.03
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	20	2.03
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD13	15	2.03
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	7	2.03
(2,547)	1:100:A:LEU:HD13	1:94:A:LEU:HA	19	2.02
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	1	2.02
(2,89)	1:125:A:LEU:HD11	1:9:A:GLY:H	4	2.02
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD13	18	2.02
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	17	2.02
(1,1240)	1:125:A:LEU:HD21	1:120:A:ARG:HD2	1	2.02
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	20	2.02
(2,1441)	1:35:A:VAL:HG22	1:34:A:GLN:HE22	2	2.01
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	2	2.01
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG13	14	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	15	2.01
(2,81)	1:3:A:LEU:HD21	1:45:A:PHE:HB2	15	2.01
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD11	7	2.01
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	4	2.01
(1,2829)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	10	2.01
(1,2810)	2:1001:A:OLA:H181	1:23:A:LEU:HD12	9	2.01
(1,2810)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	15	2.01
(1,2797)	1:116:A:TYR:HD1	1:118:A:TYR:HH	2	2.01
(1,796)	1:100:A:LEU:HD13	1:101:A:THR:H	16	2.01
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	13	2.01
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H182	17	2.0
(2,493)	1:90:A:ILE:HD12	1:79:A:GLN:HG3	11	2.0
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB2	5	2.0
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	6	2.0
(1,2829)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	19	2.0
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	8	2.0
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	16	2.0
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD13	2	2.0
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG23	15	1.99
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD22	16	1.99
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	11	1.99
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	15	1.99
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD13	2	1.99
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	18	1.99
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	20	1.99
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	10	1.99
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	20	1.99
(2,825)	1:118:A:TYR:HD2	1:127:A:MET:HG2	16	1.98
(2,810)	1:52:A:LYS:HE3	1:53:A:PRO:HD3	4	1.98
(2,547)	1:100:A:LEU:HD12	1:94:A:LEU:HA	3	1.98
(2,493)	1:90:A:ILE:HD11	1:79:A:GLN:HG3	6	1.98
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG12	3	1.98
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	19	1.98
(1,2829)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	1	1.98
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	20	1.98
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	10	1.98
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	4	1.98
(1,796)	1:100:A:LEU:HD11	1:101:A:THR:H	18	1.98
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	19	1.97
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	4	1.97
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	12	1.97
(1,1088)	1:61:A:LEU:HD23	1:62:A:THR:H	1	1.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	8	1.97
(1,217)	1:14:A:GLU:H	1:13:A:LEU:HD21	1	1.97
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	9	1.96
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD11	2	1.96
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	7	1.96
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	15	1.96
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	5	1.96
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	14	1.96
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	1	1.96
(2,810)	1:52:A:LYS:HE3	1:53:A:PRO:HD3	5	1.95
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HB2	14	1.95
(2,489)	1:90:A:ILE:HG23	1:58:A:MET:HG2	5	1.95
(2,391)	1:35:A:VAL:HG22	1:64:A:LYS:HD2	20	1.95
(2,57)	1:41:A:VAL:HG12	1:40:A:GLY:HA2	12	1.95
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG11	3	1.95
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	15	1.95
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	8	1.95
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	19	1.95
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	20	1.95
(1,1088)	1:61:A:LEU:HD22	1:62:A:THR:H	19	1.95
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	7	1.95
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HD22	1	1.94
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	19	1.94
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB2	4	1.94
(2,93)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	17	1.94
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD11	20	1.94
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD11	5	1.94
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	10	1.94
(1,2829)	2:1001:A:OLA:H181	1:23:A:LEU:HD12	9	1.94
(1,2829)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	15	1.94
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	18	1.94
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	9	1.94
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	19	1.94
(2,278)	1:35:A:VAL:HG23	2:1001:A:OLA:H10	19	1.93
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD12	20	1.93
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	8	1.93
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	16	1.93
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	10	1.93
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	18	1.93
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	16	1.93
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD22	10	1.92
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD21	9	1.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD13	13	1.92
(1,2810)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	5	1.92
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	5	1.92
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	12	1.92
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	14	1.92
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	6	1.92
(1,755)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	7	1.92
(1,128)	1:100:A:LEU:HD23	1:3:A:LEU:HD11	3	1.92
(2,624)	1:127:A:MET:HB3	1:126:A:VAL:HG11	9	1.91
(2,89)	1:125:A:LEU:HD12	1:9:A:GLY:H	14	1.91
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD12	17	1.91
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	20	1.91
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG11	11	1.91
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	12	1.91
(1,755)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	10	1.91
(1,386)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	10	1.91
(2,528)	1:143:A:GLN:HA	1:141:A:LYS:HE3	13	1.9
(2,391)	1:35:A:VAL:HG23	1:64:A:LYS:HD2	13	1.9
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	11	1.9
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	6	1.9
(1,2077)	1:23:A:LEU:HD12	1:26:A:ARG:H	6	1.9
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	7	1.9
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	20	1.9
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	7	1.9
(1,796)	1:100:A:LEU:HD12	1:101:A:THR:H	19	1.9
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	12	1.89
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG12	14	1.89
(2,493)	1:90:A:ILE:HD11	1:79:A:GLN:HB3	16	1.89
(2,82)	1:125:A:LEU:HD12	1:120:A:ARG:HD3	12	1.89
(2,75)	1:118:A:TYR:HB3	1:3:A:LEU:HD12	17	1.89
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	8	1.89
(1,796)	1:100:A:LEU:HD12	1:101:A:THR:H	14	1.89
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	8	1.89
(1,430)	1:23:A:LEU:HD22	1:37:A:LYS:HG2	3	1.89
(2,810)	1:52:A:LYS:HE3	1:53:A:PRO:HD3	8	1.88
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG12	4	1.88
(1,2810)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	13	1.88
(1,2810)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	14	1.88
(1,2810)	2:1001:A:OLA:H181	1:23:A:LEU:HD11	17	1.88
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD11	11	1.88
(2,419)	1:74:A:LEU:HD11	1:56:A:TYR:HD1	12	1.87
(2,391)	1:35:A:VAL:HG21	1:64:A:LYS:HD2	15	1.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	12	1.87
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	18	1.87
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	16	1.87
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	13	1.87
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	10	1.87
(1,797)	1:100:A:LEU:HD11	1:93:A:ASP:H	10	1.87
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	14	1.87
(1,386)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	19	1.87
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	2	1.87
(1,290)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	10	1.87
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	5	1.87
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD22	16	1.87
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD22	11	1.86
(2,82)	1:125:A:LEU:HD13	1:120:A:ARG:HD3	20	1.86
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	18	1.86
(1,2829)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	5	1.86
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	4	1.86
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	18	1.86
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	14	1.86
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	19	1.86
(2,1441)	1:34:A:GLN:HE22	1:38:A:LEU:HD23	19	1.85
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG23	12	1.85
(2,493)	1:90:A:ILE:HD13	1:79:A:GLN:HG3	19	1.85
(2,461)	1:86:A:THR:HG23	1:84:A:ASP:HB3	1	1.85
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD21	3	1.85
(2,85)	1:11:A:PHE:HD2	1:125:A:LEU:HD11	5	1.85
(2,79)	1:3:A:LEU:HD12	1:55:A:ARG:HA	9	1.85
(1,1240)	1:125:A:LEU:HD21	1:120:A:ARG:HD2	5	1.85
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD13	12	1.85
(2,825)	1:118:A:TYR:HD1	1:127:A:MET:HG2	4	1.84
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	15	1.84
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD21	12	1.84
(2,391)	1:35:A:VAL:HG22	1:64:A:LYS:HD2	3	1.84
(1,1088)	1:61:A:LEU:HD23	1:62:A:THR:H	2	1.84
(1,924)	1:125:A:LEU:HD22	1:140:A:TYR:HB3	8	1.84
(1,755)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	17	1.84
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	10	1.84
(2,493)	1:90:A:ILE:HD13	1:79:A:GLN:HG3	2	1.83
(2,489)	1:90:A:ILE:HG23	1:58:A:MET:HG2	20	1.83
(2,278)	1:35:A:VAL:HG21	2:1001:A:OLA:H10	8	1.83
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	2	1.83
(1,2077)	1:23:A:LEU:HD13	1:26:A:ARG:H	9	1.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	1	1.83
(1,290)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	19	1.83
(2,391)	1:35:A:VAL:HG21	1:64:A:LYS:HD2	1	1.82
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	4	1.82
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG13	4	1.82
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	8	1.82
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	1	1.82
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD22	19	1.82
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	18	1.82
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	15	1.81
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD23	1	1.81
(2,278)	1:35:A:VAL:HG21	2:1001:A:OLA:H10	5	1.81
(1,2829)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	13	1.81
(1,2829)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	14	1.81
(1,2829)	2:1001:A:OLA:H181	1:23:A:LEU:HD11	17	1.81
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	18	1.81
(1,2063)	1:100:A:LEU:HD12	1:101:A:THR:H	11	1.81
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	5	1.81
(1,796)	1:100:A:LEU:HD11	1:101:A:THR:H	12	1.81
(1,386)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	15	1.81
(2,1646)	1:36:A:ILE:HD13	1:33:A:ARG:HG3	19	1.8
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	8	1.8
(1,2077)	1:23:A:LEU:HD11	1:26:A:ARG:H	8	1.8
(1,2063)	1:100:A:LEU:HD12	1:101:A:THR:H	2	1.8
(1,1963)	1:100:A:LEU:HD11	1:93:A:ASP:H	19	1.8
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	2	1.8
(1,789)	1:100:A:LEU:HD23	1:3:A:LEU:HD11	3	1.8
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	3	1.8
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	16	1.8
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD12	12	1.8
(2,810)	1:52:A:LYS:HE3	1:53:A:PRO:HD3	7	1.79
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD21	18	1.79
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	2	1.79
(2,493)	1:90:A:ILE:HD12	1:79:A:GLN:HG3	20	1.79
(2,66)	1:1:A:LYS:HG2	1:74:A:LEU:HD22	19	1.79
(1,2077)	1:23:A:LEU:HD13	1:26:A:ARG:H	1	1.79
(1,2077)	1:23:A:LEU:HD12	1:26:A:ARG:H	3	1.79
(1,2077)	1:23:A:LEU:HD13	1:26:A:ARG:H	11	1.79
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	9	1.79
(1,217)	1:14:A:GLU:H	1:13:A:LEU:HD21	12	1.79
(1,128)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	5	1.79
(2,553)	1:132:A:LYS:HE2	1:134:A:VAL:HG23	5	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD23	13	1.78
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD23	5	1.78
(1,630)	1:74:A:LEU:HD12	1:3:A:LEU:H	5	1.78
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	8	1.78
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	3	1.78
(2,1589)	1:32:A:MET:HB3	2:1001:A:OLA:H183	5	1.77
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	2	1.77
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD23	6	1.77
(2,81)	1:3:A:LEU:HD23	1:45:A:PHE:HB2	6	1.77
(2,81)	1:3:A:LEU:HD21	1:45:A:PHE:HB2	18	1.77
(1,2077)	1:23:A:LEU:HD13	1:26:A:ARG:H	16	1.77
(1,797)	1:100:A:LEU:HD11	1:93:A:ASP:H	17	1.77
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD21	7	1.77
(1,290)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	15	1.77
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	16	1.77
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	13	1.76
(1,2077)	1:23:A:LEU:HD12	1:26:A:ARG:H	17	1.76
(1,796)	1:100:A:LEU:HD13	1:101:A:THR:H	15	1.76
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG22	3	1.76
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	10	1.76
(1,386)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	5	1.76
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD22	16	1.76
(1,138)	1:3:A:LEU:HD21	1:8:A:LEU:HD23	13	1.76
(2,536)	1:99:A:THR:HG22	1:117:A:GLU:HB3	6	1.75
(2,493)	1:90:A:ILE:HD13	1:87:A:GLN:HB2	17	1.75
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	8	1.75
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	17	1.75
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	19	1.75
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	13	1.75
(1,797)	1:100:A:LEU:HD12	1:93:A:ASP:H	7	1.75
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG22	15	1.75
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	1	1.75
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	19	1.75
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD21	6	1.75
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG12	13	1.74
(2,547)	1:100:A:LEU:HD12	1:94:A:LEU:HA	16	1.74
(2,543)	1:58:A:MET:HE2	1:100:A:LEU:HD21	2	1.74
(2,82)	1:125:A:LEU:HD11	1:120:A:ARG:HD3	18	1.74
(1,2819)	1:116:A:TYR:HD1	1:118:A:TYR:HH	2	1.74
(1,797)	1:100:A:LEU:HD11	1:93:A:ASP:H	2	1.74
(1,796)	1:100:A:LEU:HD11	1:101:A:THR:H	5	1.74
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	19	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD23	5	1.74
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	7	1.74
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	13	1.74
(1,180)	1:3:A:LEU:HD21	1:8:A:LEU:HD23	13	1.74
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	16	1.74
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD22	18	1.73
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HG23	5	1.73
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	11	1.73
(2,66)	1:12:A:LYS:HG3	1:141:A:LYS:HG3	9	1.73
(1,2077)	1:23:A:LEU:HD12	1:26:A:ARG:H	14	1.73
(1,2063)	1:100:A:LEU:HD13	1:101:A:THR:H	16	1.73
(1,924)	1:125:A:LEU:HD22	1:140:A:TYR:HB3	19	1.73
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	18	1.73
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD13	11	1.73
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	10	1.73
(2,1217)	1:65:A:LYS:HD2	1:63:A:THR:H	20	1.72
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD23	14	1.72
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	11	1.72
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	12	1.72
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	3	1.72
(1,796)	1:100:A:LEU:HD13	1:101:A:THR:H	3	1.72
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	1	1.72
(1,290)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	5	1.72
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD22	19	1.72
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	5	1.72
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE1	12	1.71
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG23	18	1.71
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG11	11	1.71
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD22	14	1.71
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD12	14	1.71
(2,85)	1:125:A:LEU:HD13	1:118:A:TYR:HE1	1	1.71
(1,2813)	1:127:A:MET:HE3	1:118:A:TYR:HH	19	1.71
(1,2663)	1:14:A:GLU:H	1:13:A:LEU:HD21	9	1.71
(1,1531)	1:70:A:LYS:HG2	1:68:A:HIS:HD2	19	1.71
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD12	16	1.71
(1,835)	1:89:A:LYS:H	1:107:A:VAL:HG11	16	1.71
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	18	1.71
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD23	10	1.71
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	8	1.71
(1,219)	1:13:A:LEU:HD21	1:15:A:ARG:H	9	1.71
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG13	12	1.7
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	2	1.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG12	13	1.7
(1,2326)	1:74:A:LEU:HD12	1:2:A:THR:H	12	1.7
(1,2063)	1:100:A:LEU:HD11	1:101:A:THR:H	18	1.7
(1,1264)	1:125:A:LEU:HD22	1:126:A:VAL:H	1	1.7
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	20	1.69
(2,1301)	1:13:A:LEU:HD23	1:141:A:LYS:H	1	1.69
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD21	17	1.69
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG11	2	1.69
(2,461)	1:41:A:VAL:HG23	1:60:A:ASN:HB3	20	1.69
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD11	7	1.69
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	3	1.69
(1,2793)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	12	1.69
(1,927)	1:125:A:LEU:HD22	1:119:A:ARG:H	5	1.69
(1,924)	1:125:A:LEU:HD22	1:140:A:TYR:HB3	12	1.69
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD12	12	1.69
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	8	1.69
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	15	1.69
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	6	1.69
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	1	1.69
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	7	1.69
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	18	1.69
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	8	1.69
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	11	1.69
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	18	1.69
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	13	1.68
(2,1649)	1:23:A:LEU:HD12	2:1001:A:OLA:H161	17	1.68
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG11	5	1.68
(2,730)	1:58:A:MET:HE1	1:69:A:HIS:H	14	1.68
(2,493)	1:90:A:ILE:HD11	1:87:A:GLN:HB2	7	1.68
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB1	14	1.68
(2,274)	1:61:A:LEU:HD21	1:66:A:ASP:HB3	3	1.68
(2,81)	1:125:A:LEU:HD11	1:45:A:PHE:HB2	5	1.68
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD11	12	1.68
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	20	1.68
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	20	1.68
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD12	18	1.68
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	8	1.68
(1,789)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	5	1.68
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	12	1.68
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	11	1.68
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	13	1.68
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	15	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,544)	1:100:A:LEU:HD23	1:94:A:LEU:HB2	15	1.67
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD21	5	1.67
(2,489)	1:90:A:ILE:HG23	1:58:A:MET:HG2	16	1.67
(2,391)	1:35:A:VAL:HG22	1:64:A:LYS:HD2	12	1.67
(2,391)	1:35:A:VAL:HG22	1:64:A:LYS:HD2	16	1.67
(2,82)	1:125:A:LEU:HD12	1:120:A:ARG:HD3	13	1.67
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG21	12	1.67
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	8	1.67
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	8	1.67
(1,429)	1:23:A:LEU:HD22	1:37:A:LYS:HG3	15	1.67
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG11	3	1.67
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG11	11	1.67
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	11	1.67
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	14	1.67
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	17	1.67
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	20	1.66
(2,810)	1:52:A:LYS:HE3	1:53:A:PRO:HD3	6	1.66
(2,175)	1:16:A:ASP:HB2	1:15:A:ARG:HG2	11	1.66
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD12	15	1.66
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	4	1.66
(1,2793)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	10	1.66
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG23	15	1.66
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	11	1.66
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	3	1.66
(1,797)	1:100:A:LEU:HD12	1:93:A:ASP:H	3	1.66
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	17	1.66
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	10	1.66
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD22	3	1.66
(2,544)	1:100:A:LEU:HD22	1:94:A:LEU:HB2	16	1.65
(2,82)	1:125:A:LEU:HD11	1:120:A:ARG:HD3	15	1.65
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	8	1.65
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	2	1.65
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	6	1.65
(1,2189)	1:13:A:LEU:HD21	1:15:A:ARG:H	9	1.65
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	4	1.65
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	9	1.65
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD21	6	1.65
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	13	1.65
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	9	1.65
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	14	1.65
(2,810)	1:52:A:LYS:HE3	1:50:A:SER:HB3	10	1.64
(2,740)	1:31:A:ILE:HD13	1:30:A:TRP:HZ2	9	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD11	12	1.64
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	8	1.64
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	11	1.64
(1,2793)	2:1001:A:OLA:H181	1:23:A:LEU:HD13	19	1.64
(1,2663)	1:14:A:GLU:H	1:13:A:LEU:HD21	1	1.64
(1,1621)	1:61:A:LEU:HD23	1:61:A:LEU:HA	20	1.64
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG13	10	1.64
(1,796)	1:100:A:LEU:HD12	1:101:A:THR:H	10	1.64
(1,430)	1:23:A:LEU:HD21	1:37:A:LYS:HG2	14	1.64
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	15	1.64
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD12	14	1.64
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD13	16	1.64
(1,227)	1:41:A:VAL:H	1:13:A:LEU:HD12	12	1.64
(1,138)	1:3:A:LEU:HD21	1:8:A:LEU:HD21	12	1.64
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	7	1.64
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	15	1.63
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	17	1.63
(2,740)	1:30:A:TRP:HZ2	1:31:A:ILE:HG23	11	1.63
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD11	13	1.63
(2,730)	1:58:A:MET:HE2	1:43:A:LYS:H	1	1.63
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	16	1.63
(2,493)	1:90:A:ILE:HD13	1:81:A:GLU:HB2	8	1.63
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG23	10	1.63
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	6	1.63
(1,835)	1:89:A:LYS:H	1:107:A:VAL:HG11	20	1.63
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG22	20	1.63
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	12	1.63
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	17	1.63
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	2	1.63
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD12	3	1.63
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD21	5	1.63
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	19	1.63
(2,1217)	1:63:A:THR:H	1:38:A:LEU:HB3	2	1.62
(2,570)	1:87:A:GLN:HA	1:107:A:VAL:HG21	1	1.62
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	2	1.62
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	7	1.62
(1,2793)	2:1001:A:OLA:H183	1:23:A:LEU:HD12	1	1.62
(1,2063)	1:100:A:LEU:HD12	1:101:A:THR:H	19	1.62
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	17	1.62
(1,796)	1:100:A:LEU:HD13	1:101:A:THR:H	7	1.62
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	4	1.62
(1,636)	1:61:A:LEU:HD21	1:66:A:ASP:HB2	3	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	2	1.62
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	8	1.62
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	9	1.62
(1,386)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	17	1.62
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	15	1.62
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	2	1.62
(2,1649)	1:23:A:LEU:HD11	2:1001:A:OLA:H161	10	1.61
(2,1217)	1:63:A:THR:H	1:38:A:LEU:HB3	19	1.61
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG13	13	1.61
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	7	1.61
(1,2390)	1:74:A:LEU:HD13	1:3:A:LEU:H	2	1.61
(1,2063)	1:100:A:LEU:HD12	1:101:A:THR:H	14	1.61
(1,927)	1:125:A:LEU:HD22	1:119:A:ARG:H	1	1.61
(1,430)	1:23:A:LEU:HD22	1:37:A:LYS:HG2	16	1.61
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	6	1.61
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	3	1.61
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	9	1.61
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD12	17	1.61
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	18	1.61
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	11	1.61
(1,180)	1:3:A:LEU:HD21	1:8:A:LEU:HD21	12	1.61
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	2	1.6
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	19	1.6
(2,485)	1:90:A:ILE:HG22	1:78:A:PHE:HB2	19	1.6
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD23	20	1.6
(2,82)	1:125:A:LEU:HD13	1:120:A:ARG:HD3	10	1.6
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD12	7	1.6
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	12	1.6
(1,1621)	1:61:A:LEU:HD22	1:61:A:LEU:HA	1	1.6
(1,1621)	1:61:A:LEU:HD23	1:61:A:LEU:HA	4	1.6
(1,1621)	1:61:A:LEU:HD21	1:61:A:LEU:HA	19	1.6
(1,1264)	1:125:A:LEU:HD23	1:126:A:VAL:H	5	1.6
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	3	1.6
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	13	1.6
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD22	3	1.6
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	12	1.6
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	4	1.6
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	5	1.6
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	17	1.6
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	20	1.6
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	1	1.59
(2,1394)	1:143:A:GLN:H	1:12:A:LYS:HG3	18	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1217)	1:63:A:THR:H	1:38:A:LEU:HB3	1	1.59
(2,1217)	1:65:A:LYS:HD2	1:63:A:THR:H	4	1.59
(2,840)	1:129:A:MET:HE1	1:114:A:GLU:HG3	5	1.59
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD11	14	1.59
(2,278)	1:35:A:VAL:HG23	2:1001:A:OLA:H10	13	1.59
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD11	4	1.59
(2,82)	1:125:A:LEU:HD11	1:120:A:ARG:HD3	2	1.59
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	14	1.59
(1,2793)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	15	1.59
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	14	1.59
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	19	1.59
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	3	1.59
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	7	1.59
(1,290)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	17	1.59
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD12	6	1.59
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	4	1.59
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	7	1.59
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD23	15	1.59
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	18	1.59
(2,1394)	1:143:A:GLN:H	1:12:A:LYS:HG3	15	1.58
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD11	5	1.58
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	10	1.58
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	8	1.58
(1,2793)	2:1001:A:OLA:H181	1:23:A:LEU:HD12	9	1.58
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	10	1.58
(1,796)	1:100:A:LEU:HD11	1:101:A:THR:H	20	1.58
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	5	1.58
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	16	1.58
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD13	11	1.58
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	1	1.58
(2,1646)	1:36:A:ILE:HD11	1:23:A:LEU:HB2	3	1.57
(2,1646)	1:36:A:ILE:HD12	1:33:A:ARG:HG3	8	1.57
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H183	18	1.57
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD11	11	1.57
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD13	14	1.57
(2,740)	1:31:A:ILE:HD11	1:30:A:TRP:HZ2	7	1.57
(2,740)	1:31:A:ILE:HD11	1:30:A:TRP:HZ2	10	1.57
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	15	1.57
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	1	1.57
(2,278)	1:35:A:VAL:HG21	2:1001:A:OLA:H10	2	1.57
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	14	1.57
(2,175)	1:16:A:ASP:HB2	1:15:A:ARG:HG2	18	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,86)	1:125:A:LEU:HD13	1:45:A:PHE:HE1	1	1.57
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD12	18	1.57
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB2	3	1.57
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD12	16	1.57
(1,1621)	1:61:A:LEU:HD22	1:61:A:LEU:HA	2	1.57
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	17	1.57
(1,430)	1:23:A:LEU:HD22	1:37:A:LYS:HG2	19	1.57
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	13	1.57
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	18	1.57
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	2	1.57
(2,1144)	1:105:A:ILE:H	1:110:A:PRO:HB2	7	1.56
(2,493)	1:90:A:ILE:HD13	1:81:A:GLU:HG2	1	1.56
(2,489)	1:90:A:ILE:HG21	1:58:A:MET:HG2	15	1.56
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	1	1.56
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	20	1.56
(1,1963)	1:100:A:LEU:HD11	1:93:A:ASP:H	10	1.56
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	20	1.56
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	16	1.56
(1,835)	1:89:A:LYS:H	1:107:A:VAL:HG11	17	1.56
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	2	1.56
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD22	3	1.56
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	7	1.56
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	20	1.56
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	7	1.56
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD23	15	1.56
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD13	6	1.55
(2,730)	1:58:A:MET:HE3	1:43:A:LYS:H	2	1.55
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD13	10	1.55
(2,278)	1:35:A:VAL:HG23	2:1001:A:OLA:H10	16	1.55
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HB3	19	1.55
(2,162)	1:16:A:ASP:HA	1:13:A:LEU:HD21	12	1.55
(2,89)	1:125:A:LEU:HD13	1:9:A:GLY:H	17	1.55
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD13	11	1.55
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE1	12	1.55
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	18	1.55
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG13	20	1.55
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H183	9	1.54
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	5	1.54
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	10	1.54
(2,680)	1:140:A:TYR:HE2	2:1001:A:OLA:H22	14	1.54
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	7	1.54
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG21	16	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,493)	1:90:A:ILE:HD12	1:79:A:GLN:HG3	5	1.54
(2,489)	1:90:A:ILE:HG21	1:58:A:MET:HG2	4	1.54
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG23	13	1.54
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	4	1.54
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	4	1.54
(2,93)	1:3:A:LEU:HD22	1:8:A:LEU:HD13	16	1.54
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	5	1.54
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	1	1.54
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	9	1.54
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	10	1.54
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	13	1.54
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD11	13	1.53
(2,740)	1:30:A:TRP:HZ2	1:31:A:ILE:HG23	18	1.53
(2,730)	1:58:A:MET:HE3	1:69:A:HIS:H	8	1.53
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG13	15	1.53
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	8	1.53
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	2	1.53
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	3	1.53
(2,162)	1:16:A:ASP:HA	1:13:A:LEU:HD21	1	1.53
(2,93)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	2	1.53
(2,82)	1:125:A:LEU:HD11	1:120:A:ARG:HD3	8	1.53
(1,2063)	1:100:A:LEU:HD11	1:101:A:THR:H	12	1.53
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	3	1.53
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD22	17	1.53
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE1	20	1.52
(2,730)	1:58:A:MET:HE2	1:43:A:LYS:H	12	1.52
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	19	1.52
(2,463)	1:87:A:GLN:HB3	1:82:A:ALA:HB3	16	1.52
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	18	1.52
(2,82)	1:125:A:LEU:HD11	1:120:A:ARG:HD3	6	1.52
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	1	1.52
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD12	9	1.52
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD13	18	1.52
(1,796)	1:100:A:LEU:HD12	1:101:A:THR:H	17	1.52
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	15	1.52
(1,386)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	7	1.52
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	11	1.52
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD21	5	1.52
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	4	1.52
(1,221)	1:13:A:LEU:HD22	1:14:A:GLU:HA	9	1.52
(1,138)	1:3:A:LEU:HD21	1:8:A:LEU:HD21	2	1.52
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	20	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	11	1.51
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	20	1.51
(2,299)	1:37:A:LYS:HG3	1:38:A:LEU:HD23	19	1.51
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	19	1.51
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD13	6	1.51
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	19	1.51
(1,2826)	1:127:A:MET:HE3	1:118:A:TYR:HH	19	1.51
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD13	12	1.51
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	1	1.51
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD22	12	1.51
(1,218)	1:13:A:LEU:HD21	1:139:A:TYR:H	9	1.51
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD22	8	1.51
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	8	1.51
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	10	1.5
(2,825)	1:118:A:TYR:HD1	1:127:A:MET:HG2	20	1.5
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	11	1.5
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD21	10	1.5
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG23	13	1.5
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	12	1.5
(2,391)	1:35:A:VAL:HG22	1:64:A:LYS:HD2	14	1.5
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	7	1.5
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	4	1.5
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	10	1.5
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	20	1.5
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB2	9	1.5
(1,2793)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	5	1.5
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD11	17	1.5
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	5	1.5
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	20	1.5
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG21	12	1.5
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	13	1.5
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	11	1.5
(1,186)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	17	1.5
(1,131)	1:3:A:LEU:HD13	1:7:A:PHE:HD2	12	1.5
(2,1594)	2:1001:A:OLA:H32	1:13:A:LEU:HD13	4	1.49
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	2	1.49
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	3	1.49
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD11	6	1.49
(2,1103)	1:87:A:GLN:H	1:107:A:VAL:HG13	1	1.49
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	18	1.49
(2,844)	1:107:A:VAL:H	1:82:A:ALA:HB3	8	1.49
(2,841)	1:129:A:MET:HE2	1:114:A:GLU:HG3	9	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,784)	1:35:A:VAL:HG21	1:32:A:MET:HE1	2	1.49
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD13	2	1.49
(2,616)	1:125:A:LEU:HD22	1:140:A:TYR:HD2	8	1.49
(2,162)	1:13:A:LEU:HD23	1:140:A:TYR:HA	9	1.49
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD11	20	1.49
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	8	1.49
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD22	20	1.49
(1,290)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	7	1.49
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD11	2	1.49
(1,221)	1:13:A:LEU:HD22	1:14:A:GLU:HA	1	1.49
(1,180)	1:3:A:LEU:HD21	1:8:A:LEU:HD21	2	1.49
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	2	1.49
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	2	1.48
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG13	17	1.48
(2,393)	1:89:A:LYS:HE2	1:105:A:ILE:HG21	17	1.48
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	3	1.48
(1,2063)	1:100:A:LEU:HD13	1:101:A:THR:H	15	1.48
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG12	20	1.48
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	6	1.48
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG22	6	1.48
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	4	1.48
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD13	9	1.48
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD21	7	1.48
(1,187)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	12	1.48
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD22	8	1.48
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD23	9	1.48
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	6	1.47
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE1	9	1.47
(2,57)	1:40:A:GLY:HA2	1:13:A:LEU:HD11	1	1.47
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD13	2	1.47
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	1	1.47
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD21	17	1.46
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD11	17	1.46
(2,730)	1:58:A:MET:HE3	1:43:A:LYS:H	7	1.46
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	14	1.46
(2,553)	1:132:A:LYS:HE2	1:134:A:VAL:HG23	2	1.46
(2,489)	1:90:A:ILE:HG21	1:58:A:MET:HG2	9	1.46
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	1	1.46
(2,419)	1:74:A:LEU:HD13	1:56:A:TYR:HD1	5	1.46
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	3	1.46
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	13	1.46
(1,2793)	2:1001:A:OLA:H183	1:23:A:LEU:HD13	13	1.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2793)	2:1001:A:OLA:H182	1:23:A:LEU:HD11	14	1.46
(1,2793)	2:1001:A:OLA:H181	1:23:A:LEU:HD11	17	1.46
(1,2663)	1:14:A:GLU:H	1:13:A:LEU:HD21	12	1.46
(1,2063)	1:100:A:LEU:HD11	1:101:A:THR:H	5	1.46
(1,1963)	1:100:A:LEU:HD11	1:93:A:ASP:H	17	1.46
(1,1617)	1:107:A:VAL:H	1:107:A:VAL:HG12	16	1.46
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	6	1.46
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD23	9	1.46
(1,128)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	10	1.46
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	17	1.45
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H182	15	1.45
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	10	1.45
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD23	20	1.45
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	14	1.45
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB2	18	1.45
(2,216)	1:23:A:LEU:HD23	1:33:A:ARG:HD3	7	1.45
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	5	1.45
(2,24)	1:94:A:LEU:HD11	1:4:A:PRO:HB2	18	1.45
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	5	1.45
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	7	1.45
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	20	1.45
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	5	1.45
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD23	19	1.45
(1,131)	1:3:A:LEU:HD11	1:7:A:PHE:HD2	15	1.45
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG12	11	1.44
(2,1394)	1:143:A:GLN:H	1:141:A:LYS:HD3	17	1.44
(2,840)	1:129:A:MET:HE1	1:114:A:GLU:HG3	4	1.44
(2,616)	1:125:A:LEU:HD22	1:118:A:TYR:HE1	15	1.44
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG21	2	1.44
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD13	15	1.44
(1,2063)	1:100:A:LEU:HD13	1:101:A:THR:H	3	1.44
(1,1963)	1:100:A:LEU:HD12	1:93:A:ASP:H	7	1.44
(1,1617)	1:107:A:VAL:H	1:107:A:VAL:HG12	20	1.44
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG11	20	1.44
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD23	17	1.44
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG22	19	1.44
(1,138)	1:3:A:LEU:HD21	1:8:A:LEU:HD22	10	1.44
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	18	1.44
(1,128)	1:100:A:LEU:HD23	1:3:A:LEU:HD12	20	1.44
(2,1394)	1:143:A:GLN:H	1:12:A:LYS:HG3	11	1.43
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD12	9	1.43
(2,740)	1:30:A:TRP:HZ2	1:31:A:ILE:HG21	12	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD13	8	1.43
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD13	18	1.43
(2,489)	1:77:A:GLU:HB3	1:90:A:ILE:HG22	14	1.43
(2,161)	1:13:A:LEU:HD23	1:140:A:TYR:HE2	15	1.43
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD11	3	1.43
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD11	18	1.43
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	14	1.43
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	2	1.43
(1,1963)	1:100:A:LEU:HD11	1:93:A:ASP:H	2	1.43
(1,1617)	1:107:A:VAL:H	1:107:A:VAL:HG12	17	1.43
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD22	17	1.43
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD22	15	1.43
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	4	1.43
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H183	14	1.42
(2,1581)	2:1001:A:OLA:H81	1:36:A:ILE:HD13	20	1.42
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	13	1.42
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	16	1.42
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	18	1.42
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	11	1.42
(2,70)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	12	1.42
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	18	1.42
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	19	1.42
(1,632)	1:74:A:LEU:HD12	1:3:A:LEU:HD11	5	1.42
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	15	1.42
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	5	1.42
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD23	19	1.42
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	11	1.42
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD12	5	1.42
(2,1646)	1:36:A:ILE:HD11	1:33:A:ARG:HG3	5	1.41
(2,1646)	1:36:A:ILE:HD11	1:33:A:ARG:HG3	20	1.41
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H183	11	1.41
(2,1394)	1:143:A:GLN:H	1:12:A:LYS:HG3	13	1.41
(2,825)	1:118:A:TYR:HD1	1:127:A:MET:HG2	5	1.41
(2,810)	1:52:A:LYS:HE2	1:53:A:PRO:HD3	2	1.41
(2,760)	1:127:A:MET:HE1	1:140:A:TYR:HH	11	1.41
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD21	2	1.41
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD11	16	1.41
(2,616)	1:125:A:LEU:HD23	1:11:A:PHE:HD2	2	1.41
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD22	13	1.41
(2,391)	1:35:A:VAL:HG21	1:64:A:LYS:HD2	9	1.41
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	7	1.41
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HG3	11	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	12	1.41
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	3	1.41
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	19	1.41
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD12	15	1.41
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	14	1.41
(1,557)	1:63:A:THR:HG21	1:40:A:GLY:HA2	10	1.41
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD12	17	1.41
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	4	1.41
(1,180)	1:3:A:LEU:HD21	1:8:A:LEU:HD22	10	1.41
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	18	1.41
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG11	13	1.4
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	6	1.4
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD21	11	1.4
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD13	11	1.4
(2,636)	1:134:A:VAL:HG12	1:130:A:SER:HB3	10	1.4
(2,616)	1:125:A:LEU:HD21	1:118:A:TYR:HE1	20	1.4
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	17	1.4
(2,461)	1:86:A:THR:HG22	1:84:A:ASP:HB3	15	1.4
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG22	16	1.4
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD12	13	1.4
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	16	1.4
(2,93)	1:3:A:LEU:HD21	1:8:A:LEU:HD11	12	1.4
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	5	1.4
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	10	1.4
(1,1890)	1:89:A:LYS:H	1:107:A:VAL:HG11	16	1.4
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	18	1.4
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	10	1.4
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD22	12	1.4
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	7	1.4
(2,1637)	1:64:A:LYS:HG2	1:62:A:THR:HG1	10	1.39
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	3	1.39
(2,1184)	1:61:A:LEU:HD11	1:143:A:GLN:HE22	13	1.39
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD12	10	1.39
(2,617)	1:125:A:LEU:HD23	1:127:A:MET:H	1	1.39
(2,616)	1:125:A:LEU:HD21	1:118:A:TYR:HE1	10	1.39
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	9	1.39
(2,485)	1:90:A:ILE:HG22	1:78:A:PHE:HB2	14	1.39
(2,216)	1:23:A:LEU:HD23	1:22:A:TYR:HB2	17	1.39
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	17	1.39
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	8	1.39
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	14	1.39
(2,70)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	15	1.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2619)	1:34:A:GLN:H	1:35:A:VAL:HG13	2	1.39
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	11	1.39
(1,797)	1:100:A:LEU:HD11	1:93:A:ASP:H	11	1.39
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	20	1.39
(1,282)	1:28:A:TYR:H	1:23:A:LEU:HD13	1	1.39
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD12	6	1.39
(1,138)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	1	1.39
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	20	1.39
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	10	1.38
(2,461)	1:41:A:VAL:HG21	1:60:A:ASN:HB3	6	1.38
(2,216)	1:23:A:LEU:HD23	1:33:A:ARG:HD3	5	1.38
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	20	1.38
(2,161)	1:13:A:LEU:HD21	1:140:A:TYR:HE1	20	1.38
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	9	1.38
(2,93)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	10	1.38
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD11	16	1.38
(1,796)	1:100:A:LEU:HD13	1:101:A:THR:H	8	1.38
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD22	17	1.38
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD13	12	1.38
(1,114)	1:50:A:SER:HB3	1:52:A:LYS:HB2	6	1.38
(2,1606)	1:36:A:ILE:HD13	2:1001:A:OLA:H112	6	1.37
(2,1394)	1:143:A:GLN:H	1:12:A:LYS:HG3	6	1.37
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD11	12	1.37
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	13	1.37
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG13	16	1.37
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG11	6	1.37
(2,444)	1:68:A:HIS:H	1:83:A:LEU:HD23	19	1.37
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	4	1.37
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	15	1.37
(2,426)	1:13:A:LEU:HD21	1:15:A:ARG:HB2	12	1.37
(2,376)	1:40:A:GLY:HA3	1:62:A:THR:HG21	15	1.37
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD13	6	1.37
(2,216)	1:23:A:LEU:HD23	1:33:A:ARG:HD3	6	1.37
(2,93)	1:3:A:LEU:HD22	1:8:A:LEU:HD12	8	1.37
(2,77)	1:74:A:LEU:HA	1:3:A:LEU:HD13	6	1.37
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	8	1.37
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	7	1.37
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	7	1.37
(1,797)	1:100:A:LEU:HD12	1:93:A:ASP:H	14	1.37
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	15	1.37
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	2	1.37
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD21	8	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD21	5	1.37
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	18	1.37
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	2	1.37
(1,423)	1:36:A:ILE:HD12	1:23:A:LEU:HD11	7	1.37
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD21	7	1.37
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	5	1.37
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD21	14	1.37
(1,180)	1:3:A:LEU:HD22	1:8:A:LEU:HD21	1	1.37
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	3	1.37
(2,1184)	1:142:A:LYS:HG2	1:143:A:GLN:HE22	9	1.36
(2,784)	1:35:A:VAL:HG23	1:32:A:MET:HE3	19	1.36
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	20	1.36
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	19	1.36
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	6	1.36
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	7	1.36
(2,93)	1:3:A:LEU:HD22	1:8:A:LEU:HD13	19	1.36
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB3	2	1.36
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	8	1.36
(1,2063)	1:100:A:LEU:HD12	1:101:A:THR:H	10	1.36
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	5	1.36
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	8	1.36
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	19	1.36
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	20	1.36
(1,138)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	6	1.36
(1,76)	1:96:A:ASP:HB3	1:97:A:PRO:HG2	20	1.36
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H152	15	1.35
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	11	1.35
(2,784)	1:35:A:VAL:HG21	1:32:A:MET:HE3	8	1.35
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG22	10	1.35
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB1	10	1.35
(2,391)	1:35:A:VAL:HG23	1:64:A:LYS:HD2	5	1.35
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG21	7	1.35
(2,216)	1:23:A:LEU:HD23	1:22:A:TYR:HB2	12	1.35
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	16	1.35
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD11	13	1.35
(2,66)	1:1:A:LYS:HG2	1:74:A:LEU:HD22	17	1.35
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	4	1.35
(1,1963)	1:100:A:LEU:HD12	1:93:A:ASP:H	3	1.35
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD23	10	1.35
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	17	1.35
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD13	15	1.35
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	20	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:3:A:LEU:HD11	1:7:A:PHE:HD2	6	1.35
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	14	1.35
(2,1646)	1:36:A:ILE:HD12	1:33:A:ARG:HG3	6	1.34
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	13	1.34
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H183	8	1.34
(2,1394)	1:143:A:GLN:H	1:141:A:LYS:HD3	3	1.34
(2,616)	1:125:A:LEU:HD23	1:11:A:PHE:HD2	7	1.34
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HB2	3	1.34
(2,547)	1:100:A:LEU:HD12	1:94:A:LEU:HA	15	1.34
(2,544)	1:100:A:LEU:HD21	1:94:A:LEU:HB2	4	1.34
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG21	1	1.34
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	20	1.34
(2,72)	1:3:A:LEU:HD12	1:74:A:LEU:HB2	13	1.34
(2,70)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	20	1.34
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB1	6	1.34
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG23	1	1.34
(1,2063)	1:100:A:LEU:HD13	1:101:A:THR:H	7	1.34
(1,789)	1:100:A:LEU:HD21	1:3:A:LEU:HD11	10	1.34
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD22	17	1.34
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	7	1.34
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD12	11	1.34
(1,356)	1:28:A:TYR:HE1	1:23:A:LEU:HD11	8	1.34
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD12	14	1.34
(1,187)	1:8:A:LEU:HD12	1:47:A:ASN:HD22	13	1.34
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD21	3	1.34
(1,180)	1:3:A:LEU:HD23	1:8:A:LEU:HD22	6	1.34
(2,1591)	1:41:A:VAL:HG13	2:1001:A:OLA:H72	6	1.33
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG11	19	1.33
(2,784)	1:35:A:VAL:HG23	1:32:A:MET:HE2	13	1.33
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	17	1.33
(2,707)	1:41:A:VAL:HG13	1:62:A:THR:HG1	11	1.33
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD23	3	1.33
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG23	5	1.33
(2,362)	1:61:A:LEU:HD23	1:61:A:LEU:HA	20	1.33
(2,308)	1:140:A:TYR:HB3	1:141:A:LYS:HG3	8	1.33
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	5	1.33
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	6	1.33
(2,161)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	4	1.33
(2,161)	1:13:A:LEU:HD21	1:140:A:TYR:HE1	7	1.33
(2,161)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	17	1.33
(2,93)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	14	1.33
(2,79)	1:100:A:LEU:HA	1:3:A:LEU:HD12	13	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	6	1.33
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG23	10	1.33
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE2	9	1.33
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD13	2	1.33
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	6	1.33
(1,789)	1:100:A:LEU:HD23	1:3:A:LEU:HD12	20	1.33
(1,756)	1:94:A:LEU:HD11	1:3:A:LEU:HD11	7	1.33
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	3	1.33
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	11	1.33
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD12	3	1.33
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD13	11	1.33
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	13	1.33
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD13	16	1.33
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	20	1.33
(1,229)	1:140:A:TYR:HE1	1:13:A:LEU:HD12	13	1.33
(1,76)	1:96:A:ASP:HB3	1:97:A:PRO:HG2	7	1.33
(2,1589)	1:26:A:ARG:HD3	2:1001:A:OLA:H181	13	1.32
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	3	1.32
(2,841)	1:129:A:MET:HE2	1:114:A:GLU:HG3	16	1.32
(2,784)	1:32:A:MET:HE2	1:31:A:ILE:HG23	5	1.32
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	11	1.32
(2,624)	1:127:A:MET:HB3	1:126:A:VAL:HG11	12	1.32
(2,616)	1:125:A:LEU:HD22	1:11:A:PHE:HD2	3	1.32
(2,616)	1:125:A:LEU:HD23	1:11:A:PHE:HD2	13	1.32
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HG3	6	1.32
(2,216)	1:23:A:LEU:HD23	1:22:A:TYR:HB2	19	1.32
(2,82)	1:125:A:LEU:HD13	1:120:A:ARG:HD3	3	1.32
(2,70)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	18	1.32
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	13	1.32
(1,1890)	1:89:A:LYS:H	1:107:A:VAL:HG11	20	1.32
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	15	1.32
(1,797)	1:100:A:LEU:HD13	1:93:A:ASP:H	16	1.32
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD21	10	1.32
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	11	1.32
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	14	1.32
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD22	15	1.32
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	4	1.32
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	10	1.32
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	15	1.32
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD12	17	1.32
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	2	1.32
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	13	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,76)	1:96:A:ASP:HB3	1:97:A:PRO:HG2	12	1.32
(2,1606)	1:36:A:ILE:HD13	1:23:A:LEU:HB2	19	1.31
(2,1594)	2:1001:A:OLA:H32	2:1001:A:OLA:H131	18	1.31
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HD23	4	1.31
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG22	2	1.31
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HG21	3	1.31
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD11	17	1.31
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	10	1.31
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	18	1.31
(2,216)	1:23:A:LEU:HD23	1:22:A:TYR:HB2	3	1.31
(2,88)	1:11:A:PHE:HA	1:125:A:LEU:HD13	17	1.31
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	19	1.31
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG21	4	1.31
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD12	14	1.31
(1,2640)	1:125:A:LEU:HD22	1:126:A:VAL:H	1	1.31
(1,2063)	1:100:A:LEU:HD11	1:101:A:THR:H	20	1.31
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	13	1.31
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE3	5	1.31
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD22	2	1.31
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	11	1.31
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	9	1.31
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	13	1.31
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	6	1.31
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD13	9	1.31
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	18	1.31
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	1	1.31
(2,844)	1:87:A:GLN:HE22	1:82:A:ALA:HB2	19	1.3
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE1	10	1.3
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD13	4	1.3
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG23	10	1.3
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	18	1.3
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD23	4	1.3
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG13	20	1.3
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	8	1.3
(2,160)	1:13:A:LEU:HD22	1:140:A:TYR:HD2	3	1.3
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD12	3	1.3
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD13	16	1.3
(1,2390)	1:74:A:LEU:HD12	1:3:A:LEU:H	5	1.3
(1,1982)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	12	1.3
(1,1617)	1:107:A:VAL:H	1:107:A:VAL:HG11	1	1.3
(1,1192)	1:23:A:LEU:HD12	1:32:A:MET:HE3	6	1.3
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD13	11	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	6	1.3
(1,76)	1:96:A:ASP:HB3	1:97:A:PRO:HG2	15	1.3
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	13	1.29
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	4	1.29
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD21	19	1.29
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	19	1.29
(2,636)	1:134:A:VAL:HG13	1:130:A:SER:HB3	3	1.29
(2,616)	1:125:A:LEU:HD22	1:11:A:PHE:HD2	9	1.29
(2,461)	1:41:A:VAL:HG21	1:60:A:ASN:HB3	18	1.29
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG22	19	1.29
(2,362)	1:61:A:LEU:HD22	1:61:A:LEU:HA	1	1.29
(2,311)	1:67:A:THR:HG1	1:83:A:LEU:HD23	10	1.29
(2,216)	1:23:A:LEU:HD23	1:33:A:ARG:HD3	14	1.29
(2,161)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	18	1.29
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	4	1.29
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	5	1.29
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	15	1.29
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	2	1.29
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	19	1.29
(1,287)	1:36:A:ILE:HD12	1:23:A:LEU:HD11	7	1.29
(2,1648)	2:1001:A:OLA:H172	1:36:A:ILE:HD12	9	1.28
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	7	1.28
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	13	1.28
(2,1144)	1:105:A:ILE:H	1:113:A:VAL:HB	19	1.28
(2,1029)	1:113:A:VAL:HG12	1:104:A:HIS:H	8	1.28
(2,613)	1:125:A:LEU:HD23	1:100:A:LEU:HB2	12	1.28
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	5	1.28
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	8	1.28
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG21	18	1.28
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG22	16	1.28
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	13	1.28
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD12	18	1.28
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD13	11	1.28
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	7	1.28
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB2	4	1.28
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD12	17	1.28
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	18	1.28
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	14	1.28
(1,794)	1:100:A:LEU:HD11	1:100:A:LEU:HA	3	1.28
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	1	1.28
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD13	12	1.28
(1,221)	1:13:A:LEU:HD22	1:14:A:GLU:HA	12	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	4	1.28
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	6	1.27
(2,1589)	1:32:A:MET:HB3	2:1001:A:OLA:H181	12	1.27
(2,730)	1:58:A:MET:HE3	1:43:A:LYS:H	6	1.27
(2,697)	1:65:A:LYS:HE2	1:83:A:LEU:HA	16	1.27
(2,636)	1:134:A:VAL:HG12	1:130:A:SER:HB3	5	1.27
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	9	1.27
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG22	10	1.27
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	1	1.27
(2,216)	1:23:A:LEU:HD23	1:22:A:TYR:HB2	16	1.27
(2,145)	1:11:A:PHE:HD1	1:125:A:LEU:HD11	1	1.27
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	7	1.27
(2,60)	1:0:A:SER:HB2	1:1:A:LYS:HD2	1	1.27
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	8	1.27
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	20	1.27
(1,2326)	1:74:A:LEU:HD13	1:2:A:THR:H	2	1.27
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	7	1.27
(1,868)	1:113:A:VAL:HG22	1:113:A:VAL:H	9	1.27
(1,794)	1:100:A:LEU:HD11	1:100:A:LEU:HA	8	1.27
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	15	1.27
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	4	1.27
(1,290)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	6	1.27
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD21	14	1.27
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD13	1	1.27
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD13	20	1.27
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	20	1.26
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	10	1.26
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	7	1.26
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	16	1.26
(2,840)	1:129:A:MET:HE1	1:22:A:TYR:HB2	15	1.26
(2,834)	1:68:A:HIS:HE1	1:49:A:ALA:HB1	4	1.26
(2,825)	1:118:A:TYR:HD1	1:58:A:MET:HG3	6	1.26
(2,624)	1:128:A:LYS:HD3	1:126:A:VAL:HG13	19	1.26
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HB2	19	1.26
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG22	9	1.26
(2,547)	1:100:A:LEU:HD11	1:94:A:LEU:HA	14	1.26
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	7	1.26
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG21	4	1.26
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG21	6	1.26
(2,465)	1:87:A:GLN:HG2	1:82:A:ALA:HB2	19	1.26
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	16	1.26
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB2	13	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,161)	1:13:A:LEU:HD23	1:140:A:TYR:HE1	19	1.26
(2,124)	1:10:A:THR:HB	1:44:A:LYS:HB2	4	1.26
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	16	1.26
(2,82)	1:125:A:LEU:HD11	1:120:A:ARG:HD3	11	1.26
(2,70)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	6	1.26
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD12	6	1.26
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	1	1.26
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD22	5	1.26
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	18	1.26
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	1	1.26
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	9	1.26
(1,836)	1:88:A:HIS:HA	1:107:A:VAL:HG13	20	1.26
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD23	14	1.26
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG12	4	1.26
(1,386)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	12	1.26
(1,281)	1:23:A:LEU:HA	1:23:A:LEU:HD11	2	1.26
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD13	12	1.26
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	14	1.26
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD11	15	1.26
(2,1646)	1:36:A:ILE:HD12	1:33:A:ARG:HG3	16	1.25
(2,1640)	1:140:A:TYR:HH	2:1001:A:OLA:H32	11	1.25
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H183	10	1.25
(2,1305)	1:116:A:TYR:H	1:127:A:MET:HG2	19	1.25
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	9	1.25
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	7	1.25
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB1	11	1.25
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD11	7	1.25
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG12	11	1.25
(2,620)	1:124:A:TYR:HD2	1:126:A:VAL:HG13	9	1.25
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD23	17	1.25
(2,534)	1:95:A:LYS:HB2	1:99:A:THR:HG23	10	1.25
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	5	1.25
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	15	1.25
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	18	1.25
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG13	9	1.25
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG21	4	1.25
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	17	1.25
(2,262)	1:30:A:TRP:HA	1:33:A:ARG:HG3	13	1.25
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	2	1.25
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD11	14	1.25
(2,161)	1:13:A:LEU:HD21	1:140:A:TYR:HE1	14	1.25
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	19	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	1	1.25
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG23	17	1.25
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD13	11	1.25
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG11	3	1.25
(1,1890)	1:89:A:LYS:H	1:107:A:VAL:HG11	17	1.25
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	11	1.25
(1,868)	1:113:A:VAL:HG22	1:113:A:VAL:H	10	1.25
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD23	18	1.25
(1,218)	1:13:A:LEU:HD21	1:139:A:TYR:H	12	1.25
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	8	1.25
(2,1330)	1:79:A:GLN:H	1:89:A:LYS:HB3	8	1.24
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD23	4	1.24
(2,729)	1:66:A:ASP:HA	1:59:A:GLU:HB3	18	1.24
(2,667)	1:136:A:THR:HG22	1:135:A:SER:HB2	7	1.24
(2,543)	1:58:A:MET:HE1	1:100:A:LEU:HD22	1	1.24
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	4	1.24
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG22	5	1.24
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG22	20	1.24
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	14	1.24
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD12	5	1.24
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	19	1.24
(1,2489)	1:13:A:LEU:HD21	1:17:A:GLU:H	9	1.24
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG11	11	1.24
(1,2063)	1:100:A:LEU:HD12	1:101:A:THR:H	17	1.24
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	1	1.24
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	13	1.24
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE1	19	1.24
(1,921)	1:125:A:LEU:HD21	1:125:A:LEU:HA	5	1.24
(1,794)	1:100:A:LEU:HD12	1:100:A:LEU:HA	12	1.24
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	15	1.24
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD13	17	1.24
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG12	3	1.24
(1,252)	1:20:A:ASP:HA	1:23:A:LEU:HD21	10	1.24
(1,131)	1:3:A:LEU:HD11	1:7:A:PHE:HD2	18	1.24
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	4	1.24
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	5	1.24
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD11	6	1.24
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	1	1.23
(2,1184)	1:61:A:LEU:HD11	1:143:A:GLN:HE22	8	1.23
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE2	4	1.23
(2,707)	1:67:A:THR:HG22	1:62:A:THR:HG1	12	1.23
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	18	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	3	1.23
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG21	17	1.23
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG23	12	1.23
(2,216)	1:23:A:LEU:HD23	1:22:A:TYR:HB2	15	1.23
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD11	10	1.23
(2,161)	1:13:A:LEU:HD22	1:139:A:TYR:HD1	6	1.23
(2,143)	1:42:A:THR:HG21	1:140:A:TYR:HD1	4	1.23
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	11	1.23
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD13	9	1.23
(2,70)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	11	1.23
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	10	1.23
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD12	10	1.23
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	12	1.23
(1,835)	1:89:A:LYS:H	1:107:A:VAL:HG11	1	1.23
(1,794)	1:100:A:LEU:HD11	1:100:A:LEU:HA	7	1.23
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	16	1.23
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	4	1.23
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	19	1.23
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	9	1.23
(2,784)	1:35:A:VAL:HG23	1:32:A:MET:HE2	16	1.22
(2,733)	1:58:A:MET:HE3	1:125:A:LEU:HD12	19	1.22
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	13	1.22
(2,730)	1:58:A:MET:HE3	1:43:A:LYS:H	18	1.22
(2,617)	1:125:A:LEU:HD23	1:127:A:MET:H	5	1.22
(2,534)	1:95:A:LYS:HB2	1:99:A:THR:HG23	11	1.22
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	7	1.22
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	17	1.22
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	10	1.22
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG23	15	1.22
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	3	1.22
(2,143)	1:11:A:PHE:HD2	1:10:A:THR:HG21	8	1.22
(2,82)	1:125:A:LEU:HD12	1:119:A:ARG:HD2	16	1.22
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	7	1.22
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD11	2	1.22
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	4	1.22
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	15	1.22
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	11	1.22
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	4	1.22
(1,921)	1:125:A:LEU:HD21	1:125:A:LEU:HA	1	1.22
(1,290)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	12	1.22
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	2	1.22
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	3	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	7	1.22
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD11	18	1.22
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	12	1.22
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD11	2	1.22
(2,1645)	1:140:A:TYR:HH	2:1001:A:OLA:H32	11	1.21
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD23	10	1.21
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	8	1.21
(2,784)	1:35:A:VAL:HG23	1:32:A:MET:HE2	10	1.21
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD13	15	1.21
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	4	1.21
(2,570)	1:87:A:GLN:HA	1:82:A:ALA:HB1	17	1.21
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD13	2	1.21
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	13	1.21
(2,66)	1:12:A:LYS:HG3	1:141:A:LYS:HG3	10	1.21
(2,61)	1:73:A:ALA:HB3	1:0:A:SER:HB3	12	1.21
(2,59)	1:0:A:SER:HB3	1:2:A:THR:HG23	2	1.21
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG21	19	1.21
(1,2640)	1:125:A:LEU:HD23	1:126:A:VAL:H	5	1.21
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	17	1.21
(1,2182)	1:99:A:THR:H	1:94:A:LEU:HD12	10	1.21
(1,1080)	1:56:A:TYR:HD2	1:2:A:THR:HG23	17	1.21
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	17	1.21
(1,836)	1:88:A:HIS:HA	1:107:A:VAL:HG11	1	1.21
(1,794)	1:100:A:LEU:HD13	1:100:A:LEU:HA	17	1.21
(1,637)	1:75:A:GLY:HA3	1:91:A:THR:HG23	9	1.21
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	17	1.21
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	5	1.21
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	13	1.21
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD11	11	1.21
(1,128)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	7	1.21
(2,1646)	1:36:A:ILE:HD12	2:1001:A:OLA:H112	9	1.2
(2,1640)	1:127:A:MET:HE2	1:140:A:TYR:HH	19	1.2
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	17	1.2
(2,825)	1:118:A:TYR:HD1	1:58:A:MET:HG3	1	1.2
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	1	1.2
(2,667)	1:136:A:THR:HG22	1:135:A:SER:HB2	9	1.2
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG12	17	1.2
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD12	7	1.2
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD21	9	1.2
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD23	11	1.2
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG23	11	1.2
(2,461)	1:41:A:VAL:HG23	1:60:A:ASN:HB3	5	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	20	1.2
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD12	15	1.2
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	17	1.2
(2,262)	1:30:A:TRP:HA	1:33:A:ARG:HG3	19	1.2
(2,216)	1:23:A:LEU:HD22	1:33:A:ARG:HD3	9	1.2
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	18	1.2
(2,161)	1:13:A:LEU:HD23	1:139:A:TYR:HD1	16	1.2
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD13	5	1.2
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	2	1.2
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	9	1.2
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	12	1.2
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	14	1.2
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE1	7	1.2
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD13	1	1.2
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD13	11	1.2
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD11	13	1.2
(1,794)	1:100:A:LEU:HD12	1:100:A:LEU:HA	5	1.2
(1,794)	1:100:A:LEU:HD12	1:100:A:LEU:HA	18	1.2
(1,219)	1:13:A:LEU:HD21	1:15:A:ARG:H	12	1.2
(1,186)	1:3:A:LEU:HD21	1:8:A:LEU:HD11	13	1.2
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	10	1.2
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD12	9	1.2
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	1	1.19
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	17	1.19
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG21	5	1.19
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HB2	10	1.19
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	3	1.19
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD22	20	1.19
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG21	8	1.19
(2,485)	1:78:A:PHE:HB3	1:90:A:ILE:HG22	17	1.19
(2,422)	1:74:A:LEU:HD11	1:4:A:PRO:HD2	13	1.19
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	9	1.19
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD12	8	1.19
(2,161)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	2	1.19
(2,124)	1:10:A:THR:HB	1:44:A:LYS:HB2	16	1.19
(2,114)	1:8:A:LEU:HD23	1:5:A:ASP:HA	13	1.19
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	3	1.19
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG21	13	1.19
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	4	1.19
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	8	1.19
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD11	7	1.19
(1,924)	1:125:A:LEU:HD23	1:140:A:TYR:HB3	14	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:100:A:LEU:HD13	1:100:A:LEU:HA	2	1.19
(1,794)	1:100:A:LEU:HD13	1:100:A:LEU:HA	10	1.19
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	14	1.19
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	15	1.19
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	13	1.19
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	1	1.19
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	14	1.19
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	16	1.19
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	7	1.19
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	11	1.19
(2,840)	1:129:A:MET:HE1	1:114:A:GLU:HG3	20	1.18
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE3	17	1.18
(2,760)	1:118:A:TYR:H	1:127:A:MET:HE2	10	1.18
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	9	1.18
(2,667)	1:136:A:THR:HG23	1:135:A:SER:HB2	17	1.18
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	7	1.18
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	7	1.18
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD21	18	1.18
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD11	7	1.18
(2,413)	1:73:A:ALA:HB3	1:55:A:ARG:HD2	10	1.18
(2,409)	1:70:A:LYS:HB3	1:71:A:ASP:HB2	2	1.18
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG22	5	1.18
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	9	1.18
(2,143)	1:42:A:THR:HG22	1:140:A:TYR:HD1	19	1.18
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	1	1.18
(2,83)	1:120:A:ARG:HD2	1:125:A:LEU:HD12	9	1.18
(2,77)	1:74:A:LEU:HA	1:3:A:LEU:HD11	7	1.18
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD13	6	1.18
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	10	1.18
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG22	6	1.18
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	6	1.18
(1,1387)	1:94:A:LEU:HA	1:94:A:LEU:HD21	17	1.18
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	15	1.18
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG12	4	1.18
(1,836)	1:88:A:HIS:HA	1:107:A:VAL:HG13	16	1.18
(1,794)	1:100:A:LEU:HD12	1:100:A:LEU:HA	20	1.18
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	19	1.18
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD21	18	1.18
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	10	1.18
(2,1645)	1:127:A:MET:HE2	1:140:A:TYR:HH	19	1.17
(2,1589)	1:26:A:ARG:HD2	2:1001:A:OLA:H182	19	1.17
(2,1103)	1:87:A:GLN:H	1:107:A:VAL:HG11	2	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE2	14	1.17
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG11	10	1.17
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	11	1.17
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG21	20	1.17
(2,309)	1:65:A:LYS:H	1:83:A:LEU:HD22	3	1.17
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HG3	14	1.17
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	11	1.17
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	8	1.17
(2,124)	1:10:A:THR:HB	1:44:A:LYS:HB2	5	1.17
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	2	1.17
(2,49)	1:48:A:ALA:HB1	1:55:A:ARG:HD2	11	1.17
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG21	14	1.17
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG22	16	1.17
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	19	1.17
(1,1531)	1:70:A:LYS:HG2	1:68:A:HIS:HD2	8	1.17
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	17	1.17
(1,1387)	1:94:A:LEU:HA	1:94:A:LEU:HD21	7	1.17
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	11	1.17
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD23	20	1.17
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	13	1.17
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	11	1.17
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	10	1.17
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	16	1.17
(1,219)	1:13:A:LEU:HD21	1:15:A:ARG:H	1	1.17
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	3	1.17
(1,131)	1:3:A:LEU:HD11	1:7:A:PHE:HD2	9	1.17
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD11	9	1.17
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	4	1.16
(2,1581)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	19	1.16
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD22	8	1.16
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE3	11	1.16
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	15	1.16
(2,707)	1:41:A:VAL:HG12	1:62:A:THR:HG1	1	1.16
(2,667)	1:136:A:THR:HG22	1:135:A:SER:HB2	3	1.16
(2,667)	1:136:A:THR:HG23	1:135:A:SER:HB2	15	1.16
(2,597)	1:118:A:TYR:HD2	1:102:A:GLU:HG3	8	1.16
(2,400)	1:83:A:LEU:HD13	1:65:A:LYS:HG2	10	1.16
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	5	1.16
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD11	4	1.16
(2,262)	1:30:A:TRP:HA	1:33:A:ARG:HG3	11	1.16
(2,216)	1:23:A:LEU:HD22	1:22:A:TYR:HB2	10	1.16
(2,82)	1:125:A:LEU:HD12	1:120:A:ARG:HD3	9	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG21	3	1.16
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG21	8	1.16
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD11	2	1.16
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	5	1.16
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	14	1.16
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	16	1.16
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	3	1.16
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	6	1.16
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	9	1.16
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	19	1.16
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	20	1.16
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	3	1.16
(1,868)	1:113:A:VAL:HG22	1:113:A:VAL:H	4	1.16
(1,632)	1:74:A:LEU:HD12	1:3:A:LEU:HD12	18	1.16
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD11	19	1.16
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	13	1.16
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD11	19	1.16
(1,187)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	15	1.16
(2,1648)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	12	1.15
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD23	11	1.15
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	12	1.15
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	20	1.15
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB1	3	1.15
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG13	17	1.15
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB2	14	1.15
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	9	1.15
(2,801)	1:39:A:ALA:HB2	1:41:A:VAL:HG12	7	1.15
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD12	20	1.15
(2,667)	1:136:A:THR:HG21	1:135:A:SER:HB2	1	1.15
(2,667)	1:136:A:THR:HG21	1:135:A:SER:HB2	4	1.15
(2,636)	1:134:A:VAL:HG11	1:130:A:SER:HB3	15	1.15
(2,571)	1:140:A:TYR:HB2	1:127:A:MET:HB2	16	1.15
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	9	1.15
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD21	19	1.15
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	12	1.15
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	17	1.15
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD11	11	1.15
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H152	15	1.15
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	16	1.15
(2,72)	1:4:A:PRO:HB3	1:3:A:LEU:HD13	17	1.15
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG21	20	1.15
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD13	9	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD13	18	1.15
(1,1982)	1:8:A:LEU:HD12	1:47:A:ASN:HD22	13	1.15
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	19	1.15
(1,1220)	1:118:A:TYR:HD2	1:58:A:MET:HE3	9	1.15
(1,1192)	1:23:A:LEU:HD12	1:32:A:MET:HE1	3	1.15
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	13	1.15
(1,868)	1:113:A:VAL:HG21	1:113:A:VAL:H	20	1.15
(1,755)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	4	1.15
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	9	1.15
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD23	18	1.15
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD12	12	1.15
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	2	1.15
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD12	16	1.15
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	10	1.15
(2,1646)	1:36:A:ILE:HD11	1:33:A:ARG:HG3	10	1.14
(2,1646)	2:1001:A:OLA:H111	1:36:A:ILE:HD12	18	1.14
(2,1596)	2:1001:A:OLA:H31	2:1001:A:OLA:H181	8	1.14
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	6	1.14
(2,848)	1:91:A:THR:HG23	1:91:A:THR:H	7	1.14
(2,733)	1:58:A:MET:HE2	1:125:A:LEU:HD12	3	1.14
(2,591)	1:118:A:TYR:HA	1:127:A:MET:HG2	5	1.14
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	19	1.14
(2,496)	1:90:A:ILE:HD12	1:69:A:HIS:HA	5	1.14
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	17	1.14
(2,230)	1:25:A:ALA:HB1	1:26:A:ARG:HG3	7	1.14
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	4	1.14
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	20	1.14
(2,70)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	9	1.14
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	10	1.14
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	11	1.14
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG21	14	1.14
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD11	10	1.14
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG12	13	1.14
(1,2189)	1:13:A:LEU:HD21	1:15:A:ARG:H	12	1.14
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	4	1.14
(1,1220)	1:118:A:TYR:HD2	1:58:A:MET:HE3	5	1.14
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE1	18	1.14
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD22	18	1.14
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	8	1.14
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	7	1.14
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD11	14	1.14
(2,1646)	2:1001:A:OLA:H111	1:36:A:ILE:HD11	15	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1594)	2:1001:A:OLA:H31	1:41:A:VAL:HG12	6	1.13
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG23	16	1.13
(2,591)	1:118:A:TYR:HA	1:128:A:LYS:HB3	20	1.13
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG21	4	1.13
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD22	3	1.13
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	7	1.13
(2,386)	1:35:A:VAL:HG23	1:64:A:LYS:HG2	6	1.13
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG22	12	1.13
(2,230)	1:25:A:ALA:HB1	1:26:A:ARG:HG3	4	1.13
(2,70)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	13	1.13
(2,56)	1:63:A:THR:HG21	1:40:A:GLY:HA2	10	1.13
(1,2202)	1:35:A:VAL:H	1:35:A:VAL:HG13	20	1.13
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	5	1.13
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD11	9	1.13
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD13	15	1.13
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	5	1.13
(1,1080)	1:56:A:TYR:HD2	1:2:A:THR:HG21	16	1.13
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	4	1.13
(1,914)	1:124:A:TYR:HE2	1:141:A:LYS:HB3	2	1.13
(1,794)	1:100:A:LEU:HD13	1:100:A:LEU:HA	19	1.13
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	5	1.13
(1,430)	1:23:A:LEU:HD21	1:37:A:LYS:HG2	7	1.13
(1,289)	1:20:A:ASP:HA	1:23:A:LEU:HD21	10	1.13
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD12	11	1.13
(1,227)	1:41:A:VAL:H	1:13:A:LEU:HD11	9	1.13
(2,1606)	1:36:A:ILE:HD12	1:23:A:LEU:HB2	8	1.12
(2,1581)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	17	1.12
(2,1029)	1:105:A:ILE:HD13	1:104:A:HIS:H	9	1.12
(2,825)	1:118:A:TYR:HD1	1:58:A:MET:HG3	14	1.12
(2,714)	1:127:A:MET:H	1:125:A:LEU:HD11	14	1.12
(2,624)	1:127:A:MET:HB3	1:126:A:VAL:HG13	18	1.12
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HB2	18	1.12
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	16	1.12
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	12	1.12
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD22	8	1.12
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG23	8	1.12
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD12	1	1.12
(2,262)	1:30:A:TRP:HA	1:33:A:ARG:HG3	9	1.12
(2,230)	1:25:A:ALA:HB1	1:26:A:ARG:HB3	3	1.12
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB2	11	1.12
(2,175)	1:15:A:ARG:HG2	1:16:A:ASP:HB3	15	1.12
(2,143)	1:11:A:PHE:HD2	1:10:A:THR:HG22	6	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:8:A:LEU:HD23	1:5:A:ASP:HA	9	1.12
(2,72)	1:3:A:LEU:HD13	1:74:A:LEU:HB2	7	1.12
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	2	1.12
(2,5)	1:34:A:GLN:H	1:31:A:ILE:HG22	15	1.12
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	1	1.12
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	16	1.12
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	11	1.12
(1,934)	1:137:A:SER:HB3	1:126:A:VAL:HG13	9	1.12
(1,448)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	15	1.12
(1,218)	1:13:A:LEU:HD21	1:139:A:TYR:H	1	1.12
(2,1029)	1:105:A:ILE:HD11	1:104:A:HIS:H	10	1.11
(2,784)	1:32:A:MET:HE3	1:31:A:ILE:HG23	15	1.11
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD23	16	1.11
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG12	1	1.11
(2,624)	1:128:A:LYS:HD3	1:126:A:VAL:HG11	2	1.11
(2,553)	1:89:A:LYS:HE3	1:103:A:THR:HG22	18	1.11
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD12	8	1.11
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD23	1	1.11
(2,461)	1:86:A:THR:HG23	1:84:A:ASP:HB3	12	1.11
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	3	1.11
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	2	1.11
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	7	1.11
(1,2189)	1:13:A:LEU:HD21	1:15:A:ARG:H	1	1.11
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	18	1.11
(1,836)	1:88:A:HIS:HA	1:107:A:VAL:HG13	17	1.11
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	20	1.11
(1,229)	1:140:A:TYR:HE1	1:13:A:LEU:HD11	5	1.11
(2,1641)	1:140:A:TYR:HH	2:1001:A:OLA:H32	11	1.1
(2,1606)	1:36:A:ILE:HD12	1:23:A:LEU:HB2	16	1.1
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H152	15	1.1
(2,1217)	1:61:A:LEU:HB2	1:63:A:THR:H	15	1.1
(2,1184)	1:61:A:LEU:HD11	1:143:A:GLN:HE22	17	1.1
(2,1103)	1:87:A:GLN:H	1:107:A:VAL:HG11	12	1.1
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	20	1.1
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD21	6	1.1
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG23	4	1.1
(2,535)	1:117:A:GLU:HB2	1:99:A:THR:HG21	1	1.1
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	6	1.1
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	3	1.1
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	11	1.1
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD11	9	1.1
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG22	14	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	13	1.1
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD11	19	1.1
(2,70)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	16	1.1
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG22	2	1.1
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD11	11	1.1
(1,2063)	1:100:A:LEU:HD13	1:101:A:THR:H	8	1.1
(1,1277)	1:127:A:MET:HE3	1:118:A:TYR:HH	19	1.1
(1,794)	1:100:A:LEU:HD13	1:100:A:LEU:HA	11	1.1
(1,789)	1:100:A:LEU:HD22	1:3:A:LEU:HD11	7	1.1
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	2	1.1
(1,755)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	14	1.1
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD13	8	1.1
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD13	16	1.1
(2,1646)	1:36:A:ILE:HD13	1:33:A:ARG:HG3	17	1.09
(2,1330)	1:79:A:GLN:H	1:89:A:LYS:HB3	1	1.09
(2,1330)	1:79:A:GLN:H	1:89:A:LYS:HB3	5	1.09
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	12	1.09
(2,784)	1:32:A:MET:HE2	1:31:A:ILE:HG22	6	1.09
(2,757)	1:58:A:MET:HE3	1:43:A:LYS:HD2	14	1.09
(2,751)	1:83:A:LEU:HD13	1:104:A:HIS:HE1	11	1.09
(2,616)	1:125:A:LEU:HD22	1:118:A:TYR:HE1	16	1.09
(2,543)	1:100:A:LEU:HD22	1:74:A:LEU:HB2	19	1.09
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG11	10	1.09
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB2	15	1.09
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	17	1.09
(2,420)	1:106:A:LYS:HG2	1:105:A:ILE:HA	15	1.09
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HB3	13	1.09
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	1	1.09
(2,77)	1:74:A:LEU:HA	1:3:A:LEU:HD11	16	1.09
(2,59)	1:94:A:LEU:HB3	1:0:A:SER:HB3	17	1.09
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD13	12	1.09
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	2	1.09
(1,755)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	11	1.09
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD11	7	1.09
(1,186)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	2	1.09
(1,131)	1:3:A:LEU:HD11	1:7:A:PHE:HD2	11	1.09
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	18	1.09
(2,1184)	1:143:A:GLN:HE22	1:61:A:LEU:HD22	4	1.08
(2,1112)	1:143:A:GLN:HE21	1:141:A:LYS:HG3	14	1.08
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	11	1.08
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	17	1.08
(2,544)	1:8:A:LEU:HG	1:100:A:LEU:HD21	9	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	2	1.08
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD21	9	1.08
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	5	1.08
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD13	10	1.08
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	2	1.08
(2,330)	1:41:A:VAL:HG21	1:43:A:LYS:HE3	14	1.08
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	6	1.08
(2,293)	2:1001:A:OLA:H172	1:36:A:ILE:HD12	9	1.08
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	15	1.08
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG11	16	1.08
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	20	1.08
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	9	1.08
(1,1963)	1:100:A:LEU:HD11	1:93:A:ASP:H	11	1.08
(1,1387)	1:94:A:LEU:HA	1:94:A:LEU:HD22	10	1.08
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD23	5	1.08
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD13	6	1.08
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	18	1.08
(1,429)	1:23:A:LEU:HD22	1:37:A:LYS:HG3	12	1.08
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	4	1.08
(1,187)	1:8:A:LEU:HD12	1:47:A:ASN:HD22	7	1.08
(1,129)	1:3:A:LEU:HA	1:3:A:LEU:HD13	13	1.08
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	12	1.08
(2,1581)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	6	1.07
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	11	1.07
(2,616)	1:125:A:LEU:HD22	1:118:A:TYR:HE1	11	1.07
(2,486)	1:90:A:ILE:HG22	1:104:A:HIS:HB3	18	1.07
(2,461)	1:41:A:VAL:HG22	1:60:A:ASN:HB3	2	1.07
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	4	1.07
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	12	1.07
(2,420)	1:106:A:LYS:HG2	1:105:A:ILE:HA	14	1.07
(2,419)	1:74:A:LEU:HD11	1:7:A:PHE:HD2	7	1.07
(2,414)	1:73:A:ALA:HB1	1:76:A:GLU:HG2	19	1.07
(2,377)	1:41:A:VAL:HG11	1:62:A:THR:HG21	16	1.07
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HG3	2	1.07
(2,230)	1:25:A:ALA:HB1	1:26:A:ARG:HG3	17	1.07
(2,160)	1:13:A:LEU:HD22	1:41:A:VAL:H	7	1.07
(2,125)	1:35:A:VAL:HG13	1:64:A:LYS:HE3	3	1.07
(2,72)	1:3:A:LEU:HD11	1:58:A:MET:HG2	3	1.07
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG21	11	1.07
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG11	9	1.07
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	4	1.07
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	8	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	9	1.07
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD13	6	1.07
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	11	1.07
(2,1646)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	2	1.06
(2,733)	1:58:A:MET:HE1	1:125:A:LEU:HD11	9	1.06
(2,707)	1:67:A:THR:HG22	1:62:A:THR:HG1	18	1.06
(2,667)	1:136:A:THR:HG21	1:135:A:SER:HB2	8	1.06
(2,624)	1:128:A:LYS:HD3	1:126:A:VAL:HG13	14	1.06
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	2	1.06
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	17	1.06
(2,494)	1:90:A:ILE:HD12	1:104:A:HIS:HB3	12	1.06
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG22	3	1.06
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	20	1.06
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	12	1.06
(2,124)	1:10:A:THR:HB	1:44:A:LYS:HB2	14	1.06
(2,77)	1:2:A:THR:HA	1:3:A:LEU:HD13	1	1.06
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	3	1.06
(1,2746)	1:28:A:TYR:H	1:23:A:LEU:HD13	1	1.06
(1,1963)	1:100:A:LEU:HD12	1:93:A:ASP:H	14	1.06
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	15	1.06
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	17	1.06
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE1	8	1.06
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD13	14	1.06
(1,386)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	3	1.06
(1,386)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	16	1.06
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	7	1.06
(1,187)	1:8:A:LEU:HD13	1:47:A:ASN:HD22	10	1.06
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	7	1.06
(2,1641)	1:127:A:MET:HE2	1:140:A:TYR:HH	19	1.05
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H151	13	1.05
(2,1441)	1:38:A:LEU:HD11	1:34:A:GLN:HE22	10	1.05
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	14	1.05
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE2	2	1.05
(2,616)	1:125:A:LEU:HD22	1:11:A:PHE:HD2	19	1.05
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HD22	6	1.05
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD22	12	1.05
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	15	1.05
(2,496)	1:90:A:ILE:HD12	1:69:A:HIS:HA	1	1.05
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	5	1.05
(2,79)	1:3:A:LEU:HD13	1:55:A:ARG:HA	4	1.05
(2,77)	1:74:A:LEU:HA	1:3:A:LEU:HD11	2	1.05
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG22	12	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	8	1.05
(1,1364)	1:70:A:LYS:H	1:70:A:LYS:HE3	9	1.05
(1,870)	1:105:A:ILE:HG12	1:113:A:VAL:HG12	17	1.05
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	16	1.05
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	13	1.05
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD13	16	1.05
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	13	1.05
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	7	1.05
(2,1648)	1:36:A:ILE:HD11	2:1001:A:OLA:H152	7	1.04
(2,1029)	1:113:A:VAL:HG11	1:104:A:HIS:H	4	1.04
(2,636)	1:134:A:VAL:HG11	1:130:A:SER:HB3	19	1.04
(2,553)	1:103:A:THR:HG21	1:89:A:LYS:HE2	13	1.04
(2,534)	1:95:A:LYS:HB2	1:99:A:THR:HG21	20	1.04
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	4	1.04
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HB3	20	1.04
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD22	12	1.04
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	3	1.04
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD12	5	1.04
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	3	1.04
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD12	6	1.04
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	6	1.03
(2,1605)	2:1001:A:OLA:H172	1:36:A:ILE:HD12	9	1.03
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE3	5	1.03
(2,840)	1:129:A:MET:HE1	1:22:A:TYR:HB2	2	1.03
(2,840)	1:129:A:MET:HE2	1:22:A:TYR:HB2	19	1.03
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD11	10	1.03
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG23	10	1.03
(2,707)	1:41:A:VAL:HG11	1:62:A:THR:HG1	20	1.03
(2,616)	1:125:A:LEU:HD21	1:118:A:TYR:HE1	4	1.03
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	14	1.03
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD22	7	1.03
(2,510)	1:92:A:PHE:HB3	1:94:A:LEU:HD21	14	1.03
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	10	1.03
(2,386)	1:35:A:VAL:HG21	1:64:A:LYS:HG2	2	1.03
(2,230)	1:25:A:ALA:HB3	1:26:A:ARG:HG3	10	1.03
(2,230)	1:25:A:ALA:HB2	1:26:A:ARG:HB3	18	1.03
(2,143)	1:127:A:MET:HG3	1:140:A:TYR:HD2	5	1.03
(2,93)	1:120:A:ARG:HG2	1:125:A:LEU:HD12	4	1.03
(2,81)	1:125:A:LEU:HD12	1:45:A:PHE:HB2	4	1.03
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	14	1.03
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD12	5	1.03
(1,1192)	1:23:A:LEU:HD12	1:32:A:MET:HE1	17	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD12	20	1.03
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	8	1.03
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	12	1.03
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	15	1.03
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD13	12	1.03
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	5	1.03
(1,114)	1:50:A:SER:HB3	1:52:A:LYS:HB2	18	1.03
(2,1646)	1:36:A:ILE:HD12	1:33:A:ARG:HG3	14	1.02
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	18	1.02
(2,1029)	1:113:A:VAL:HG13	1:104:A:HIS:H	6	1.02
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD21	7	1.02
(2,919)	1:125:A:LEU:HD22	1:100:A:LEU:H	1	1.02
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE3	7	1.02
(2,714)	1:127:A:MET:H	1:125:A:LEU:HD13	4	1.02
(2,604)	1:124:A:TYR:HE2	1:14:A:GLU:HG2	12	1.02
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	18	1.02
(2,420)	1:74:A:LEU:HD12	1:55:A:ARG:HA	8	1.02
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	4	1.02
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB3	9	1.02
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	1	1.02
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	7	1.02
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	11	1.02
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	17	1.02
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD13	11	1.02
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	10	1.02
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG21	9	1.02
(1,2520)	1:143:A:GLN:HE22	1:12:A:LYS:HB2	14	1.02
(1,2489)	1:13:A:LEU:HD21	1:17:A:GLU:H	12	1.02
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD12	8	1.02
(1,2123)	1:82:A:ALA:H	1:81:A:GLU:HG3	14	1.02
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	5	1.02
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	14	1.02
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	2	1.02
(1,300)	1:143:A:GLN:H	1:12:A:LYS:HG3	19	1.02
(1,290)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	3	1.02
(1,290)	1:23:A:LEU:HD21	1:33:A:ARG:HD2	16	1.02
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	5	1.02
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	8	1.02
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	2	1.02
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H151	20	1.01
(2,1594)	2:1001:A:OLA:H31	1:41:A:VAL:HG12	19	1.01
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG12	20	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	3	1.01
(2,707)	1:41:A:VAL:HG12	1:62:A:THR:HG1	14	1.01
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG22	6	1.01
(2,517)	1:96:A:ASP:H	1:94:A:LEU:HD22	10	1.01
(2,442)	1:83:A:LEU:H	1:83:A:LEU:HD23	15	1.01
(2,414)	1:73:A:ALA:HB2	1:76:A:GLU:HG2	10	1.01
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	13	1.01
(2,144)	1:126:A:VAL:HG23	1:124:A:TYR:HD2	2	1.01
(2,143)	1:11:A:PHE:HD2	1:10:A:THR:HG21	18	1.01
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	13	1.01
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	5	1.01
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD22	15	1.01
(1,1963)	1:100:A:LEU:HD13	1:93:A:ASP:H	16	1.01
(1,1087)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	12	1.01
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG12	3	1.01
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	11	1.01
(1,448)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	19	1.01
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD11	9	1.01
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG11	5	1.01
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	13	1.01
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	19	1.01
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD13	1	1.01
(2,1589)	1:129:A:MET:HB3	2:1001:A:OLA:H181	16	1.0
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD13	16	1.0
(2,1216)	1:34:A:GLN:HE22	1:33:A:ARG:HG2	1	1.0
(2,1098)	1:132:A:LYS:HB3	1:131:A:TRP:HE1	2	1.0
(2,810)	1:52:A:LYS:HE3	1:50:A:SER:HB3	15	1.0
(2,636)	1:134:A:VAL:HG12	1:130:A:SER:HB3	8	1.0
(2,597)	1:118:A:TYR:HD2	1:127:A:MET:HG3	14	1.0
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD21	17	1.0
(2,486)	1:90:A:ILE:HG21	1:104:A:HIS:HB3	2	1.0
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	11	1.0
(2,423)	1:3:A:LEU:HD23	1:74:A:LEU:HD13	2	1.0
(2,409)	1:70:A:LYS:HB3	1:71:A:ASP:HB2	4	1.0
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	20	1.0
(2,274)	1:83:A:LEU:HD21	1:66:A:ASP:HB3	20	1.0
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	10	1.0
(2,161)	1:13:A:LEU:HD23	1:140:A:TYR:HE1	11	1.0
(2,143)	1:11:A:PHE:HD2	1:10:A:THR:HG22	12	1.0
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	3	1.0
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD21	2	1.0
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD11	16	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,448)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	20	1.0
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD13	6	1.0
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG12	11	1.0
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	1	1.0
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD13	15	1.0
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	4	0.99
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	4	0.99
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	6	0.99
(2,1029)	1:105:A:ILE:HD12	1:104:A:HIS:H	20	0.99
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	15	0.99
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	6	0.99
(2,667)	1:136:A:THR:HG21	1:135:A:SER:HB2	16	0.99
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	13	0.99
(2,613)	1:125:A:LEU:HD23	1:100:A:LEU:HB2	8	0.99
(2,536)	1:99:A:THR:HG23	1:117:A:GLU:HB3	14	0.99
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	10	0.99
(2,409)	1:70:A:LYS:HB3	1:71:A:ASP:HB2	14	0.99
(2,309)	1:39:A:ALA:H	1:38:A:LEU:HD11	9	0.99
(2,286)	2:1001:A:OLA:H172	1:36:A:ILE:HG21	13	0.99
(2,278)	1:35:A:VAL:HG21	2:1001:A:OLA:H10	15	0.99
(2,262)	1:30:A:TRP:HA	1:33:A:ARG:HG3	2	0.99
(2,216)	1:23:A:LEU:HD21	1:22:A:TYR:HB2	13	0.99
(2,160)	1:13:A:LEU:HD23	1:140:A:TYR:HD1	10	0.99
(2,160)	1:13:A:LEU:HD23	1:41:A:VAL:H	14	0.99
(2,82)	1:125:A:LEU:HD12	1:120:A:ARG:HD3	7	0.99
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD21	17	0.99
(1,1216)	1:70:A:LYS:HG2	1:68:A:HIS:HD2	19	0.99
(1,1172)	1:125:A:LEU:HD21	1:120:A:ARG:HD2	1	0.99
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	1	0.99
(1,557)	1:63:A:THR:HG21	1:40:A:GLY:HA2	17	0.99
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	1	0.99
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD11	17	0.99
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	18	0.99
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	12	0.99
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD12	14	0.99
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD11	3	0.99
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	5	0.99
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD11	18	0.99
(1,114)	1:50:A:SER:HB3	1:52:A:LYS:HB2	13	0.99
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD12	7	0.98
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	9	0.98
(2,1112)	1:143:A:GLN:HE21	1:142:A:LYS:HG2	2	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	16	0.98
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE1	1	0.98
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE3	11	0.98
(2,684)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	4	0.98
(2,684)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	17	0.98
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG12	10	0.98
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	3	0.98
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG23	19	0.98
(2,400)	1:83:A:LEU:HD12	1:65:A:LYS:HG2	5	0.98
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG22	6	0.98
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	17	0.98
(2,316)	1:41:A:VAL:HG22	1:41:A:VAL:H	3	0.98
(2,278)	1:35:A:VAL:HG23	2:1001:A:OLA:H10	10	0.98
(2,125)	1:35:A:VAL:HG11	1:64:A:LYS:HE3	14	0.98
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	3	0.98
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD23	8	0.98
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD23	13	0.98
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD23	12	0.98
(1,1192)	1:23:A:LEU:HD12	1:32:A:MET:HE3	14	0.98
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE3	16	0.98
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	8	0.98
(1,1087)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	15	0.98
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG13	3	0.98
(1,794)	1:100:A:LEU:HD12	1:100:A:LEU:HA	16	0.98
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	8	0.98
(1,557)	1:63:A:THR:HG21	1:40:A:GLY:HA2	15	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD12	3	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD13	11	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	13	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD13	16	0.98
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	20	0.98
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	11	0.98
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	1	0.98
(2,1648)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	18	0.97
(2,1646)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	4	0.97
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HB2	14	0.97
(2,1029)	1:113:A:VAL:HG13	1:104:A:HIS:H	16	0.97
(2,1029)	1:113:A:VAL:HG12	1:104:A:HIS:H	18	0.97
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	16	0.97
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	12	0.97
(2,691)	1:141:A:LYS:HD2	1:141:A:LYS:H	14	0.97
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG22	12	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	18	0.97
(2,616)	1:125:A:LEU:HD23	1:140:A:TYR:HD2	18	0.97
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG23	6	0.97
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	10	0.97
(2,561)	1:106:A:LYS:HA	1:105:A:ILE:HG22	1	0.97
(2,533)	1:99:A:THR:HG21	1:95:A:LYS:HE3	13	0.97
(2,498)	1:90:A:ILE:HD13	1:78:A:PHE:HD2	18	0.97
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	12	0.97
(2,391)	1:35:A:VAL:HG22	1:64:A:LYS:HD2	19	0.97
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG22	8	0.97
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG12	2	0.97
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG12	15	0.97
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	8	0.97
(2,178)	1:134:A:VAL:HG13	1:18:A:ASN:HB2	16	0.97
(2,84)	1:3:A:LEU:HD21	1:7:A:PHE:H	17	0.97
(2,26)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	4	0.97
(1,2813)	1:127:A:MET:HE3	1:118:A:TYR:HH	1	0.97
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD23	5	0.97
(1,1982)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	15	0.97
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	18	0.97
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	14	0.97
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	15	0.97
(1,448)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	13	0.97
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	18	0.97
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD13	4	0.97
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	10	0.97
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	4	0.97
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	10	0.97
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	15	0.97
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD12	17	0.97
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD11	7	0.97
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD11	9	0.97
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	1	0.97
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	8	0.97
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD12	18	0.97
(2,1606)	1:36:A:ILE:HD11	1:23:A:LEU:HB2	3	0.96
(2,1606)	1:36:A:ILE:HD12	1:23:A:LEU:HB2	14	0.96
(2,1590)	2:1001:A:OLA:H31	1:19:A:PHE:HE1	17	0.96
(2,1567)	1:36:A:ILE:HG12	2:1001:A:OLA:H82	7	0.96
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	5	0.96
(2,919)	1:125:A:LEU:HD22	1:100:A:LEU:H	5	0.96
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	10	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,836)	1:49:A:ALA:HB1	1:48:A:ALA:HA	19	0.96
(2,835)	1:37:A:LYS:HA	1:37:A:LYS:HE2	2	0.96
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	7	0.96
(2,718)	1:73:A:ALA:HB2	1:0:A:SER:HA	2	0.96
(2,691)	1:141:A:LYS:HD2	1:141:A:LYS:H	9	0.96
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG21	19	0.96
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	5	0.96
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	19	0.96
(2,616)	1:125:A:LEU:HD23	1:118:A:TYR:HE1	12	0.96
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	2	0.96
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	16	0.96
(2,534)	1:99:A:THR:HG23	1:95:A:LYS:HD3	8	0.96
(2,527)	1:95:A:LYS:H	1:95:A:LYS:HD3	20	0.96
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG11	5	0.96
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	2	0.96
(2,422)	1:74:A:LEU:HD12	1:4:A:PRO:HD2	5	0.96
(2,414)	1:73:A:ALA:HB1	1:76:A:GLU:HG2	14	0.96
(2,400)	1:83:A:LEU:HD13	1:65:A:LYS:HG2	8	0.96
(2,377)	1:41:A:VAL:HG12	1:62:A:THR:HG23	9	0.96
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	12	0.96
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG23	19	0.96
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD13	3	0.96
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	19	0.96
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	11	0.96
(1,1092)	1:44:A:LYS:HA	1:10:A:THR:HG23	14	0.96
(1,755)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	16	0.96
(1,442)	1:38:A:LEU:HD23	1:38:A:LEU:HB2	10	0.96
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD13	9	0.96
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	18	0.96
(1,186)	1:3:A:LEU:HD21	1:8:A:LEU:HD11	12	0.96
(2,1637)	2:1001:A:OLA:H71	1:62:A:THR:HG1	14	0.95
(2,1591)	1:41:A:VAL:HG11	2:1001:A:OLA:H72	17	0.95
(2,1029)	1:113:A:VAL:HG12	1:104:A:HIS:H	12	0.95
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG21	2	0.95
(2,707)	1:41:A:VAL:HG13	1:62:A:THR:HG1	19	0.95
(2,691)	1:141:A:LYS:HD2	1:141:A:LYS:H	2	0.95
(2,628)	1:116:A:TYR:HB3	1:127:A:MET:HG3	13	0.95
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG22	11	0.95
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	13	0.95
(2,553)	1:103:A:THR:HG21	1:89:A:LYS:HE2	7	0.95
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	2	0.95
(2,459)	1:86:A:THR:HB	1:107:A:VAL:HB	16	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	18	0.95
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	10	0.95
(2,316)	1:41:A:VAL:HG21	1:41:A:VAL:H	10	0.95
(2,293)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	12	0.95
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	18	0.95
(2,161)	1:13:A:LEU:HD22	1:140:A:TYR:HE1	10	0.95
(2,125)	1:35:A:VAL:HG11	1:64:A:LYS:HE3	7	0.95
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	18	0.95
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	2	0.95
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD12	20	0.95
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD21	11	0.95
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	19	0.95
(1,591)	1:70:A:LYS:HE3	1:70:A:LYS:HB3	11	0.95
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	16	0.95
(1,442)	1:38:A:LEU:HD22	1:38:A:LEU:HB2	12	0.95
(1,442)	1:38:A:LEU:HD22	1:38:A:LEU:HB2	13	0.95
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	3	0.95
(2,1670)	2:1001:A:OLA:H82	2:1001:A:OLA:H181	9	0.94
(2,1488)	1:81:A:GLU:H	1:87:A:GLN:HE21	2	0.94
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	1	0.94
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	3	0.94
(2,1175)	1:83:A:LEU:HD23	1:64:A:LYS:H	11	0.94
(2,836)	1:49:A:ALA:HB3	1:50:A:SER:HB3	14	0.94
(2,760)	1:127:A:MET:HE1	1:140:A:TYR:HH	5	0.94
(2,730)	1:58:A:MET:HE2	1:43:A:LYS:H	20	0.94
(2,555)	1:88:A:HIS:HB2	1:105:A:ILE:HG21	6	0.94
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD12	3	0.94
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	17	0.94
(2,442)	1:83:A:LEU:H	1:83:A:LEU:HD23	4	0.94
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG23	6	0.94
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB2	19	0.94
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD13	16	0.94
(1,1226)	1:49:A:ALA:HB2	1:51:A:GLY:H	12	0.94
(1,1220)	1:118:A:TYR:HD2	1:58:A:MET:HE3	10	0.94
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	11	0.94
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	18	0.94
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	19	0.94
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	13	0.94
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	8	0.94
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD11	2	0.94
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD12	6	0.94
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD11	6	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:3:A:LEU:HD21	1:8:A:LEU:HD12	10	0.94
(2,1648)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	5	0.93
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	8	0.93
(2,1606)	1:36:A:ILE:HD13	1:23:A:LEU:HB2	17	0.93
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	4	0.93
(2,1112)	1:143:A:GLN:HE21	1:142:A:LYS:HG2	13	0.93
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD13	2	0.93
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	1	0.93
(2,836)	1:49:A:ALA:HB2	1:50:A:SER:HB3	9	0.93
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	18	0.93
(2,784)	1:35:A:VAL:HG23	1:32:A:MET:HE3	3	0.93
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	13	0.93
(2,714)	1:127:A:MET:H	1:125:A:LEU:HD12	17	0.93
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG23	19	0.93
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG13	15	0.93
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	15	0.93
(2,604)	1:124:A:TYR:HE2	1:139:A:TYR:HB2	15	0.93
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	15	0.93
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	12	0.93
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	4	0.93
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	13	0.93
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	12	0.93
(2,377)	1:41:A:VAL:HG11	1:62:A:THR:HG21	3	0.93
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG12	18	0.93
(2,119)	1:8:A:LEU:HD11	1:9:A:GLY:H	19	0.93
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	14	0.93
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	5	0.93
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD11	19	0.93
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD23	8	0.93
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG11	14	0.93
(1,1092)	1:44:A:LYS:HA	1:10:A:THR:HG21	16	0.93
(1,1087)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	20	0.93
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	19	0.93
(1,227)	1:41:A:VAL:H	1:13:A:LEU:HD11	1	0.93
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD12	8	0.93
(2,1217)	1:63:A:THR:H	1:38:A:LEU:HB3	18	0.92
(2,1027)	1:39:A:ALA:H	1:36:A:ILE:HG22	13	0.92
(2,825)	1:118:A:TYR:HD1	1:58:A:MET:HG3	12	0.92
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD23	9	0.92
(2,691)	1:141:A:LYS:HD2	1:141:A:LYS:H	5	0.92
(2,590)	1:117:A:GLU:HG2	1:115:A:THR:HG22	10	0.92
(2,590)	1:117:A:GLU:HG2	1:101:A:THR:HG23	13	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	15	0.92
(2,500)	1:90:A:ILE:HD13	1:88:A:HIS:H	10	0.92
(2,496)	1:90:A:ILE:HD12	1:69:A:HIS:HA	20	0.92
(2,461)	1:41:A:VAL:HG23	1:60:A:ASN:HB3	17	0.92
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	15	0.92
(2,420)	1:74:A:LEU:HD12	1:55:A:ARG:HA	4	0.92
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG13	12	0.92
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG13	13	0.92
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG13	14	0.92
(2,161)	1:13:A:LEU:HD21	1:140:A:TYR:HE1	8	0.92
(2,144)	1:126:A:VAL:HG22	1:124:A:TYR:HD2	14	0.92
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	11	0.92
(2,26)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	14	0.92
(1,1890)	1:89:A:LYS:H	1:107:A:VAL:HG11	1	0.92
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE3	17	0.92
(1,1092)	1:44:A:LYS:HA	1:10:A:THR:HG22	4	0.92
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG21	7	0.92
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	1	0.92
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD21	19	0.92
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	11	0.92
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	20	0.92
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD13	1	0.92
(1,186)	1:3:A:LEU:HD22	1:8:A:LEU:HD13	19	0.92
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	8	0.91
(2,1112)	1:143:A:GLN:HE21	1:61:A:LEU:HD11	8	0.91
(2,1103)	1:87:A:GLN:H	1:107:A:VAL:HG13	9	0.91
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD11	19	0.91
(2,1029)	1:105:A:ILE:HD13	1:104:A:HIS:H	11	0.91
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	5	0.91
(2,734)	1:58:A:MET:HE1	1:100:A:LEU:HD22	1	0.91
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	8	0.91
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	4	0.91
(2,616)	1:125:A:LEU:HD23	1:118:A:TYR:HE1	14	0.91
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HD21	13	0.91
(2,590)	1:117:A:GLU:HG2	1:101:A:THR:HG21	5	0.91
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	14	0.91
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	5	0.91
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	16	0.91
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB1	16	0.91
(2,435)	1:88:A:HIS:HB3	1:82:A:ALA:HB3	19	0.91
(2,413)	1:73:A:ALA:HB3	1:54:A:ASP:HB3	5	0.91
(2,377)	1:41:A:VAL:HG13	1:62:A:THR:HG23	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG11	4	0.91
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG13	5	0.91
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG11	6	0.91
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG12	17	0.91
(2,183)	1:21:A:GLU:HA	1:24:A:LYS:HE3	19	0.91
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	8	0.91
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	19	0.91
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	10	0.91
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	20	0.91
(2,26)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	11	0.91
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD21	2	0.91
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE1	6	0.91
(1,1087)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	18	0.91
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	15	0.91
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG13	8	0.91
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	10	0.91
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG11	13	0.91
(1,794)	1:100:A:LEU:HD11	1:100:A:LEU:HA	14	0.91
(1,794)	1:100:A:LEU:HD12	1:100:A:LEU:HA	15	0.91
(1,792)	1:100:A:LEU:HD13	1:118:A:TYR:HD2	14	0.91
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD11	19	0.91
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD12	1	0.91
(1,275)	1:23:A:LEU:HA	1:23:A:LEU:HD11	2	0.91
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	4	0.91
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	11	0.91
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	2	0.91
(2,1605)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	12	0.9
(2,1469)	1:52:A:LYS:HE2	1:52:A:LYS:H	4	0.9
(2,1112)	1:143:A:GLN:HE21	1:61:A:LEU:HD11	17	0.9
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD22	20	0.9
(2,1079)	1:89:A:LYS:H	1:79:A:GLN:HB3	8	0.9
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG21	20	0.9
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	19	0.9
(2,820)	1:41:A:VAL:HG22	1:43:A:LYS:HE2	8	0.9
(2,751)	1:104:A:HIS:HE1	1:82:A:ALA:HB3	9	0.9
(2,732)	1:58:A:MET:HE1	1:67:A:THR:HG1	3	0.9
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HG	20	0.9
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	18	0.9
(2,707)	1:67:A:THR:HG23	1:62:A:THR:HG1	9	0.9
(2,707)	1:67:A:THR:HG22	1:62:A:THR:HG1	17	0.9
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	6	0.9
(2,684)	1:13:A:LEU:HD21	1:140:A:TYR:HE1	14	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,616)	1:125:A:LEU:HD23	1:140:A:TYR:HD2	6	0.9
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HB2	20	0.9
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	17	0.9
(2,590)	1:117:A:GLU:HG2	1:101:A:THR:HG23	14	0.9
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	3	0.9
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG23	4	0.9
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG22	5	0.9
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG22	9	0.9
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	12	0.9
(2,571)	1:106:A:LYS:HB3	1:109:A:ASP:HB2	8	0.9
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	12	0.9
(2,486)	1:90:A:ILE:HG21	1:104:A:HIS:HB3	10	0.9
(2,486)	1:90:A:ILE:HG22	1:104:A:HIS:HB3	15	0.9
(2,426)	1:13:A:LEU:HD21	1:15:A:ARG:HB2	1	0.9
(2,414)	1:73:A:ALA:HB1	1:76:A:GLU:HG2	8	0.9
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG13	1	0.9
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG12	20	0.9
(2,301)	1:37:A:LYS:H	1:37:A:LYS:HE3	19	0.9
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	2	0.9
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	12	0.9
(2,161)	1:13:A:LEU:HD21	1:140:A:TYR:HE2	3	0.9
(2,82)	1:125:A:LEU:HD12	1:120:A:ARG:HD3	4	0.9
(2,49)	1:52:A:LYS:HE2	1:48:A:ALA:HB3	17	0.9
(1,2489)	1:13:A:LEU:HD21	1:17:A:GLU:H	1	0.9
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD13	20	0.9
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	6	0.9
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	16	0.9
(1,1217)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	1	0.9
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	2	0.9
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	18	0.9
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG13	4	0.9
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD12	5	0.9
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	4	0.9
(1,594)	1:70:A:LYS:HG2	1:69:A:HIS:HA	19	0.9
(1,448)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	4	0.9
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD13	18	0.9
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	20	0.9
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	9	0.9
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	2	0.89
(2,1439)	1:13:A:LEU:H	1:143:A:GLN:HE21	12	0.89
(2,1283)	1:127:A:MET:HE2	1:127:A:MET:H	9	0.89
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD12	1	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1037)	1:42:A:THR:H	1:41:A:VAL:HG22	12	0.89
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG23	8	0.89
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB3	4	0.89
(2,731)	1:58:A:MET:HE1	1:61:A:LEU:H	6	0.89
(2,727)	1:3:A:LEU:HD22	1:7:A:PHE:HA	16	0.89
(2,707)	1:67:A:THR:HG22	1:62:A:THR:HG1	3	0.89
(2,707)	1:41:A:VAL:HG12	1:62:A:THR:HG1	13	0.89
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG23	14	0.89
(2,635)	1:130:A:SER:HB3	1:128:A:LYS:HD2	2	0.89
(2,604)	1:124:A:TYR:HE2	1:14:A:GLU:HG2	11	0.89
(2,597)	1:118:A:TYR:HD2	1:99:A:THR:HG23	11	0.89
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG22	1	0.89
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	17	0.89
(2,536)	1:99:A:THR:HG23	1:117:A:GLU:HB3	10	0.89
(2,486)	1:90:A:ILE:HG21	1:104:A:HIS:HB3	16	0.89
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB2	16	0.89
(2,420)	1:106:A:LYS:HG2	1:105:A:ILE:HA	1	0.89
(2,414)	1:73:A:ALA:HB3	1:76:A:GLU:HG2	9	0.89
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	3	0.89
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	11	0.89
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG22	14	0.89
(2,380)	1:65:A:LYS:HB2	2:1001:A:OLA:H9	15	0.89
(2,279)	1:107:A:VAL:HA	1:107:A:VAL:HG21	18	0.89
(2,107)	1:120:A:ARG:HB2	1:7:A:PHE:HB3	16	0.89
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	6	0.89
(2,77)	1:74:A:LEU:HA	1:3:A:LEU:HD13	11	0.89
(2,59)	1:0:A:SER:HB3	1:2:A:THR:HG21	1	0.89
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG23	10	0.89
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD22	15	0.89
(1,2138)	1:107:A:VAL:H	1:107:A:VAL:HG12	16	0.89
(1,1982)	1:8:A:LEU:HD12	1:47:A:ASN:HD22	7	0.89
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE1	20	0.89
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG11	15	0.89
(1,632)	1:74:A:LEU:HD12	1:3:A:LEU:HD13	14	0.89
(1,557)	1:63:A:THR:HG21	1:40:A:GLY:HA2	12	0.89
(1,442)	1:38:A:LEU:HD22	1:38:A:LEU:HB2	7	0.89
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	17	0.89
(1,430)	1:23:A:LEU:HD21	1:37:A:LYS:HG2	10	0.89
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG13	19	0.89
(1,186)	1:3:A:LEU:HD23	1:8:A:LEU:HD12	14	0.89
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	7	0.89
(2,1640)	1:140:A:TYR:HH	1:62:A:THR:HG22	9	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1579)	1:41:A:VAL:HG11	2:1001:A:OLA:H21	13	0.88
(2,1330)	1:79:A:GLN:H	1:89:A:LYS:HB3	16	0.88
(2,825)	1:118:A:TYR:HD2	1:58:A:MET:HG3	17	0.88
(2,825)	1:118:A:TYR:HD2	1:58:A:MET:HG3	18	0.88
(2,791)	1:131:A:TRP:HB2	1:131:A:TRP:HZ2	6	0.88
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	7	0.88
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG23	16	0.88
(2,518)	1:96:A:ASP:H	1:94:A:LEU:HD11	5	0.88
(2,486)	1:90:A:ILE:HG22	1:104:A:HIS:HB3	4	0.88
(2,461)	1:41:A:VAL:HG23	1:60:A:ASN:HB3	19	0.88
(2,446)	1:83:A:LEU:HD13	1:60:A:ASN:HD21	15	0.88
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	13	0.88
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	7	0.88
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	4	0.88
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	20	0.88
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG11	19	0.88
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	5	0.88
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG12	19	0.88
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	12	0.88
(2,125)	1:35:A:VAL:HG12	1:64:A:LYS:HE3	4	0.88
(1,2138)	1:107:A:VAL:H	1:107:A:VAL:HG12	20	0.88
(1,1982)	1:8:A:LEU:HD13	1:47:A:ASN:HD22	10	0.88
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	5	0.88
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	4	0.88
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE1	3	0.88
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE1	19	0.88
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD12	17	0.88
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	10	0.88
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	4	0.88
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG11	9	0.88
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD13	3	0.88
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	18	0.88
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	3	0.88
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	19	0.88
(1,429)	1:23:A:LEU:HD21	1:37:A:LYS:HG3	14	0.88
(1,131)	1:3:A:LEU:HD13	1:7:A:PHE:HD2	20	0.88
(2,1439)	1:13:A:LEU:H	1:143:A:GLN:HE21	1	0.87
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	1	0.87
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG23	14	0.87
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG21	19	0.87
(2,904)	1:106:A:LYS:H	1:106:A:LYS:HE2	7	0.87
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG21	20	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,841)	1:129:A:MET:HE3	1:114:A:GLU:HG3	3	0.87
(2,825)	1:118:A:TYR:HD2	1:58:A:MET:HG3	3	0.87
(2,791)	1:131:A:TRP:HB2	1:131:A:TRP:HZ2	10	0.87
(2,791)	1:131:A:TRP:HB2	1:131:A:TRP:HZ2	14	0.87
(2,791)	1:131:A:TRP:HB2	1:131:A:TRP:HZ2	16	0.87
(2,707)	1:41:A:VAL:HG11	1:62:A:THR:HG1	2	0.87
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG21	8	0.87
(2,561)	1:106:A:LYS:HA	1:105:A:ILE:HG23	20	0.87
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD23	13	0.87
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	12	0.87
(2,500)	1:90:A:ILE:HD11	1:88:A:HIS:H	15	0.87
(2,486)	1:90:A:ILE:HG23	1:104:A:HIS:HB3	1	0.87
(2,386)	1:64:A:LYS:HG3	1:35:A:VAL:HG21	1	0.87
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG11	8	0.87
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG23	9	0.87
(2,278)	1:35:A:VAL:HG22	2:1001:A:OLA:H10	1	0.87
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB1	7	0.87
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB3	20	0.87
(2,188)	1:134:A:VAL:HG12	1:21:A:GLU:HG2	18	0.87
(2,160)	1:13:A:LEU:HD23	1:41:A:VAL:H	17	0.87
(2,143)	1:42:A:THR:HG23	1:140:A:TYR:HD1	20	0.87
(2,114)	1:8:A:LEU:HD22	1:5:A:ASP:HA	5	0.87
(2,114)	1:8:A:LEU:HD23	1:5:A:ASP:HA	19	0.87
(2,82)	1:125:A:LEU:HD13	1:120:A:ARG:HD3	19	0.87
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD21	10	0.87
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	13	0.87
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	15	0.87
(1,2138)	1:107:A:VAL:H	1:107:A:VAL:HG12	17	0.87
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG12	12	0.87
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE3	4	0.87
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE2	9	0.87
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE2	20	0.87
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD12	10	0.87
(1,1092)	1:44:A:LYS:HA	1:10:A:THR:HG23	5	0.87
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	5	0.87
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG23	6	0.87
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	11	0.87
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	17	0.87
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	5	0.87
(1,288)	1:23:A:LEU:HD21	1:33:A:ARG:HA	15	0.87
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	5	0.87
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	8	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	12	0.87
(2,1658)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	8	0.86
(2,1469)	1:52:A:LYS:HE3	1:52:A:LYS:H	7	0.86
(2,1037)	1:42:A:THR:H	1:41:A:VAL:HG21	6	0.86
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG23	17	0.86
(2,840)	1:129:A:MET:HE1	1:114:A:GLU:HG3	11	0.86
(2,791)	1:131:A:TRP:HB2	1:131:A:TRP:HZ2	5	0.86
(2,791)	1:131:A:TRP:HB2	1:131:A:TRP:HZ2	8	0.86
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD23	4	0.86
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	14	0.86
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	15	0.86
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	19	0.86
(2,697)	1:65:A:LYS:HE2	1:83:A:LEU:HA	13	0.86
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	16	0.86
(2,543)	1:58:A:MET:HE3	1:100:A:LEU:HD21	13	0.86
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD11	12	0.86
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB2	9	0.86
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	15	0.86
(2,415)	1:0:A:SER:HB2	1:73:A:ALA:HB3	15	0.86
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HD11	14	0.86
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	1	0.86
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD23	7	0.86
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	8	0.86
(2,81)	1:125:A:LEU:HD13	1:45:A:PHE:HB2	17	0.86
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG23	7	0.86
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	15	0.86
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG12	8	0.86
(1,1278)	1:113:A:VAL:H	1:113:A:VAL:HG13	7	0.86
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE3	13	0.86
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE2	2	0.86
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE3	4	0.86
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	7	0.86
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	20	0.86
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	2	0.86
(1,448)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	1	0.86
(1,448)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	2	0.86
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	20	0.86
(2,1606)	2:1001:A:OLA:H111	1:36:A:ILE:HD12	5	0.85
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG13	7	0.85
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	11	0.85
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	11	0.85
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD13	4	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1037)	1:42:A:THR:H	1:41:A:VAL:HG22	13	0.85
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG21	15	0.85
(2,1029)	1:113:A:VAL:HG11	1:104:A:HIS:H	14	0.85
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	18	0.85
(2,836)	1:49:A:ALA:HB3	1:48:A:ALA:HA	1	0.85
(2,836)	1:49:A:ALA:HB1	1:48:A:ALA:HA	11	0.85
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	6	0.85
(2,751)	1:104:A:HIS:HE1	1:82:A:ALA:HB3	7	0.85
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	17	0.85
(2,707)	1:41:A:VAL:HG13	1:62:A:THR:HG1	6	0.85
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG22	13	0.85
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD23	15	0.85
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	1	0.85
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	10	0.85
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	2	0.85
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG23	19	0.85
(2,320)	1:67:A:THR:HG22	1:60:A:ASN:HD21	15	0.85
(2,316)	1:41:A:VAL:HG22	1:41:A:VAL:H	16	0.85
(2,293)	1:36:A:ILE:HD11	2:1001:A:OLA:H152	7	0.85
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	14	0.85
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	20	0.85
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG22	14	0.85
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	1	0.85
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE3	19	0.85
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE1	2	0.85
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE1	8	0.85
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE3	10	0.85
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE2	12	0.85
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE3	16	0.85
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	6	0.85
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG11	14	0.85
(1,868)	1:113:A:VAL:HG23	1:113:A:VAL:H	17	0.85
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG11	12	0.85
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG11	14	0.85
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG11	18	0.85
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD21	12	0.85
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD22	20	0.85
(1,784)	1:45:A:PHE:HD2	1:100:A:LEU:HD21	19	0.85
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	16	0.85
(1,448)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	14	0.85
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD13	16	0.85
(1,430)	1:23:A:LEU:HD21	1:37:A:LYS:HG2	5	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD13	8	0.85
(1,288)	1:23:A:LEU:HD21	1:33:A:ARG:HA	17	0.85
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	18	0.85
(2,1645)	1:140:A:TYR:HH	1:62:A:THR:HG22	9	0.84
(2,1579)	1:41:A:VAL:HG13	2:1001:A:OLA:H21	2	0.84
(2,1544)	1:134:A:VAL:HG13	1:21:A:GLU:H	5	0.84
(2,1488)	1:81:A:GLU:H	1:87:A:GLN:HE21	8	0.84
(2,1466)	1:98:A:ASN:H	1:95:A:LYS:HD3	3	0.84
(2,1330)	1:79:A:GLN:H	1:89:A:LYS:HB3	18	0.84
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	2	0.84
(2,1283)	1:127:A:MET:HE3	1:127:A:MET:H	7	0.84
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG23	19	0.84
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	20	0.84
(2,760)	1:127:A:MET:HE2	1:140:A:TYR:HH	19	0.84
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	4	0.84
(2,707)	1:67:A:THR:HG23	1:62:A:THR:HG1	8	0.84
(2,707)	1:41:A:VAL:HG11	1:62:A:THR:HG1	15	0.84
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	1	0.84
(2,613)	1:125:A:LEU:HD22	1:100:A:LEU:HB2	17	0.84
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG22	14	0.84
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	6	0.84
(2,577)	1:110:A:PRO:HG3	1:105:A:ILE:HG23	20	0.84
(2,561)	1:106:A:LYS:HA	1:105:A:ILE:HG21	17	0.84
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD23	6	0.84
(2,486)	1:90:A:ILE:HG22	1:104:A:HIS:HB3	13	0.84
(2,446)	1:83:A:LEU:HD13	1:60:A:ASN:HD21	6	0.84
(2,376)	1:40:A:GLY:HA3	1:62:A:THR:HG22	18	0.84
(2,315)	1:41:A:VAL:H	1:41:A:VAL:HG11	11	0.84
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	8	0.84
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	11	0.84
(2,184)	1:24:A:LYS:HD2	1:21:A:GLU:HA	12	0.84
(2,66)	1:1:A:LYS:HG2	1:74:A:LEU:HD21	13	0.84
(2,65)	1:1:A:LYS:HG2	1:1:A:LYS:HE3	12	0.84
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	16	0.84
(1,1474)	1:105:A:ILE:HD13	1:106:A:LYS:H	3	0.84
(1,1474)	1:105:A:ILE:HD13	1:106:A:LYS:H	15	0.84
(1,1464)	1:8:A:LEU:HD11	1:45:A:PHE:HB2	15	0.84
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	1	0.84
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	7	0.84
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE3	10	0.84
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE1	11	0.84
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE2	20	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE1	17	0.84
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE1	17	0.84
(1,1087)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	6	0.84
(1,785)	1:100:A:LEU:HD22	1:45:A:PHE:HE2	3	0.84
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	9	0.84
(1,591)	1:70:A:LYS:HE3	1:70:A:LYS:HB3	13	0.84
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	7	0.84
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	8	0.84
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	9	0.84
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	1	0.84
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	10	0.84
(2,1591)	1:41:A:VAL:HG12	2:1001:A:OLA:H72	10	0.83
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	18	0.83
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	5	0.83
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	11	0.83
(2,840)	1:129:A:MET:HE3	1:114:A:GLU:HG3	1	0.83
(2,825)	1:118:A:TYR:HD1	1:127:A:MET:HG2	11	0.83
(2,786)	1:32:A:MET:HE2	1:36:A:ILE:HA	1	0.83
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	11	0.83
(2,730)	1:58:A:MET:HE3	1:43:A:LYS:H	4	0.83
(2,730)	1:58:A:MET:HE1	1:43:A:LYS:H	5	0.83
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG22	15	0.83
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	19	0.83
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD21	5	0.83
(2,486)	1:90:A:ILE:HG21	1:104:A:HIS:HB3	14	0.83
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	19	0.83
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB2	12	0.83
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	5	0.83
(2,377)	1:41:A:VAL:HG13	1:62:A:THR:HG21	10	0.83
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	16	0.83
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	17	0.83
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	9	0.83
(2,59)	1:94:A:LEU:HB3	1:0:A:SER:HB3	9	0.83
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG22	18	0.83
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG22	5	0.83
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG21	20	0.83
(1,1925)	1:107:A:VAL:HG23	1:79:A:GLN:HE22	15	0.83
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	8	0.83
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	20	0.83
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD13	18	0.83
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE2	1	0.83
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	1	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	19	0.83
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	13	0.83
(1,591)	1:70:A:LYS:HE3	1:70:A:LYS:HB3	19	0.83
(1,548)	1:62:A:THR:HG22	1:60:A:ASN:HB2	8	0.83
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	13	0.83
(1,114)	1:50:A:SER:HB3	1:52:A:LYS:HB2	16	0.83
(2,1581)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	14	0.82
(2,1560)	1:11:A:PHE:H	1:44:A:LYS:HG3	6	0.82
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	15	0.82
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG21	5	0.82
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG23	18	0.82
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG23	10	0.82
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	11	0.82
(2,727)	1:3:A:LEU:HD21	1:7:A:PHE:HA	10	0.82
(2,707)	1:41:A:VAL:HG13	1:62:A:THR:HG1	4	0.82
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	1	0.82
(2,543)	1:58:A:MET:HE2	1:100:A:LEU:HD23	14	0.82
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD23	16	0.82
(2,486)	1:90:A:ILE:HG22	1:104:A:HIS:HB3	3	0.82
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG12	8	0.82
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB1	4	0.82
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	4	0.82
(2,422)	1:74:A:LEU:HD11	1:4:A:PRO:HD2	19	0.82
(2,409)	1:52:A:LYS:HD3	1:71:A:ASP:HB2	3	0.82
(2,393)	1:89:A:LYS:HE2	1:105:A:ILE:HG21	8	0.82
(2,316)	1:41:A:VAL:HG23	1:41:A:VAL:H	9	0.82
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	3	0.82
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	2	0.82
(2,65)	1:1:A:LYS:HG2	1:1:A:LYS:HE3	9	0.82
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	16	0.82
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG23	16	0.82
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG21	2	0.82
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	7	0.82
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD21	12	0.82
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD23	1	0.82
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG12	18	0.82
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	10	0.82
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	14	0.82
(1,1192)	1:23:A:LEU:HD11	1:32:A:MET:HE1	15	0.82
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE3	14	0.82
(1,1172)	1:125:A:LEU:HD21	1:120:A:ARG:HD2	5	0.82
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE1	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	15	0.82
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	13	0.82
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	18	0.82
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	2	0.82
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	1	0.81
(2,1606)	1:36:A:ILE:HD11	1:23:A:LEU:HB2	20	0.81
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	10	0.81
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG22	2	0.81
(2,1027)	1:39:A:ALA:H	1:36:A:ILE:HG21	10	0.81
(2,860)	1:64:A:LYS:HB2	2:1001:A:OLA:H9	2	0.81
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG21	11	0.81
(2,841)	1:129:A:MET:HE2	1:114:A:GLU:HG3	8	0.81
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE3	15	0.81
(2,836)	1:49:A:ALA:HB1	1:48:A:ALA:HA	2	0.81
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	5	0.81
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	3	0.81
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	16	0.81
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	18	0.81
(2,782)	1:127:A:MET:HE2	1:116:A:TYR:HA	13	0.81
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	9	0.81
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	3	0.81
(2,706)	1:41:A:VAL:HG22	1:62:A:THR:HG1	7	0.81
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	17	0.81
(2,618)	1:125:A:LEU:HD22	1:100:A:LEU:H	7	0.81
(2,606)	1:124:A:TYR:HE1	1:141:A:LYS:HD3	9	0.81
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG23	18	0.81
(2,561)	1:106:A:LYS:HA	1:105:A:ILE:HG21	16	0.81
(2,553)	1:103:A:THR:HG21	1:89:A:LYS:HE2	11	0.81
(2,486)	1:90:A:ILE:HG22	1:104:A:HIS:HB3	12	0.81
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HB2	19	0.81
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB2	11	0.81
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB3	12	0.81
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	6	0.81
(2,409)	1:52:A:LYS:HB3	1:71:A:ASP:HB2	17	0.81
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	16	0.81
(2,188)	1:134:A:VAL:HG12	1:21:A:GLU:HG2	9	0.81
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	13	0.81
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	11	0.81
(2,160)	1:13:A:LEU:HD21	1:41:A:VAL:H	2	0.81
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	14	0.81
(2,81)	1:125:A:LEU:HD13	1:45:A:PHE:HB2	14	0.81
(2,45)	1:49:A:ALA:HB2	1:48:A:ALA:HA	3	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:49:A:ALA:HB1	1:48:A:ALA:HA	14	0.81
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	5	0.81
(1,1464)	1:8:A:LEU:HD12	1:45:A:PHE:HB2	9	0.81
(1,1245)	1:11:A:PHE:H	1:44:A:LYS:HG2	9	0.81
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	2	0.81
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	11	0.81
(1,1087)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	11	0.81
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	4	0.81
(1,1034)	1:124:A:TYR:HE2	1:141:A:LYS:HB3	2	0.81
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD22	14	0.81
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	5	0.81
(1,448)	1:41:A:VAL:HG22	1:140:A:TYR:HE1	18	0.81
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD13	14	0.81
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	7	0.81
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	19	0.81
(2,1605)	1:36:A:ILE:HD11	2:1001:A:OLA:H152	7	0.8
(2,1601)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	1	0.8
(2,1579)	1:41:A:VAL:HG13	2:1001:A:OLA:H21	7	0.8
(2,1561)	1:66:A:ASP:H	1:65:A:LYS:HD2	5	0.8
(2,1037)	1:42:A:THR:H	1:41:A:VAL:HG22	1	0.8
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB1	15	0.8
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	5	0.8
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	15	0.8
(2,825)	1:118:A:TYR:HD1	1:127:A:MET:HG2	15	0.8
(2,819)	1:36:A:ILE:HG23	2:1001:A:OLA:H82	19	0.8
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	14	0.8
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG22	5	0.8
(2,731)	1:58:A:MET:HE1	1:61:A:LEU:H	19	0.8
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	3	0.8
(2,707)	1:67:A:THR:HG21	1:62:A:THR:HG1	5	0.8
(2,667)	1:130:A:SER:HB2	1:136:A:THR:HG21	2	0.8
(2,597)	1:118:A:TYR:HD2	1:127:A:MET:HG3	12	0.8
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG12	9	0.8
(2,571)	1:106:A:LYS:HB3	1:109:A:ASP:HB2	1	0.8
(2,568)	1:113:A:VAL:HG23	1:113:A:VAL:HA	1	0.8
(2,568)	1:113:A:VAL:HG23	1:113:A:VAL:HA	2	0.8
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG23	5	0.8
(2,568)	1:113:A:VAL:HG23	1:113:A:VAL:HA	15	0.8
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	15	0.8
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	3	0.8
(2,486)	1:90:A:ILE:HG23	1:104:A:HIS:HB3	6	0.8
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB1	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,391)	1:35:A:VAL:HG23	1:64:A:LYS:HD2	8	0.8
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	4	0.8
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB1	17	0.8
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	13	0.8
(2,188)	1:134:A:VAL:HG12	1:21:A:GLU:HG2	15	0.8
(2,119)	1:8:A:LEU:HD12	1:9:A:GLY:H	9	0.8
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG22	4	0.8
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG22	4	0.8
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	4	0.8
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE3	8	0.8
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE3	18	0.8
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	10	0.8
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG23	9	0.8
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	6	0.8
(1,786)	1:45:A:PHE:HZ	1:100:A:LEU:HD21	2	0.8
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	2	0.8
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	17	0.8
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	6	0.8
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	12	0.79
(2,1591)	1:41:A:VAL:HG13	2:1001:A:OLA:H72	19	0.79
(2,1521)	1:7:A:PHE:H	1:8:A:LEU:HB3	18	0.79
(2,1313)	1:125:A:LEU:HA	1:124:A:TYR:H	8	0.79
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	7	0.79
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	14	0.79
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	18	0.79
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG23	11	0.79
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	3	0.79
(2,840)	1:129:A:MET:HE3	1:114:A:GLU:HG3	7	0.79
(2,836)	1:49:A:ALA:HB3	1:48:A:ALA:HA	7	0.79
(2,819)	1:36:A:ILE:HG22	2:1001:A:OLA:H82	17	0.79
(2,760)	1:127:A:MET:HE3	1:140:A:TYR:HH	8	0.79
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD23	19	0.79
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG11	10	0.79
(2,545)	1:100:A:LEU:HD22	1:94:A:LEU:HD22	14	0.79
(2,502)	1:90:A:ILE:HD11	1:90:A:ILE:H	9	0.79
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	18	0.79
(2,486)	1:90:A:ILE:HG21	1:104:A:HIS:HB3	20	0.79
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	17	0.79
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	2	0.79
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	12	0.79
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB1	6	0.79
(2,274)	1:61:A:LEU:HD22	1:66:A:ASP:HB3	18	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG12	6	0.79
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	6	0.79
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD23	19	0.79
(2,65)	1:12:A:LYS:HE3	1:12:A:LYS:HG3	11	0.79
(2,7)	1:31:A:ILE:HD12	1:34:A:GLN:HB2	17	0.79
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG23	9	0.79
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG23	18	0.79
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	10	0.79
(1,1474)	1:105:A:ILE:HD13	1:106:A:LYS:H	20	0.79
(1,1464)	1:8:A:LEU:HD11	1:45:A:PHE:HB2	16	0.79
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	5	0.79
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	19	0.79
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	10	0.79
(1,1173)	1:125:A:LEU:HD21	1:120:A:ARG:HD3	1	0.79
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	9	0.79
(1,721)	1:102:A:GLU:HG2	1:90:A:ILE:HG23	1	0.79
(1,441)	1:38:A:LEU:HD23	1:38:A:LEU:HA	20	0.79
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD13	16	0.79
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	10	0.79
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	19	0.79
(1,194)	1:10:A:THR:H	1:10:A:THR:HG23	9	0.79
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	19	0.79
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD13	12	0.79
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	14	0.79
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD11	15	0.79
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD13	20	0.79
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	11	0.78
(2,1627)	1:83:A:LEU:HB2	1:84:A:ASP:HB3	8	0.78
(2,1583)	2:1001:A:OLA:H22	1:127:A:MET:HG3	10	0.78
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG12	19	0.78
(2,1537)	1:41:A:VAL:H	1:41:A:VAL:HG13	12	0.78
(2,1313)	1:125:A:LEU:HA	1:124:A:TYR:H	4	0.78
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	2	0.78
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	6	0.78
(2,1232)	1:85:A:SER:H	1:81:A:GLU:HB2	11	0.78
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE3	20	0.78
(2,819)	1:36:A:ILE:HG23	2:1001:A:OLA:H82	6	0.78
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	10	0.78
(2,727)	1:3:A:LEU:HD21	1:7:A:PHE:HA	2	0.78
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG22	3	0.78
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	11	0.78
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	10	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	6	0.78
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	7	0.78
(2,435)	1:104:A:HIS:HB2	1:82:A:ALA:HB2	9	0.78
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB1	4	0.78
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	2	0.78
(2,144)	1:11:A:PHE:HD1	1:141:A:LYS:HG3	15	0.78
(2,114)	1:8:A:LEU:HD23	1:5:A:ASP:HA	15	0.78
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	4	0.78
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	4	0.78
(1,2826)	1:127:A:MET:HE3	1:118:A:TYR:HH	1	0.78
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	13	0.78
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	15	0.78
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	12	0.78
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	13	0.78
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	8	0.78
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	14	0.78
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE3	7	0.78
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	19	0.78
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	5	0.78
(1,600)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	9	0.78
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	7	0.78
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	4	0.78
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	6	0.78
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG21	6	0.78
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG23	18	0.78
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG23	19	0.78
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD13	9	0.78
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	18	0.78
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	4	0.78
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	9	0.78
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	10	0.78
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	11	0.78
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	8	0.78
(2,1670)	2:1001:A:OLA:H82	2:1001:A:OLA:H183	13	0.77
(2,1591)	1:41:A:VAL:HG11	2:1001:A:OLA:H72	16	0.77
(2,1561)	1:66:A:ASP:H	1:65:A:LYS:HD2	7	0.77
(2,1521)	1:7:A:PHE:H	1:8:A:LEU:HB3	1	0.77
(2,1424)	1:41:A:VAL:HG11	1:64:A:LYS:H	18	0.77
(2,1283)	1:127:A:MET:HE1	1:127:A:MET:H	11	0.77
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	7	0.77
(2,1117)	1:95:A:LYS:HD3	1:99:A:THR:H	13	0.77
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG23	8	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	12	0.77
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	16	0.77
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	4	0.77
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD23	15	0.77
(2,731)	1:58:A:MET:HE1	1:61:A:LEU:H	2	0.77
(2,731)	1:58:A:MET:HE3	1:61:A:LEU:H	14	0.77
(2,706)	1:41:A:VAL:HG22	1:62:A:THR:HG1	12	0.77
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG23	9	0.77
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG11	19	0.77
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	15	0.77
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG11	4	0.77
(2,534)	1:99:A:THR:HG23	1:95:A:LYS:HD3	5	0.77
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	13	0.77
(2,320)	1:67:A:THR:HG22	1:60:A:ASN:HD21	20	0.77
(2,316)	1:41:A:VAL:HG23	1:41:A:VAL:H	7	0.77
(2,301)	1:37:A:LYS:H	1:37:A:LYS:HE3	3	0.77
(2,293)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	18	0.77
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG23	10	0.77
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG22	17	0.77
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB3	15	0.77
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	1	0.77
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	14	0.77
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	16	0.77
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG22	5	0.77
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	13	0.77
(2,51)	1:48:A:ALA:HB3	1:56:A:TYR:HB3	6	0.77
(2,26)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	16	0.77
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG23	1	0.77
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG22	3	0.77
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	20	0.77
(1,2463)	1:111:A:THR:HG23	1:113:A:VAL:H	14	0.77
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD23	7	0.77
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	6	0.77
(1,1220)	1:118:A:TYR:HD2	1:58:A:MET:HE3	13	0.77
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	3	0.77
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	10	0.77
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	8	0.77
(1,743)	1:93:A:ASP:HB2	1:91:A:THR:HG21	9	0.77
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG12	8	0.77
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG13	18	0.77
(1,630)	1:74:A:LEU:HD13	1:3:A:LEU:H	12	0.77
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	5	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	20	0.77
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	6	0.77
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	1	0.77
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	12	0.77
(1,288)	1:23:A:LEU:HD23	1:33:A:ARG:HA	10	0.77
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	18	0.77
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	16	0.77
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	4	0.77
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD11	6	0.77
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD11	15	0.77
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	16	0.76
(2,1648)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	3	0.76
(2,1537)	1:41:A:VAL:H	1:41:A:VAL:HG13	1	0.76
(2,1439)	1:13:A:LEU:H	1:143:A:GLN:HE21	3	0.76
(2,1216)	1:34:A:GLN:HE22	1:33:A:ARG:HG2	4	0.76
(2,1125)	1:118:A:TYR:H	1:127:A:MET:HB3	6	0.76
(2,1027)	1:39:A:ALA:H	1:36:A:ILE:HG21	12	0.76
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE1	4	0.76
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	3	0.76
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	8	0.76
(2,830)	2:1001:A:OLA:H81	1:36:A:ILE:HA	17	0.76
(2,826)	1:59:A:GLU:HB3	1:61:A:LEU:HD13	16	0.76
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	18	0.76
(2,819)	1:36:A:ILE:HG21	2:1001:A:OLA:H82	18	0.76
(2,789)	1:26:A:ARG:HD3	1:131:A:TRP:HZ3	3	0.76
(2,783)	1:127:A:MET:HE1	1:140:A:TYR:HE2	3	0.76
(2,782)	1:127:A:MET:HE2	1:116:A:TYR:HA	5	0.76
(2,779)	1:119:A:ARG:HA	1:119:A:ARG:HD2	7	0.76
(2,760)	1:127:A:MET:HE2	1:140:A:TYR:HH	12	0.76
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD22	15	0.76
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG23	7	0.76
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG23	12	0.76
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG21	17	0.76
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	6	0.76
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG22	2	0.76
(2,543)	1:100:A:LEU:HD22	1:74:A:LEU:HB2	18	0.76
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	18	0.76
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	13	0.76
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	6	0.76
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB1	18	0.76
(2,414)	1:73:A:ALA:HB3	1:76:A:GLU:HG2	1	0.76
(2,380)	2:1001:A:OLA:H9	1:64:A:LYS:HB3	20	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB3	1	0.76
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	15	0.76
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	3	0.76
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	10	0.76
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	20	0.76
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	13	0.76
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	15	0.76
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD23	9	0.76
(2,49)	1:57:A:ASP:HB3	1:48:A:ALA:HB1	8	0.76
(2,7)	1:31:A:ILE:HD13	1:34:A:GLN:HB2	19	0.76
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG23	11	0.76
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG22	5	0.76
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	18	0.76
(1,1474)	1:105:A:ILE:HD13	1:106:A:LYS:H	14	0.76
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	18	0.76
(1,1464)	1:8:A:LEU:HD12	1:45:A:PHE:HB2	3	0.76
(1,1464)	1:8:A:LEU:HD12	1:45:A:PHE:HB2	18	0.76
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE3	5	0.76
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	11	0.76
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD11	10	0.76
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	6	0.76
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	8	0.76
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	18	0.76
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG21	2	0.76
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	20	0.76
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD11	9	0.76
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	4	0.76
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	18	0.76
(1,246)	1:136:A:THR:HG1	1:18:A:ASN:HB2	19	0.76
(1,194)	1:10:A:THR:H	1:10:A:THR:HG23	6	0.76
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	5	0.76
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	19	0.76
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD12	6	0.76
(2,1656)	1:19:A:PHE:HZ	2:1001:A:OLA:H172	9	0.75
(2,1648)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	19	0.75
(2,1646)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	12	0.75
(2,1635)	1:83:A:LEU:HG	1:62:A:THR:HG1	13	0.75
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	4	0.75
(2,1581)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	18	0.75
(2,1521)	1:7:A:PHE:H	1:8:A:LEU:HB3	7	0.75
(2,1488)	1:81:A:GLU:H	1:78:A:PHE:HE2	1	0.75
(2,1488)	1:81:A:GLU:H	1:78:A:PHE:HE2	9	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD22	14	0.75
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	3	0.75
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG22	5	0.75
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB1	1	0.75
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	13	0.75
(2,836)	1:49:A:ALA:HB1	1:48:A:ALA:HA	15	0.75
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	17	0.75
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG23	12	0.75
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	15	0.75
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	4	0.75
(2,613)	1:125:A:LEU:HD21	1:100:A:LEU:HD23	9	0.75
(2,568)	1:113:A:VAL:HG22	1:113:A:VAL:HA	3	0.75
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG21	13	0.75
(2,552)	1:131:A:TRP:H	1:134:A:VAL:HG22	19	0.75
(2,533)	1:95:A:LYS:HE2	1:99:A:THR:HG21	12	0.75
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG21	1	0.75
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	13	0.75
(2,500)	1:90:A:ILE:HD11	1:88:A:HIS:H	14	0.75
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	9	0.75
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD12	13	0.75
(2,437)	1:86:A:THR:HB	1:82:A:ALA:HB2	4	0.75
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	2	0.75
(2,422)	1:74:A:LEU:HD12	1:4:A:PRO:HD2	18	0.75
(2,422)	1:74:A:LEU:HD11	1:4:A:PRO:HD2	20	0.75
(2,393)	1:35:A:VAL:HG23	1:64:A:LYS:HE3	6	0.75
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	14	0.75
(2,378)	1:83:A:LEU:HD12	1:62:A:THR:HG22	6	0.75
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	20	0.75
(2,178)	1:134:A:VAL:HG13	1:18:A:ASN:HB2	13	0.75
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	2	0.75
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	5	0.75
(2,86)	1:125:A:LEU:HD13	1:45:A:PHE:HE1	5	0.75
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG21	7	0.75
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	16	0.75
(1,1464)	1:8:A:LEU:HD11	1:45:A:PHE:HB2	19	0.75
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	15	0.75
(1,1014)	1:137:A:SER:HB3	1:126:A:VAL:HG13	9	0.75
(1,792)	1:100:A:LEU:HD11	1:118:A:TYR:HD2	16	0.75
(1,448)	1:41:A:VAL:HG22	1:140:A:TYR:HE1	11	0.75
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	11	0.75
(1,194)	1:10:A:THR:H	1:10:A:THR:HG23	10	0.75
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	7	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	14	0.75
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD11	19	0.75
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD12	17	0.75
(2,1658)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	12	0.74
(2,1596)	1:83:A:LEU:HD21	2:1001:A:OLA:H32	1	0.74
(2,1596)	2:1001:A:OLA:H32	1:83:A:LEU:HD12	16	0.74
(2,1583)	2:1001:A:OLA:H161	2:1001:A:OLA:H21	3	0.74
(2,1581)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	16	0.74
(2,1521)	1:7:A:PHE:H	1:8:A:LEU:HB3	6	0.74
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	17	0.74
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG23	20	0.74
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	16	0.74
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG21	12	0.74
(2,825)	1:118:A:TYR:HD2	1:58:A:MET:HG3	19	0.74
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD22	5	0.74
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG22	5	0.74
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	4	0.74
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	9	0.74
(2,624)	1:128:A:LYS:HD3	1:126:A:VAL:HG13	6	0.74
(2,617)	1:125:A:LEU:HD21	1:127:A:MET:H	11	0.74
(2,558)	1:105:A:ILE:HD13	1:105:A:ILE:HA	19	0.74
(2,496)	1:90:A:ILE:HD11	1:69:A:HIS:HA	16	0.74
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG23	6	0.74
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	7	0.74
(2,461)	1:41:A:VAL:HG22	1:60:A:ASN:HB3	4	0.74
(2,419)	1:74:A:LEU:HD11	1:56:A:TYR:HD1	13	0.74
(2,414)	1:73:A:ALA:HB2	1:76:A:GLU:HG2	4	0.74
(2,356)	1:49:A:ALA:HB3	1:57:A:ASP:HB2	7	0.74
(2,331)	1:44:A:LYS:HA	1:11:A:PHE:HB2	5	0.74
(2,331)	1:44:A:LYS:HA	1:11:A:PHE:HB2	17	0.74
(2,293)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	5	0.74
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	8	0.74
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	2	0.74
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	19	0.74
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	4	0.74
(2,139)	1:14:A:GLU:HG2	1:124:A:TYR:HD2	10	0.74
(2,121)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	6	0.74
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	20	0.74
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	4	0.74
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD22	10	0.74
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB1	14	0.74
(2,54)	1:49:A:ALA:HB3	1:50:A:SER:HB2	10	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	6	0.74
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD23	7	0.74
(1,1464)	1:8:A:LEU:HD11	1:45:A:PHE:HB2	6	0.74
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG21	10	0.74
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	1	0.74
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	4	0.74
(1,429)	1:23:A:LEU:HD21	1:37:A:LYS:HG3	10	0.74
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	1	0.74
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD11	17	0.74
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	2	0.74
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD12	6	0.74
(1,220)	1:13:A:LEU:HD23	1:13:A:LEU:HA	12	0.74
(1,194)	1:10:A:THR:H	1:10:A:THR:HG23	2	0.74
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	3	0.74
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD11	18	0.74
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD11	8	0.74
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD12	13	0.74
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD11	16	0.74
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	9	0.73
(2,1641)	1:140:A:TYR:HH	1:62:A:THR:HG22	9	0.73
(2,1626)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	8	0.73
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	18	0.73
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	16	0.73
(2,1581)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	10	0.73
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	20	0.73
(2,1283)	1:127:A:MET:HE3	1:127:A:MET:H	15	0.73
(2,1274)	1:113:A:VAL:HG13	1:105:A:ILE:H	1	0.73
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	2	0.73
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	12	0.73
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	16	0.73
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	10	0.73
(2,1217)	1:63:A:THR:H	1:83:A:LEU:HG	14	0.73
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD12	19	0.73
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG22	4	0.73
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	14	0.73
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE1	19	0.73
(2,838)	1:127:A:MET:HE1	1:116:A:TYR:HE2	11	0.73
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD23	11	0.73
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	2	0.73
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	15	0.73
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	10	0.73
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	8	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	12	0.73
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG13	20	0.73
(2,555)	1:89:A:LYS:HE2	1:105:A:ILE:HG22	7	0.73
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	14	0.73
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	8	0.73
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	1	0.73
(2,446)	1:83:A:LEU:HD12	1:60:A:ASN:HD21	10	0.73
(2,420)	1:41:A:VAL:HA	1:61:A:LEU:HD11	18	0.73
(2,415)	1:0:A:SER:HB2	1:73:A:ALA:HB1	17	0.73
(2,414)	1:73:A:ALA:HB2	1:76:A:GLU:HG2	5	0.73
(2,413)	1:73:A:ALA:HB3	1:54:A:ASP:HB3	17	0.73
(2,326)	1:140:A:TYR:HE2	1:43:A:LYS:HE3	18	0.73
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG23	7	0.73
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB1	3	0.73
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	18	0.73
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	11	0.73
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD21	20	0.73
(2,61)	1:0:A:SER:HB3	1:1:A:LYS:HG2	15	0.73
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	14	0.73
(2,49)	1:48:A:ALA:HB2	1:55:A:ARG:HD2	16	0.73
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	19	0.73
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	8	0.73
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	16	0.73
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	12	0.73
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG23	7	0.73
(1,2138)	1:107:A:VAL:H	1:107:A:VAL:HG11	1	0.73
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	17	0.73
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	3	0.73
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD11	7	0.73
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	15	0.73
(1,1087)	1:3:A:LEU:HD11	1:4:A:PRO:HD2	9	0.73
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	11	0.73
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	13	0.73
(1,792)	1:100:A:LEU:HD12	1:118:A:TYR:HD2	6	0.73
(1,570)	1:66:A:ASP:H	1:65:A:LYS:HD2	5	0.73
(1,448)	1:41:A:VAL:HG22	1:140:A:TYR:HE1	6	0.73
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	19	0.73
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	18	0.73
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD11	11	0.73
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD12	1	0.73
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD12	3	0.73
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD13	4	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD13	14	0.73
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD13	19	0.73
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	2	0.72
(2,1605)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	18	0.72
(2,1283)	1:127:A:MET:HE3	1:127:A:MET:H	2	0.72
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	9	0.72
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	20	0.72
(2,1079)	1:89:A:LYS:H	1:79:A:GLN:HB3	1	0.72
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG21	5	0.72
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	17	0.72
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	20	0.72
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	16	0.72
(2,786)	1:32:A:MET:HE2	1:36:A:ILE:HA	20	0.72
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG22	10	0.72
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG22	20	0.72
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG13	4	0.72
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	8	0.72
(2,518)	1:96:A:ASP:H	1:94:A:LEU:HD11	13	0.72
(2,502)	1:90:A:ILE:HD11	1:90:A:ILE:H	16	0.72
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	12	0.72
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	11	0.72
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	14	0.72
(2,463)	1:87:A:GLN:HB3	1:107:A:VAL:HG11	19	0.72
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	1	0.72
(2,419)	1:74:A:LEU:HD13	1:56:A:TYR:HD1	15	0.72
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	8	0.72
(2,374)	1:62:A:THR:HG22	1:83:A:LEU:HG	3	0.72
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	3	0.72
(2,320)	1:67:A:THR:HG21	1:60:A:ASN:HD21	1	0.72
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB1	7	0.72
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	8	0.72
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	4	0.72
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	7	0.72
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	11	0.72
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	4	0.72
(2,143)	1:127:A:MET:HG3	1:140:A:TYR:HD2	17	0.72
(2,125)	1:35:A:VAL:HG11	1:64:A:LYS:HE3	12	0.72
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD22	13	0.72
(2,72)	1:74:A:LEU:HG	1:3:A:LEU:HD12	15	0.72
(2,65)	1:1:A:LYS:HG2	1:1:A:LYS:HE3	16	0.72
(2,62)	1:0:A:SER:HB3	1:2:A:THR:H	17	0.72
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	14	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	12	0.72
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD12	3	0.72
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	9	0.72
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	4	0.72
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	13	0.72
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE1	19	0.72
(1,914)	1:124:A:TYR:HE2	1:141:A:LYS:HB3	9	0.72
(1,792)	1:100:A:LEU:HD12	1:118:A:TYR:HD2	13	0.72
(1,755)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	2	0.72
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	15	0.72
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	19	0.72
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG22	11	0.72
(1,443)	1:40:A:GLY:HA2	1:39:A:ALA:HA	7	0.72
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD13	4	0.72
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	10	0.72
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	8	0.72
(1,220)	1:13:A:LEU:HD23	1:13:A:LEU:HA	9	0.72
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	1	0.72
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	13	0.72
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	12	0.72
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	10	0.72
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	8	0.72
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	1	0.72
(1,14)	1:32:A:MET:H	1:31:A:ILE:HD13	20	0.72
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	3	0.71
(2,1648)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	2	0.71
(2,1627)	2:1001:A:OLA:H151	1:84:A:ASP:HB3	14	0.71
(2,1579)	1:41:A:VAL:HG11	2:1001:A:OLA:H21	12	0.71
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	2	0.71
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	15	0.71
(2,1306)	1:49:A:ALA:HB2	1:72:A:TRP:H	3	0.71
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB1	20	0.71
(2,1184)	1:143:A:GLN:HE22	1:61:A:LEU:HD21	2	0.71
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	11	0.71
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	11	0.71
(2,1103)	1:87:A:GLN:H	1:107:A:VAL:HG11	10	0.71
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB3	16	0.71
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	8	0.71
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	13	0.71
(2,801)	1:41:A:VAL:HG12	2:1001:A:OLA:H72	9	0.71
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	7	0.71
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	10	0.71
(2,783)	1:127:A:MET:HE3	1:140:A:TYR:HE2	9	0.71
(2,779)	1:119:A:ARG:HA	1:119:A:ARG:HD2	8	0.71
(2,731)	1:58:A:MET:HE3	1:61:A:LEU:H	3	0.71
(2,707)	1:67:A:THR:HG22	1:62:A:THR:HG1	7	0.71
(2,698)	1:142:A:LYS:HG2	1:142:A:LYS:HE3	1	0.71
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	7	0.71
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	20	0.71
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	19	0.71
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG23	14	0.71
(2,533)	1:99:A:THR:HG21	1:96:A:ASP:HB2	10	0.71
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	15	0.71
(2,501)	1:90:A:ILE:HD13	1:80:A:ASP:H	15	0.71
(2,500)	1:90:A:ILE:HD13	1:88:A:HIS:H	8	0.71
(2,486)	1:90:A:ILE:HG21	1:104:A:HIS:HB3	5	0.71
(2,444)	1:36:A:ILE:H	1:38:A:LEU:HD13	10	0.71
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB2	5	0.71
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	20	0.71
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	15	0.71
(2,419)	1:74:A:LEU:HD11	1:56:A:TYR:HD1	11	0.71
(2,409)	1:70:A:LYS:HB3	1:71:A:ASP:HB2	18	0.71
(2,400)	1:83:A:LEU:HD11	1:65:A:LYS:HG2	2	0.71
(2,350)	1:33:A:ARG:HG2	1:34:A:GLN:H	10	0.71
(2,338)	1:57:A:ASP:HB2	1:46:A:ARG:HG3	7	0.71
(2,326)	1:45:A:PHE:HE1	1:43:A:LYS:HE3	15	0.71
(2,320)	1:67:A:THR:HG21	1:60:A:ASN:HD21	14	0.71
(2,274)	1:61:A:LEU:HD21	1:66:A:ASP:HB3	9	0.71
(2,139)	1:14:A:GLU:HG2	1:124:A:TYR:HD2	3	0.71
(2,132)	1:85:A:SER:H	1:65:A:LYS:HE2	16	0.71
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	7	0.71
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	6	0.71
(2,107)	1:120:A:ARG:HB2	1:7:A:PHE:HB3	20	0.71
(2,56)	1:63:A:THR:HG21	1:40:A:GLY:HA2	17	0.71
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	6	0.71
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	5	0.71
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	15	0.71
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	6	0.71
(1,1474)	1:105:A:ILE:HD13	1:106:A:LYS:H	19	0.71
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	14	0.71
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD12	11	0.71
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	18	0.71
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	14	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1112)	1:58:A:MET:HE3	1:43:A:LYS:HE3	8	0.71
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	2	0.71
(1,1087)	1:3:A:LEU:HD13	1:4:A:PRO:HD2	13	0.71
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	18	0.71
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG11	20	0.71
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	9	0.71
(1,792)	1:100:A:LEU:HD12	1:118:A:TYR:HD2	4	0.71
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	4	0.71
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	8	0.71
(1,386)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	14	0.71
(1,288)	1:23:A:LEU:HD21	1:33:A:ARG:HA	16	0.71
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD11	3	0.71
(1,111)	1:48:A:ALA:HB2	1:71:A:ASP:HB2	13	0.71
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	12	0.71
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD12	15	0.71
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD11	20	0.71
(2,1678)	2:1001:A:OLA:H141	2:1001:A:OLA:H152	14	0.7
(2,1678)	2:1001:A:OLA:H152	2:1001:A:OLA:H142	16	0.7
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	19	0.7
(2,1608)	1:19:A:PHE:HZ	2:1001:A:OLA:H172	9	0.7
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	15	0.7
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG12	6	0.7
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	12	0.7
(2,1521)	1:7:A:PHE:H	1:8:A:LEU:HB3	14	0.7
(2,1469)	1:52:A:LYS:HE2	1:52:A:LYS:H	2	0.7
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG22	18	0.7
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	15	0.7
(2,841)	1:129:A:MET:HE3	1:114:A:GLU:HG3	6	0.7
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	13	0.7
(2,783)	1:127:A:MET:HE2	1:140:A:TYR:HE2	13	0.7
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD11	14	0.7
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	8	0.7
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	2	0.7
(2,706)	1:41:A:VAL:HG22	1:62:A:THR:HG1	9	0.7
(2,698)	1:142:A:LYS:HG2	1:142:A:LYS:HE3	20	0.7
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	18	0.7
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG23	10	0.7
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG22	16	0.7
(2,635)	1:130:A:SER:HB3	1:128:A:LYS:HD2	19	0.7
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	5	0.7
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	7	0.7
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD21	16	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,502)	1:90:A:ILE:HD11	1:90:A:ILE:H	6	0.7
(2,496)	1:90:A:ILE:HD11	1:69:A:HIS:HA	6	0.7
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	13	0.7
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	15	0.7
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	15	0.7
(2,443)	1:143:A:GLN:H	1:142:A:LYS:HG2	1	0.7
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	1	0.7
(2,435)	1:104:A:HIS:HB2	1:82:A:ALA:HB2	11	0.7
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB1	20	0.7
(2,409)	1:70:A:LYS:HB3	1:71:A:ASP:HB2	9	0.7
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	17	0.7
(2,229)	1:25:A:ALA:HB2	1:132:A:LYS:HE2	12	0.7
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	20	0.7
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	12	0.7
(2,144)	1:11:A:PHE:HD1	1:141:A:LYS:HG3	5	0.7
(2,114)	1:8:A:LEU:HD22	1:5:A:ASP:HA	6	0.7
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	9	0.7
(2,56)	1:63:A:THR:HG21	1:40:A:GLY:HA2	15	0.7
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	4	0.7
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG3	1	0.7
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	19	0.7
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	19	0.7
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG21	9	0.7
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	15	0.7
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD21	15	0.7
(1,1762)	1:8:A:LEU:HD13	1:47:A:ASN:HD21	14	0.7
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	5	0.7
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	4	0.7
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	8	0.7
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD11	4	0.7
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD12	9	0.7
(1,570)	1:66:A:ASP:H	1:65:A:LYS:HD2	7	0.7
(1,558)	1:63:A:THR:HG22	1:62:A:THR:H	6	0.7
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	9	0.7
(1,430)	1:23:A:LEU:HD22	1:37:A:LYS:HG2	17	0.7
(1,220)	1:13:A:LEU:HD23	1:13:A:LEU:HA	1	0.7
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD22	3	0.7
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD11	9	0.7
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	13	0.7
(2,1678)	2:1001:A:OLA:H121	2:1001:A:OLA:H131	19	0.69
(2,1656)	1:19:A:PHE:HZ	2:1001:A:OLA:H172	13	0.69
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	11	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1605)	2:1001:A:OLA:H172	1:36:A:ILE:HD13	5	0.69
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	8	0.69
(2,1583)	2:1001:A:OLA:H161	2:1001:A:OLA:H21	7	0.69
(2,1540)	1:119:A:ARG:HG2	1:100:A:LEU:H	20	0.69
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	1	0.69
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	11	0.69
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	17	0.69
(2,1217)	1:63:A:THR:H	1:83:A:LEU:HG	10	0.69
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	11	0.69
(2,1125)	1:118:A:TYR:H	1:95:A:LYS:HB2	11	0.69
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	13	0.69
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG23	17	0.69
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	1	0.69
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD22	6	0.69
(2,706)	1:41:A:VAL:HG21	1:62:A:THR:HG1	3	0.69
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG22	5	0.69
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG23	20	0.69
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG22	11	0.69
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	20	0.69
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	14	0.69
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG22	11	0.69
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG23	20	0.69
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	17	0.69
(2,555)	1:89:A:LYS:HE2	1:105:A:ILE:HG22	11	0.69
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD21	4	0.69
(2,502)	1:90:A:ILE:HD11	1:90:A:ILE:H	4	0.69
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	7	0.69
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	10	0.69
(2,496)	1:90:A:ILE:HD11	1:69:A:HIS:HA	4	0.69
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	16	0.69
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB3	16	0.69
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	17	0.69
(2,419)	1:74:A:LEU:HD11	1:56:A:TYR:HD1	16	0.69
(2,415)	1:73:A:ALA:HB3	1:0:A:SER:HB3	12	0.69
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	18	0.69
(2,320)	1:67:A:THR:HG21	1:60:A:ASN:HD21	12	0.69
(2,274)	1:61:A:LEU:HD21	1:66:A:ASP:HB3	11	0.69
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	1	0.69
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	2	0.69
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	12	0.69
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	13	0.69
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB1	17	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	11	0.69
(2,154)	1:12:A:LYS:HE2	1:13:A:LEU:H	19	0.69
(2,119)	1:8:A:LEU:HD11	1:9:A:GLY:H	6	0.69
(2,119)	1:8:A:LEU:HD12	1:9:A:GLY:H	12	0.69
(2,98)	1:8:A:LEU:HD23	1:5:A:ASP:HA	13	0.69
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD22	2	0.69
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG22	6	0.69
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD22	12	0.69
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB1	10	0.69
(2,24)	1:4:A:PRO:HB2	1:94:A:LEU:HD23	17	0.69
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE1	9	0.69
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	17	0.69
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	14	0.69
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	7	0.69
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	8	0.69
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	2	0.69
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	11	0.69
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	19	0.69
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	5	0.69
(1,1226)	1:49:A:ALA:HB3	1:51:A:GLY:H	15	0.69
(1,1168)	1:32:A:MET:HE3	1:35:A:VAL:H	5	0.69
(1,792)	1:100:A:LEU:HD12	1:118:A:TYR:HD2	9	0.69
(1,558)	1:63:A:THR:HG22	1:62:A:THR:H	1	0.69
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	18	0.69
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	1	0.69
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	14	0.69
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	4	0.69
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	18	0.69
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	3	0.69
(1,288)	1:23:A:LEU:HD23	1:33:A:ARG:HA	14	0.69
(1,194)	1:10:A:THR:H	1:10:A:THR:HG21	7	0.69
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD22	11	0.69
(1,131)	1:3:A:LEU:HD12	1:7:A:PHE:HD2	10	0.69
(1,111)	1:48:A:ALA:HB1	1:71:A:ASP:HB2	15	0.69
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD12	16	0.69
(2,1678)	2:1001:A:OLA:H151	2:1001:A:OLA:H142	5	0.68
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	16	0.68
(2,1646)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	11	0.68
(2,1646)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	13	0.68
(2,1596)	2:1001:A:OLA:H31	2:1001:A:OLA:H181	14	0.68
(2,1488)	1:81:A:GLU:H	1:78:A:PHE:HE2	11	0.68
(2,1473)	1:6:A:LYS:H	1:6:A:LYS:HE2	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1313)	1:125:A:LEU:HA	1:124:A:TYR:H	9	0.68
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG23	13	0.68
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD12	1	0.68
(2,1117)	1:95:A:LYS:HD3	1:99:A:THR:H	3	0.68
(2,1029)	1:105:A:ILE:HD11	1:104:A:HIS:H	17	0.68
(2,825)	1:118:A:TYR:HD2	1:58:A:MET:HG3	8	0.68
(2,760)	1:127:A:MET:HE3	1:140:A:TYR:HH	9	0.68
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG23	16	0.68
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	10	0.68
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	11	0.68
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG22	4	0.68
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG23	6	0.68
(2,635)	1:128:A:LYS:HD3	1:130:A:SER:HB3	5	0.68
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG11	14	0.68
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD23	3	0.68
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	1	0.68
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	4	0.68
(2,533)	1:99:A:THR:HG21	1:95:A:LYS:HE3	15	0.68
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	2	0.68
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	17	0.68
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	19	0.68
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	4	0.68
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	15	0.68
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG22	14	0.68
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	10	0.68
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	13	0.68
(2,154)	1:13:A:LEU:H	1:12:A:LYS:HE3	4	0.68
(2,144)	1:11:A:PHE:HD1	1:141:A:LYS:HG3	3	0.68
(2,144)	1:11:A:PHE:HD1	1:141:A:LYS:HG3	11	0.68
(2,123)	1:10:A:THR:HB	1:143:A:GLN:HB2	5	0.68
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	2	0.68
(2,65)	1:1:A:LYS:HG2	1:1:A:LYS:HE3	1	0.68
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	5	0.68
(2,49)	1:48:A:ALA:HB1	1:55:A:ARG:HD2	13	0.68
(2,49)	1:48:A:ALA:HB3	1:55:A:ARG:HD2	14	0.68
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	7	0.68
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	9	0.68
(1,1474)	1:105:A:ILE:HD11	1:106:A:LYS:H	11	0.68
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	13	0.68
(1,1087)	1:3:A:LEU:HD12	1:4:A:PRO:HD2	16	0.68
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	13	0.68
(1,792)	1:100:A:LEU:HD11	1:118:A:TYR:HD2	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:94:A:LEU:HD13	1:3:A:LEU:HD13	17	0.68
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD23	13	0.68
(1,558)	1:63:A:THR:HG22	1:62:A:THR:H	2	0.68
(1,557)	1:63:A:THR:HG23	1:40:A:GLY:HA2	20	0.68
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG21	1	0.68
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	4	0.68
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	8	0.68
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	2	0.68
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	5	0.68
(1,448)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	5	0.68
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	1	0.68
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD11	2	0.68
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	3	0.68
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	8	0.68
(1,194)	1:10:A:THR:H	1:10:A:THR:HG23	20	0.68
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	8	0.68
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD21	15	0.68
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	2	0.68
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	6	0.68
(2,1648)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	14	0.67
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	1	0.67
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	2	0.67
(2,1581)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	8	0.67
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	18	0.67
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	6	0.67
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	8	0.67
(2,1037)	1:42:A:THR:H	1:42:A:THR:HG23	19	0.67
(2,843)	1:17:A:GLU:HG3	1:139:A:TYR:HD1	11	0.67
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	12	0.67
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD13	19	0.67
(2,783)	1:127:A:MET:HE1	1:140:A:TYR:HE2	7	0.67
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD22	8	0.67
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG22	1	0.67
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG23	11	0.67
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG22	18	0.67
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG22	16	0.67
(2,571)	1:106:A:LYS:HB3	1:109:A:ASP:HB2	19	0.67
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	11	0.67
(2,500)	1:90:A:ILE:HD12	1:88:A:HIS:H	4	0.67
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	5	0.67
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	17	0.67
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB2	3	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	8	0.67
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD11	6	0.67
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	9	0.67
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	1	0.67
(2,350)	1:33:A:ARG:HG2	1:34:A:GLN:H	17	0.67
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG23	14	0.67
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG22	15	0.67
(2,209)	1:23:A:LEU:HD11	1:36:A:ILE:HG21	3	0.67
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	14	0.67
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	14	0.67
(2,144)	1:11:A:PHE:HD1	1:141:A:LYS:HG3	12	0.67
(2,143)	1:127:A:MET:HG3	1:140:A:TYR:HD2	2	0.67
(2,123)	1:10:A:THR:HB	1:143:A:GLN:HB2	4	0.67
(2,123)	1:10:A:THR:HB	1:143:A:GLN:HB2	16	0.67
(2,119)	1:8:A:LEU:HD12	1:9:A:GLY:H	13	0.67
(2,114)	1:8:A:LEU:HD22	1:5:A:ASP:HA	20	0.67
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	3	0.67
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	2	0.67
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	3	0.67
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	10	0.67
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	8	0.67
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG12	9	0.67
(1,1464)	1:8:A:LEU:HD12	1:45:A:PHE:HB2	12	0.67
(1,1292)	1:111:A:THR:HG21	1:112:A:ASP:H	15	0.67
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	7	0.67
(1,1226)	1:49:A:ALA:HB2	1:51:A:GLY:H	7	0.67
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	13	0.67
(1,1185)	1:32:A:MET:HG2	1:32:A:MET:HE1	18	0.67
(1,1184)	1:36:A:ILE:HG13	1:32:A:MET:HE1	7	0.67
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	3	0.67
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	16	0.67
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG23	17	0.67
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	15	0.67
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	5	0.67
(1,397)	1:35:A:VAL:HG21	1:36:A:ILE:H	13	0.67
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	20	0.67
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	20	0.67
(1,290)	1:23:A:LEU:HD23	1:33:A:ARG:HD2	14	0.67
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	11	0.67
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	20	0.67
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	7	0.67
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD12	16	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	3	0.67
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD11	14	0.67
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD13	17	0.67
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	12	0.66
(2,1614)	1:58:A:MET:HE1	1:60:A:ASN:H	2	0.66
(2,1593)	1:84:A:ASP:HA	2:1001:A:OLA:H112	15	0.66
(2,1487)	1:67:A:THR:HG23	1:65:A:LYS:H	13	0.66
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	16	0.66
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	19	0.66
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG23	10	0.66
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG23	14	0.66
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB1	17	0.66
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	12	0.66
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB2	16	0.66
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD21	18	0.66
(2,1079)	1:89:A:LYS:H	1:79:A:GLN:HB3	18	0.66
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	18	0.66
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	6	0.66
(2,836)	1:49:A:ALA:HB2	1:48:A:ALA:HA	18	0.66
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG23	13	0.66
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	20	0.66
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	16	0.66
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	18	0.66
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG23	11	0.66
(2,532)	1:118:A:TYR:HD2	1:99:A:THR:HG22	16	0.66
(2,528)	1:143:A:GLN:HA	1:141:A:LYS:HE3	17	0.66
(2,523)	1:95:A:LYS:HG2	1:96:A:ASP:H	11	0.66
(2,494)	1:90:A:ILE:HD13	1:104:A:HIS:HB3	1	0.66
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	11	0.66
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	3	0.66
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD13	6	0.66
(2,418)	1:106:A:LYS:HG2	1:107:A:VAL:H	17	0.66
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	19	0.66
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG23	6	0.66
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	14	0.66
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	3	0.66
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	5	0.66
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	19	0.66
(2,123)	1:10:A:THR:HB	1:143:A:GLN:HB2	14	0.66
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	17	0.66
(2,7)	1:31:A:ILE:HD12	1:34:A:GLN:HB2	1	0.66
(2,5)	1:30:A:TRP:HE3	1:31:A:ILE:HG21	12	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	4	0.66
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD12	15	0.66
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	12	0.66
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD12	17	0.66
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	2	0.66
(1,1192)	1:23:A:LEU:HD13	1:32:A:MET:HE2	1	0.66
(1,1186)	1:127:A:MET:HE3	1:125:A:LEU:HD12	19	0.66
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE1	6	0.66
(1,1112)	1:58:A:MET:HE2	1:43:A:LYS:HE3	13	0.66
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	12	0.66
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE3	14	0.66
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	14	0.66
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	6	0.66
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	19	0.66
(1,601)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	5	0.66
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	13	0.66
(1,558)	1:63:A:THR:HG21	1:62:A:THR:H	17	0.66
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	8	0.66
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	20	0.66
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	9	0.66
(1,397)	1:35:A:VAL:HG22	1:36:A:ILE:H	5	0.66
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	12	0.66
(1,386)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	8	0.66
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	4	0.66
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD21	10	0.66
(1,130)	1:3:A:LEU:HD13	1:7:A:PHE:HB3	20	0.66
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	14	0.66
(2,1678)	2:1001:A:OLA:H61	2:1001:A:OLA:H161	18	0.65
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	6	0.65
(2,1601)	2:1001:A:OLA:H22	2:1001:A:OLA:H182	12	0.65
(2,1511)	1:61:A:LEU:HB2	1:67:A:THR:H	9	0.65
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	3	0.65
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	4	0.65
(2,1313)	1:125:A:LEU:HA	1:124:A:TYR:H	1	0.65
(2,1313)	1:125:A:LEU:HA	1:124:A:TYR:H	5	0.65
(2,1139)	1:100:A:LEU:H	1:119:A:ARG:HB3	1	0.65
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	4	0.65
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	7	0.65
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	20	0.65
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	13	0.65
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE2	1	0.65
(2,836)	1:49:A:ALA:HB1	1:48:A:ALA:HA	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,780)	1:109:A:ASP:H	1:106:A:LYS:HD2	20	0.65
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	1	0.65
(2,732)	1:58:A:MET:HE1	1:67:A:THR:HG1	2	0.65
(2,727)	1:3:A:LEU:HD22	1:7:A:PHE:HA	19	0.65
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG21	7	0.65
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	16	0.65
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	2	0.65
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	7	0.65
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG21	7	0.65
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG23	7	0.65
(2,570)	1:87:A:GLN:HA	1:82:A:ALA:HB1	20	0.65
(2,568)	1:113:A:VAL:HG22	1:113:A:VAL:HA	19	0.65
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG13	3	0.65
(2,545)	1:100:A:LEU:HD21	1:94:A:LEU:HD23	9	0.65
(2,545)	1:100:A:LEU:HD21	1:94:A:LEU:HD23	15	0.65
(2,517)	1:96:A:ASP:H	1:94:A:LEU:HD21	7	0.65
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	2	0.65
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	20	0.65
(2,478)	1:88:A:HIS:HB2	1:90:A:ILE:HG13	13	0.65
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	17	0.65
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	14	0.65
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	20	0.65
(2,437)	1:86:A:THR:HB	1:82:A:ALA:HB2	19	0.65
(2,420)	1:106:A:LYS:HG2	1:105:A:ILE:HA	20	0.65
(2,414)	1:73:A:ALA:HB3	1:76:A:GLU:HG2	2	0.65
(2,413)	1:73:A:ALA:HB3	1:54:A:ASP:HB3	14	0.65
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	5	0.65
(2,158)	1:41:A:VAL:HA	1:13:A:LEU:HB3	11	0.65
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	17	0.65
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD13	16	0.65
(2,82)	1:125:A:LEU:HD13	1:120:A:ARG:HD3	14	0.65
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB3	2	0.65
(2,45)	1:49:A:ALA:HB1	1:48:A:ALA:HA	11	0.65
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	4	0.65
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	7	0.65
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	18	0.65
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	18	0.65
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	1	0.65
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG21	18	0.65
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	12	0.65
(1,1762)	1:8:A:LEU:HD11	1:47:A:ASN:HD21	6	0.65
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD23	19	0.65
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	6	0.65
(1,1226)	1:49:A:ALA:HB3	1:51:A:GLY:H	2	0.65
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD13	4	0.65
(1,1186)	1:127:A:MET:HE2	1:125:A:LEU:HD12	17	0.65
(1,1112)	1:58:A:MET:HE1	1:43:A:LYS:HE3	7	0.65
(1,1112)	1:58:A:MET:HE2	1:43:A:LYS:HE3	10	0.65
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	14	0.65
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	3	0.65
(1,558)	1:63:A:THR:HG22	1:62:A:THR:H	5	0.65
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	20	0.65
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	9	0.65
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG23	15	0.65
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD11	17	0.65
(1,194)	1:10:A:THR:H	1:10:A:THR:HG22	15	0.65
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD22	2	0.65
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	14	0.65
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD22	16	0.65
(2,1608)	1:19:A:PHE:HZ	2:1001:A:OLA:H172	13	0.64
(2,1596)	1:83:A:LEU:HD23	2:1001:A:OLA:H32	17	0.64
(2,1540)	1:94:A:LEU:HG	1:100:A:LEU:H	18	0.64
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD22	3	0.64
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD21	6	0.64
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	13	0.64
(2,727)	1:3:A:LEU:HD23	1:7:A:PHE:HA	20	0.64
(2,706)	1:41:A:VAL:HG21	1:62:A:THR:HG1	16	0.64
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	19	0.64
(2,571)	1:106:A:LYS:HB3	1:109:A:ASP:HB2	6	0.64
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	4	0.64
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG22	9	0.64
(2,544)	1:100:A:LEU:HD22	1:94:A:LEU:HB2	5	0.64
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	1	0.64
(2,502)	1:90:A:ILE:HD13	1:90:A:ILE:H	3	0.64
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	14	0.64
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	8	0.64
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB2	2	0.64
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB1	2	0.64
(2,410)	1:70:A:LYS:HG2	1:71:A:ASP:HB3	10	0.64
(2,388)	1:63:A:THR:HB	1:64:A:LYS:HD3	6	0.64
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	3	0.64
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG21	10	0.64
(2,280)	1:68:A:HIS:H	1:67:A:THR:HG23	18	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	16	0.64
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	18	0.64
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD12	20	0.64
(2,160)	1:13:A:LEU:HD22	1:41:A:VAL:H	11	0.64
(2,160)	1:13:A:LEU:HD22	1:41:A:VAL:H	16	0.64
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG21	10	0.64
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	8	0.64
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD22	13	0.64
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD23	1	0.64
(2,87)	1:72:A:TRP:HZ3	1:3:A:LEU:HD23	16	0.64
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	19	0.64
(2,24)	1:94:A:LEU:HD13	1:4:A:PRO:HB2	8	0.64
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG21	4	0.64
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	2	0.64
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	3	0.64
(1,1955)	1:125:A:LEU:HD22	1:119:A:ARG:H	5	0.64
(1,1474)	1:105:A:ILE:HD12	1:106:A:LYS:H	17	0.64
(1,1330)	1:126:A:VAL:H	1:125:A:LEU:HD12	17	0.64
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG22	10	0.64
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	20	0.64
(1,1226)	1:49:A:ALA:HB3	1:51:A:GLY:H	10	0.64
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	20	0.64
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG21	14	0.64
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	13	0.64
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	5	0.64
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	12	0.64
(1,583)	1:65:A:LYS:HA	1:66:A:ASP:HB2	2	0.64
(1,558)	1:63:A:THR:HG21	1:62:A:THR:H	10	0.64
(1,558)	1:63:A:THR:HG22	1:62:A:THR:H	11	0.64
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	16	0.64
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG23	2	0.64
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	20	0.64
(1,383)	1:23:A:LEU:HD21	1:33:A:ARG:HA	15	0.64
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD21	9	0.64
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG23	16	0.64
(2,1678)	2:1001:A:OLA:H122	2:1001:A:OLA:H141	11	0.63
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	7	0.63
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG11	12	0.63
(2,1461)	1:136:A:THR:H	1:128:A:LYS:HB3	8	0.63
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	9	0.63
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG22	4	0.63
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	20	0.63
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	13	0.63
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG22	19	0.63
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB1	13	0.63
(2,731)	1:58:A:MET:HE3	1:61:A:LEU:H	7	0.63
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG22	6	0.63
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	1	0.63
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG23	3	0.63
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	12	0.63
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG21	4	0.63
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD23	6	0.63
(2,558)	1:105:A:ILE:HD13	1:105:A:ILE:HA	3	0.63
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	10	0.63
(2,555)	1:89:A:LYS:HE3	1:105:A:ILE:HG23	5	0.63
(2,543)	1:100:A:LEU:HD22	1:58:A:MET:HG2	4	0.63
(2,526)	1:95:A:LYS:HG2	1:99:A:THR:HB	2	0.63
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	20	0.63
(2,498)	1:90:A:ILE:HD13	1:78:A:PHE:HD2	15	0.63
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	5	0.63
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	12	0.63
(2,447)	1:84:A:ASP:HA	2:1001:A:OLA:H82	3	0.63
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	7	0.63
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	9	0.63
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	3	0.63
(2,400)	1:83:A:LEU:HD11	1:65:A:LYS:HG2	4	0.63
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	6	0.63
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB3	9	0.63
(2,209)	1:23:A:LEU:HD12	1:36:A:ILE:HG22	11	0.63
(2,144)	1:11:A:PHE:HD1	1:141:A:LYS:HG3	16	0.63
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	18	0.63
(2,98)	1:8:A:LEU:HD23	1:5:A:ASP:HA	9	0.63
(2,62)	1:0:A:SER:HB3	1:2:A:THR:H	11	0.63
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	11	0.63
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	19	0.63
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	12	0.63
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	14	0.63
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	11	0.63
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	8	0.63
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	10	0.63
(1,2559)	1:85:A:SER:H	1:65:A:LYS:HE2	6	0.63
(1,2559)	1:85:A:SER:H	1:65:A:LYS:HE2	12	0.63
(1,2243)	1:23:A:LEU:HD21	1:37:A:LYS:H	5	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1464)	1:8:A:LEU:HD12	1:45:A:PHE:HB2	7	0.63
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	12	0.63
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD11	8	0.63
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD12	18	0.63
(1,1113)	1:43:A:LYS:HD3	1:58:A:MET:HE2	11	0.63
(1,1104)	1:58:A:MET:HE3	1:118:A:TYR:HE2	9	0.63
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	7	0.63
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD13	8	0.63
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	4	0.63
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	9	0.63
(1,558)	1:63:A:THR:HG22	1:62:A:THR:H	13	0.63
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	3	0.63
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG23	12	0.63
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	1	0.63
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG22	17	0.63
(1,290)	1:23:A:LEU:HD22	1:33:A:ARG:HD2	8	0.63
(1,194)	1:10:A:THR:H	1:10:A:THR:HG23	12	0.63
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD12	8	0.63
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	14	0.62
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	10	0.62
(2,1596)	1:83:A:LEU:HD23	2:1001:A:OLA:H32	2	0.62
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	15	0.62
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	19	0.62
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	7	0.62
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	20	0.62
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	4	0.62
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG22	12	0.62
(2,836)	1:49:A:ALA:HB1	1:48:A:ALA:HA	4	0.62
(2,789)	1:26:A:ARG:HD2	1:131:A:TRP:HZ3	16	0.62
(2,783)	1:127:A:MET:HE1	1:140:A:TYR:HE2	4	0.62
(2,760)	1:127:A:MET:HE3	1:140:A:TYR:HH	2	0.62
(2,760)	1:127:A:MET:HE2	1:140:A:TYR:HH	17	0.62
(2,727)	1:3:A:LEU:HD22	1:7:A:PHE:HA	8	0.62
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	3	0.62
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG11	5	0.62
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG23	12	0.62
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	5	0.62
(2,582)	1:113:A:VAL:HA	1:113:A:VAL:HG11	17	0.62
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG12	10	0.62
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	9	0.62
(2,558)	1:105:A:ILE:HD13	1:105:A:ILE:HA	20	0.62
(2,548)	1:92:A:PHE:HB3	1:100:A:LEU:HD12	14	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	12	0.62
(2,496)	1:90:A:ILE:HD12	1:69:A:HIS:HA	10	0.62
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	6	0.62
(2,415)	1:0:A:SER:HB2	1:73:A:ALA:HB2	9	0.62
(2,414)	1:73:A:ALA:HB1	1:76:A:GLU:HG2	11	0.62
(2,391)	1:64:A:LYS:HD3	1:35:A:VAL:HG23	18	0.62
(2,331)	1:44:A:LYS:HA	1:11:A:PHE:HB2	13	0.62
(2,309)	1:65:A:LYS:H	1:83:A:LEU:HD22	20	0.62
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG22	2	0.62
(2,188)	1:134:A:VAL:HG12	1:21:A:GLU:HG2	19	0.62
(2,160)	1:13:A:LEU:HD21	1:41:A:VAL:H	19	0.62
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	12	0.62
(2,114)	1:8:A:LEU:HD22	1:5:A:ASP:HA	10	0.62
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	11	0.62
(2,45)	1:49:A:ALA:HB1	1:48:A:ALA:HA	2	0.62
(2,7)	1:31:A:ILE:HD12	1:34:A:GLN:HB2	3	0.62
(2,7)	1:31:A:ILE:HD13	1:34:A:GLN:HB2	20	0.62
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	12	0.62
(1,2818)	1:83:A:LEU:HD21	1:62:A:THR:HG1	4	0.62
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	14	0.62
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG21	7	0.62
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	2	0.62
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD21	9	0.62
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD22	18	0.62
(1,1762)	1:8:A:LEU:HD11	1:47:A:ASN:HD21	19	0.62
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD22	4	0.62
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	16	0.62
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE1	1	0.62
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	6	0.62
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	1	0.62
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	1	0.62
(1,785)	1:100:A:LEU:HD21	1:45:A:PHE:HE2	8	0.62
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD22	10	0.62
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG11	11	0.62
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD22	7	0.62
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD23	16	0.62
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	11	0.62
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	17	0.62
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG22	6	0.62
(1,430)	1:23:A:LEU:HD23	1:37:A:LYS:HG2	1	0.62
(1,420)	1:36:A:ILE:HD13	1:36:A:ILE:HB	7	0.62
(1,383)	1:23:A:LEU:HD21	1:33:A:ARG:HA	17	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	18	0.62
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	20	0.62
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	13	0.62
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	4	0.62
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	8	0.61
(2,1652)	1:32:A:MET:HE3	1:35:A:VAL:HG12	3	0.61
(2,1626)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	12	0.61
(2,1591)	1:41:A:VAL:HG13	2:1001:A:OLA:H72	8	0.61
(2,1521)	1:7:A:PHE:H	1:120:A:ARG:HB2	15	0.61
(2,1466)	1:98:A:ASN:H	1:95:A:LYS:HD3	4	0.61
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	18	0.61
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	14	0.61
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	15	0.61
(2,1029)	1:113:A:VAL:HG11	1:104:A:HIS:H	13	0.61
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	1	0.61
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	4	0.61
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB1	10	0.61
(2,841)	1:129:A:MET:HE2	1:114:A:GLU:HG3	18	0.61
(2,834)	1:68:A:HIS:HE1	1:49:A:ALA:HB2	18	0.61
(2,786)	1:32:A:MET:HE2	1:36:A:ILE:HA	9	0.61
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE3	17	0.61
(2,782)	1:127:A:MET:HE3	1:116:A:TYR:HA	18	0.61
(2,706)	1:41:A:VAL:HG23	1:62:A:THR:HG1	10	0.61
(2,706)	1:41:A:VAL:HG23	1:62:A:THR:HG1	14	0.61
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	6	0.61
(2,533)	1:99:A:THR:HG21	1:96:A:ASP:HB2	11	0.61
(2,501)	1:90:A:ILE:HD11	1:80:A:ASP:H	4	0.61
(2,447)	1:84:A:ASP:HA	2:1001:A:OLA:H112	12	0.61
(2,435)	1:104:A:HIS:HB3	1:82:A:ALA:HB2	5	0.61
(2,414)	1:73:A:ALA:HB2	1:76:A:GLU:HG2	17	0.61
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB3	15	0.61
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	1	0.61
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	12	0.61
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG22	4	0.61
(2,252)	1:26:A:ARG:HD3	1:131:A:TRP:HB3	19	0.61
(2,250)	1:26:A:ARG:HD2	1:131:A:TRP:HD1	20	0.61
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	12	0.61
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	10	0.61
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	1	0.61
(2,143)	1:127:A:MET:HG3	1:140:A:TYR:HD2	11	0.61
(2,120)	1:8:A:LEU:HD12	1:7:A:PHE:H	19	0.61
(2,107)	1:120:A:ARG:HB2	1:7:A:PHE:HB3	13	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:0:A:SER:HB3	1:2:A:THR:H	2	0.61
(2,61)	1:73:A:ALA:HB3	1:0:A:SER:HB3	8	0.61
(2,56)	1:63:A:THR:HG21	1:40:A:GLY:HA2	12	0.61
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB2	11	0.61
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	16	0.61
(2,51)	1:48:A:ALA:HB2	1:56:A:TYR:HB3	18	0.61
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	18	0.61
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	11	0.61
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	12	0.61
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	5	0.61
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	8	0.61
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG22	4	0.61
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	9	0.61
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD22	8	0.61
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD22	18	0.61
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	10	0.61
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	3	0.61
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	1	0.61
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	2	0.61
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	3	0.61
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	17	0.61
(1,1112)	1:58:A:MET:HE2	1:43:A:LYS:HE3	17	0.61
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD23	16	0.61
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG23	8	0.61
(1,558)	1:63:A:THR:HG21	1:62:A:THR:H	12	0.61
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG22	13	0.61
(1,429)	1:23:A:LEU:HD21	1:37:A:LYS:HG3	7	0.61
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	13	0.61
(1,124)	1:3:A:LEU:HA	1:3:A:LEU:HD13	13	0.61
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	1	0.61
(1,16)	1:32:A:MET:HA	1:31:A:ILE:HD11	4	0.61
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG22	1	0.61
(2,1678)	2:1001:A:OLA:H161	2:1001:A:OLA:H152	6	0.6
(2,1652)	1:32:A:MET:HE2	2:1001:A:OLA:H131	18	0.6
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	5	0.6
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	15	0.6
(2,1606)	1:36:A:ILE:HD11	1:23:A:LEU:HB2	10	0.6
(2,1244)	1:28:A:TYR:H	1:26:A:ARG:HD2	17	0.6
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD12	14	0.6
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	2	0.6
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	5	0.6
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	13	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,860)	1:64:A:LYS:HB2	2:1001:A:OLA:H9	6	0.6
(2,811)	1:89:A:LYS:HE3	1:89:A:LYS:H	13	0.6
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	3	0.6
(2,782)	1:127:A:MET:HE2	1:116:A:TYR:HA	10	0.6
(2,732)	1:58:A:MET:HE1	1:67:A:THR:HG1	4	0.6
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	10	0.6
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HG	11	0.6
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	14	0.6
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD22	12	0.6
(2,571)	1:106:A:LYS:HB3	1:109:A:ASP:HB2	13	0.6
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG12	11	0.6
(2,533)	1:99:A:THR:HG21	1:96:A:ASP:HB2	16	0.6
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	18	0.6
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	3	0.6
(2,311)	1:38:A:LEU:HA	1:38:A:LEU:HD12	2	0.6
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	5	0.6
(2,287)	1:36:A:ILE:HD12	1:33:A:ARG:HA	7	0.6
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG22	2	0.6
(2,188)	1:134:A:VAL:HG12	1:21:A:GLU:HG2	6	0.6
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	19	0.6
(2,144)	1:124:A:TYR:HD2	1:141:A:LYS:HG3	1	0.6
(2,143)	1:127:A:MET:HG3	1:140:A:TYR:HD2	14	0.6
(2,132)	1:10:A:THR:H	1:142:A:LYS:HE3	6	0.6
(2,114)	1:8:A:LEU:HD22	1:5:A:ASP:HA	8	0.6
(2,114)	1:8:A:LEU:HD21	1:5:A:ASP:HA	12	0.6
(2,93)	1:125:A:LEU:HD12	1:127:A:MET:HG3	7	0.6
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	19	0.6
(2,51)	1:48:A:ALA:HB3	1:56:A:TYR:HB3	15	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	5	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	7	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	9	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	10	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	11	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	13	0.6
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	19	0.6
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	2	0.6
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG21	14	0.6
(1,1629)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	17	0.6
(1,1464)	1:8:A:LEU:HD12	1:45:A:PHE:HB2	13	0.6
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	18	0.6
(1,1225)	1:127:A:MET:HE3	1:128:A:LYS:H	7	0.6
(1,1225)	1:127:A:MET:HE1	1:128:A:LYS:H	19	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	2	0.6
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	6	0.6
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD23	6	0.6
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	6	0.6
(1,558)	1:63:A:THR:HG21	1:62:A:THR:H	15	0.6
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	14	0.6
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG22	16	0.6
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG22	17	0.6
(2,1670)	2:1001:A:OLA:H82	2:1001:A:OLA:H182	1	0.59
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	3	0.59
(2,1614)	1:106:A:LYS:HB2	1:111:A:THR:H	8	0.59
(2,1606)	1:36:A:ILE:HD12	2:1001:A:OLA:H112	9	0.59
(2,1599)	1:61:A:LEU:HD11	1:44:A:LYS:HG2	13	0.59
(2,1577)	2:1001:A:OLA:H72	1:36:A:ILE:HG22	7	0.59
(2,1495)	1:13:A:LEU:H	1:42:A:THR:HG21	2	0.59
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	20	0.59
(2,1411)	1:13:A:LEU:H	1:143:A:GLN:HE22	7	0.59
(2,1360)	1:52:A:LYS:H	1:52:A:LYS:HG3	17	0.59
(2,1184)	1:61:A:LEU:HD11	1:143:A:GLN:HE22	5	0.59
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD11	2	0.59
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	9	0.59
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	9	0.59
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	10	0.59
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG23	4	0.59
(2,820)	1:41:A:VAL:HG23	1:43:A:LYS:HE2	12	0.59
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	8	0.59
(2,785)	1:32:A:MET:HE3	1:35:A:VAL:HG12	3	0.59
(2,783)	1:127:A:MET:HE3	1:140:A:TYR:HE2	15	0.59
(2,780)	1:109:A:ASP:H	1:106:A:LYS:HD2	3	0.59
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	16	0.59
(2,727)	1:3:A:LEU:HD22	1:7:A:PHE:HA	9	0.59
(2,667)	1:135:A:SER:HB3	1:136:A:THR:HG21	18	0.59
(2,558)	1:105:A:ILE:HD13	1:105:A:ILE:HA	14	0.59
(2,558)	1:105:A:ILE:HD13	1:105:A:ILE:HA	15	0.59
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD23	1	0.59
(2,534)	1:95:A:LYS:HB2	1:99:A:THR:HG23	16	0.59
(2,527)	1:95:A:LYS:H	1:95:A:LYS:HD2	10	0.59
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	5	0.59
(2,501)	1:90:A:ILE:HD13	1:80:A:ASP:H	13	0.59
(2,501)	1:90:A:ILE:HD13	1:80:A:ASP:H	14	0.59
(2,488)	1:102:A:GLU:HB3	1:90:A:ILE:HG22	12	0.59
(2,441)	1:141:A:LYS:H	1:141:A:LYS:HG3	17	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD11	16	0.59
(2,400)	1:65:A:LYS:HG2	1:83:A:LEU:HD21	3	0.59
(2,378)	1:83:A:LEU:HD12	1:62:A:THR:HG21	2	0.59
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	9	0.59
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB1	4	0.59
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	10	0.59
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	7	0.59
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	7	0.59
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	17	0.59
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	13	0.59
(2,119)	1:8:A:LEU:HD12	1:9:A:GLY:H	7	0.59
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	12	0.59
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	6	0.59
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	8	0.59
(2,7)	1:31:A:ILE:HD11	1:34:A:GLN:HB2	16	0.59
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	15	0.59
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	16	0.59
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	14	0.59
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	7	0.59
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	14	0.59
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD23	1	0.59
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	11	0.59
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	6	0.59
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	16	0.59
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE3	11	0.59
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE3	13	0.59
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	9	0.59
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	1	0.59
(1,756)	1:94:A:LEU:HD12	1:3:A:LEU:HD11	10	0.59
(1,754)	1:94:A:LEU:HD11	1:100:A:LEU:HA	5	0.59
(1,719)	1:90:A:ILE:HG21	1:104:A:HIS:HD2	19	0.59
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	8	0.59
(1,558)	1:63:A:THR:HG23	1:62:A:THR:H	14	0.59
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG21	11	0.59
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG22	15	0.59
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	2	0.59
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	20	0.59
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD22	1	0.59
(1,111)	1:48:A:ALA:HB3	1:71:A:ASP:HB2	17	0.59
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	3	0.59
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	8	0.59
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	20	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG23	20	0.59
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	11	0.59
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG23	18	0.59
(2,1652)	1:32:A:MET:HE1	2:1001:A:OLA:H131	5	0.58
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	14	0.58
(2,1488)	1:81:A:GLU:H	1:87:A:GLN:HE21	19	0.58
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	8	0.58
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	15	0.58
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	17	0.58
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	2	0.58
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	3	0.58
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	13	0.58
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	14	0.58
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG21	11	0.58
(2,1217)	1:63:A:THR:H	1:38:A:LEU:HB3	5	0.58
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	3	0.58
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	3	0.58
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG21	9	0.58
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	12	0.58
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE1	20	0.58
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	20	0.58
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	11	0.58
(2,732)	1:58:A:MET:HE3	1:67:A:THR:HG1	12	0.58
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	17	0.58
(2,731)	1:58:A:MET:HE1	1:61:A:LEU:H	4	0.58
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	5	0.58
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG21	14	0.58
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG13	8	0.58
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG11	12	0.58
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	13	0.58
(2,478)	1:88:A:HIS:HB2	1:90:A:ILE:HG13	3	0.58
(2,437)	1:81:A:GLU:HA	1:82:A:ALA:HB1	18	0.58
(2,412)	1:73:A:ALA:HB1	1:55:A:ARG:H	9	0.58
(2,388)	1:65:A:LYS:HA	1:64:A:LYS:HD2	18	0.58
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB1	7	0.58
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB3	14	0.58
(2,227)	1:24:A:LYS:H	1:25:A:ALA:HB2	11	0.58
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	3	0.58
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	7	0.58
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD13	7	0.58
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	16	0.58
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	7	0.58
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	17	0.58
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	20	0.58
(2,7)	1:31:A:ILE:HD13	1:34:A:GLN:HB2	4	0.58
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG23	5	0.58
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	11	0.58
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	1	0.58
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	3	0.58
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	16	0.58
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	13	0.58
(1,2243)	1:23:A:LEU:HD22	1:37:A:LYS:H	12	0.58
(1,2182)	1:99:A:THR:H	1:94:A:LEU:HD13	17	0.58
(1,2029)	1:114:A:GLU:H	1:103:A:THR:HG23	11	0.58
(1,1292)	1:111:A:THR:HG21	1:112:A:ASP:H	9	0.58
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	5	0.58
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	13	0.58
(1,989)	1:134:A:VAL:HG13	1:22:A:TYR:HB3	3	0.58
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	14	0.58
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	15	0.58
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	14	0.58
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	19	0.58
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG11	2	0.58
(1,636)	1:61:A:LEU:HD23	1:66:A:ASP:HB2	10	0.58
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG23	18	0.58
(1,441)	1:38:A:LEU:HD23	1:38:A:LEU:HA	1	0.58
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	9	0.58
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	18	0.58
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	8	0.58
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	15	0.58
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	12	0.58
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG23	1	0.58
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG21	14	0.58
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG22	15	0.58
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	12	0.58
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	1	0.57
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	12	0.57
(2,1594)	2:1001:A:OLA:H32	1:41:A:VAL:HG12	9	0.57
(2,1581)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	15	0.57
(2,1480)	1:46:A:ARG:HG3	1:71:A:ASP:H	1	0.57
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG13	17	0.57
(2,1394)	1:143:A:GLN:H	1:141:A:LYS:HD3	19	0.57
(2,1360)	1:52:A:LYS:HG2	1:52:A:LYS:H	15	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1330)	1:79:A:GLN:H	1:89:A:LYS:HB3	14	0.57
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	13	0.57
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD12	2	0.57
(2,1144)	1:105:A:ILE:H	1:113:A:VAL:HB	4	0.57
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	16	0.57
(2,906)	1:41:A:VAL:HG12	1:40:A:GLY:H	12	0.57
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG23	9	0.57
(2,838)	1:127:A:MET:HE2	1:116:A:TYR:HE1	9	0.57
(2,836)	1:49:A:ALA:HB3	1:48:A:ALA:HA	12	0.57
(2,819)	2:1001:A:OLA:H81	1:36:A:ILE:HG21	20	0.57
(2,787)	1:39:A:ALA:HB2	1:40:A:GLY:H	13	0.57
(2,785)	1:32:A:MET:HE2	2:1001:A:OLA:H131	18	0.57
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	14	0.57
(2,740)	1:31:A:ILE:HD13	1:30:A:TRP:HZ2	4	0.57
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	8	0.57
(2,713)	1:3:A:LEU:HB2	1:8:A:LEU:HD21	12	0.57
(2,636)	1:129:A:MET:HB2	1:130:A:SER:HB3	11	0.57
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG23	2	0.57
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	6	0.57
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG11	9	0.57
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	13	0.57
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	16	0.57
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD23	1	0.57
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG22	1	0.57
(2,527)	1:95:A:LYS:H	1:95:A:LYS:HD2	16	0.57
(2,523)	1:95:A:LYS:HG2	1:96:A:ASP:H	14	0.57
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD12	16	0.57
(2,330)	1:41:A:VAL:HG23	1:43:A:LYS:HE3	16	0.57
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	13	0.57
(2,247)	1:26:A:ARG:HD3	1:131:A:TRP:HE3	19	0.57
(2,209)	1:23:A:LEU:HD11	1:36:A:ILE:HG22	6	0.57
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	17	0.57
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	10	0.57
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	12	0.57
(2,144)	1:124:A:TYR:HD2	1:141:A:LYS:HG3	18	0.57
(2,143)	1:127:A:MET:HG3	1:140:A:TYR:HD2	15	0.57
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	16	0.57
(2,51)	1:48:A:ALA:HB2	1:56:A:TYR:HB3	20	0.57
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	5	0.57
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	9	0.57
(2,40)	1:53:A:PRO:HA	1:53:A:PRO:HG2	3	0.57
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG22	19	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	1	0.57
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	1	0.57
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	10	0.57
(1,1330)	1:126:A:VAL:H	1:125:A:LEU:HD13	4	0.57
(1,1240)	1:125:A:LEU:HD22	1:120:A:ARG:HD2	4	0.57
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	4	0.57
(1,1225)	1:127:A:MET:HE1	1:128:A:LYS:H	8	0.57
(1,1222)	1:127:A:MET:HE2	1:118:A:TYR:HD1	11	0.57
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE2	3	0.57
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE2	5	0.57
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	2	0.57
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	13	0.57
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	5	0.57
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	12	0.57
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	16	0.57
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	18	0.57
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	1	0.57
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	4	0.57
(1,743)	1:93:A:ASP:HB2	1:91:A:THR:HG23	7	0.57
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG13	3	0.57
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD23	11	0.57
(1,628)	1:74:A:LEU:HD11	1:74:A:LEU:H	2	0.57
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	3	0.57
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	6	0.57
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG22	7	0.57
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG23	3	0.57
(1,397)	1:35:A:VAL:HG21	1:36:A:ILE:H	16	0.57
(1,373)	1:32:A:MET:HA	1:35:A:VAL:HG12	18	0.57
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD13	11	0.57
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	5	0.57
(1,137)	1:3:A:LEU:HD21	1:7:A:PHE:HB3	10	0.57
(1,131)	1:3:A:LEU:HD13	1:7:A:PHE:HD2	13	0.57
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	7	0.57
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	3	0.57
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	7	0.57
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	9	0.57
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	10	0.57
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	4	0.56
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	18	0.56
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	8	0.56
(2,1623)	2:1001:A:OLA:H81	1:36:A:ILE:HA	17	0.56
(2,1610)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	12	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	1	0.56
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	4	0.56
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	19	0.56
(2,1360)	1:52:A:LYS:H	1:52:A:LYS:HG3	10	0.56
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD12	2	0.56
(2,1184)	1:61:A:LEU:HD12	1:143:A:GLN:HE22	18	0.56
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	15	0.56
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	11	0.56
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD23	18	0.56
(2,928)	1:90:A:ILE:H	1:89:A:LYS:HE3	12	0.56
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	6	0.56
(2,787)	1:39:A:ALA:HB2	1:40:A:GLY:H	12	0.56
(2,785)	1:32:A:MET:HE1	2:1001:A:OLA:H131	5	0.56
(2,730)	1:58:A:MET:HE1	1:69:A:HIS:H	3	0.56
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	11	0.56
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD23	20	0.56
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG11	15	0.56
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	5	0.56
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	7	0.56
(2,535)	1:117:A:GLU:HB2	1:99:A:THR:HG21	7	0.56
(2,500)	1:90:A:ILE:HD11	1:88:A:HIS:H	13	0.56
(2,498)	1:90:A:ILE:HD13	1:69:A:HIS:HD2	4	0.56
(2,478)	1:88:A:HIS:HB2	1:90:A:ILE:HG13	18	0.56
(2,418)	1:106:A:LYS:HG2	1:107:A:VAL:H	19	0.56
(2,350)	1:52:A:LYS:H	1:52:A:LYS:HD2	4	0.56
(2,301)	1:24:A:LYS:H	1:24:A:LYS:HE2	14	0.56
(2,293)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	3	0.56
(2,232)	1:132:A:LYS:HG2	1:25:A:ALA:HB1	2	0.56
(2,184)	1:21:A:GLU:HA	1:24:A:LYS:HD3	2	0.56
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	6	0.56
(2,171)	1:15:A:ARG:HD3	1:16:A:ASP:H	7	0.56
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	3	0.56
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD11	18	0.56
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	3	0.56
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	15	0.56
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	20	0.56
(2,122)	1:9:A:GLY:HA3	1:142:A:LYS:HE2	8	0.56
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	1	0.56
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	4	0.56
(2,115)	1:8:A:LEU:HD22	1:8:A:LEU:HB2	9	0.56
(2,51)	1:48:A:ALA:HB2	1:56:A:TYR:HB3	9	0.56
(1,2836)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	11	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2813)	1:127:A:MET:HE3	1:118:A:TYR:HH	18	0.56
(1,2809)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	11	0.56
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	2	0.56
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	1	0.56
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG22	18	0.56
(1,2182)	1:99:A:THR:H	1:94:A:LEU:HD11	7	0.56
(1,1955)	1:125:A:LEU:HD22	1:119:A:ARG:H	1	0.56
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD22	3	0.56
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	3	0.56
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	2	0.56
(1,1344)	1:105:A:ILE:HD11	1:105:A:ILE:H	14	0.56
(1,1330)	1:126:A:VAL:H	1:125:A:LEU:HD11	14	0.56
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	1	0.56
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG22	20	0.56
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD11	15	0.56
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE1	13	0.56
(1,954)	1:129:A:MET:HG3	1:116:A:TYR:HD2	2	0.56
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	2	0.56
(1,755)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	20	0.56
(1,632)	1:74:A:LEU:HD13	1:3:A:LEU:HD11	1	0.56
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	7	0.56
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG23	10	0.56
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	4	0.56
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	2	0.56
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	20	0.56
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD12	14	0.56
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD21	13	0.56
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	17	0.56
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB2	7	0.56
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG21	6	0.56
(2,1670)	2:1001:A:OLA:H181	2:1001:A:OLA:H21	6	0.55
(2,1664)	1:102:A:GLU:HG3	1:118:A:TYR:HE2	12	0.55
(2,1659)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	12	0.55
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	19	0.55
(2,1640)	2:1001:A:OLA:H31	1:140:A:TYR:HH	2	0.55
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG13	18	0.55
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	12	0.55
(2,1216)	1:34:A:GLN:HE22	1:33:A:ARG:HG2	3	0.55
(2,1075)	1:94:A:LEU:HD23	1:93:A:ASP:H	4	0.55
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD21	5	0.55
(2,906)	1:41:A:VAL:HG12	1:40:A:GLY:H	1	0.55
(2,811)	1:89:A:LYS:HE3	1:89:A:LYS:H	7	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE3	16	0.55
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD11	11	0.55
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	10	0.55
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	11	0.55
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	3	0.55
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	8	0.55
(2,675)	1:139:A:TYR:HA	1:139:A:TYR:HE2	15	0.55
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG23	15	0.55
(2,533)	1:99:A:THR:HG21	1:95:A:LYS:HE3	19	0.55
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	6	0.55
(2,422)	1:74:A:LEU:HD12	1:4:A:PRO:HD2	14	0.55
(2,374)	2:1001:A:OLA:H81	1:62:A:THR:HG23	20	0.55
(2,367)	1:83:A:LEU:H	1:83:A:LEU:HD13	4	0.55
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	17	0.55
(2,293)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	19	0.55
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	10	0.55
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB2	6	0.55
(2,183)	1:24:A:LYS:HE2	1:21:A:GLU:HA	5	0.55
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	14	0.55
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	16	0.55
(2,154)	1:13:A:LEU:H	1:12:A:LYS:HE3	2	0.55
(2,143)	1:11:A:PHE:HD2	1:10:A:THR:HG21	1	0.55
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	3	0.55
(2,115)	1:8:A:LEU:HD21	1:8:A:LEU:HB2	5	0.55
(2,115)	1:8:A:LEU:HD21	1:8:A:LEU:HB2	6	0.55
(2,115)	1:8:A:LEU:HD22	1:8:A:LEU:HB2	13	0.55
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	18	0.55
(2,115)	1:8:A:LEU:HD22	1:8:A:LEU:HB2	19	0.55
(2,115)	1:8:A:LEU:HD21	1:8:A:LEU:HB2	20	0.55
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	9	0.55
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	13	0.55
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	10	0.55
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG21	1	0.55
(1,2325)	1:90:A:ILE:H	1:77:A:GLU:HG2	14	0.55
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG23	12	0.55
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	20	0.55
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	4	0.55
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	16	0.55
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD21	20	0.55
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	8	0.55
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	16	0.55
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	4	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	18	0.55
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	9	0.55
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	7	0.55
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	11	0.55
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	17	0.55
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG13	20	0.55
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	11	0.55
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD21	12	0.55
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	10	0.55
(1,632)	1:74:A:LEU:HD11	1:3:A:LEU:HD12	13	0.55
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD13	3	0.55
(1,448)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	12	0.55
(1,448)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	17	0.55
(1,441)	1:38:A:LEU:HD23	1:38:A:LEU:HA	4	0.55
(1,429)	1:23:A:LEU:HD21	1:37:A:LYS:HG3	5	0.55
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	5	0.55
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD13	6	0.55
(1,397)	1:35:A:VAL:HG21	1:36:A:ILE:H	6	0.55
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	4	0.55
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	9	0.55
(1,187)	1:8:A:LEU:HD13	1:47:A:ASN:HD22	14	0.55
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB2	8	0.55
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG21	3	0.55
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG21	8	0.55
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	14	0.55
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	11	0.54
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	1	0.54
(2,1593)	1:84:A:ASP:HA	2:1001:A:OLA:H112	5	0.54
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	11	0.54
(2,1473)	1:6:A:LYS:HE3	1:6:A:LYS:H	7	0.54
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD21	15	0.54
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	6	0.54
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	7	0.54
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	14	0.54
(2,1139)	1:100:A:LEU:H	1:119:A:ARG:HB3	18	0.54
(2,1117)	1:95:A:LYS:HD3	1:99:A:THR:H	15	0.54
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	18	0.54
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD22	16	0.54
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	8	0.54
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	17	0.54
(2,821)	1:14:A:GLU:HB2	1:141:A:LYS:HG3	2	0.54
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	12	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,789)	1:114:A:GLU:HB3	1:131:A:TRP:HZ3	11	0.54
(2,787)	1:127:A:MET:HE2	1:117:A:GLU:H	10	0.54
(2,787)	1:39:A:ALA:HB1	1:40:A:GLY:H	18	0.54
(2,760)	1:118:A:TYR:H	1:127:A:MET:HE2	3	0.54
(2,716)	1:5:A:ASP:H	1:2:A:THR:HG21	17	0.54
(2,707)	1:67:A:THR:HG22	1:62:A:THR:HG1	16	0.54
(2,697)	1:65:A:LYS:HE2	1:83:A:LEU:HA	6	0.54
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	12	0.54
(2,692)	1:142:A:LYS:H	1:141:A:LYS:HD2	13	0.54
(2,684)	1:13:A:LEU:HD21	1:140:A:TYR:HE2	3	0.54
(2,635)	1:130:A:SER:HB3	1:128:A:LYS:HD2	3	0.54
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	1	0.54
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	17	0.54
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	8	0.54
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	11	0.54
(2,543)	1:100:A:LEU:HD23	1:74:A:LEU:HB2	20	0.54
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	11	0.54
(2,522)	1:101:A:THR:HG23	1:95:A:LYS:HB2	1	0.54
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	2	0.54
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	4	0.54
(2,437)	1:86:A:THR:HB	1:82:A:ALA:HB1	14	0.54
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	3	0.54
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	16	0.54
(2,350)	1:52:A:LYS:H	1:52:A:LYS:HD2	1	0.54
(2,349)	1:52:A:LYS:H	1:52:A:LYS:HG3	17	0.54
(2,333)	1:42:A:THR:HG23	1:44:A:LYS:HA	14	0.54
(2,290)	1:36:A:ILE:HD12	1:36:A:ILE:HA	13	0.54
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	9	0.54
(2,229)	1:25:A:ALA:HB3	1:132:A:LYS:HE2	3	0.54
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	8	0.54
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	11	0.54
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	1	0.54
(2,160)	1:13:A:LEU:HD23	1:41:A:VAL:H	8	0.54
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	8	0.54
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	13	0.54
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	15	0.54
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	18	0.54
(2,119)	1:8:A:LEU:HD11	1:9:A:GLY:H	1	0.54
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	2	0.54
(2,115)	1:8:A:LEU:HD21	1:8:A:LEU:HB2	10	0.54
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	11	0.54
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	15	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	3	0.54
(2,51)	1:48:A:ALA:HB3	1:56:A:TYR:HB3	5	0.54
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	12	0.54
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD12	14	0.54
(2,7)	1:31:A:ILE:HD12	1:34:A:GLN:HB2	13	0.54
(2,7)	1:31:A:ILE:HD13	1:34:A:GLN:HB2	14	0.54
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	9	0.54
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG22	6	0.54
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	7	0.54
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	5	0.54
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG21	9	0.54
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	15	0.54
(1,1459)	1:55:A:ARG:H	1:55:A:ARG:HD3	4	0.54
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	5	0.54
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	14	0.54
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	5	0.54
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	8	0.54
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	3	0.54
(1,1088)	1:61:A:LEU:HD22	1:62:A:THR:H	8	0.54
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	4	0.54
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG23	2	0.54
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	16	0.54
(1,952)	1:129:A:MET:HB2	1:136:A:THR:HG22	19	0.54
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	8	0.54
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	4	0.54
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	10	0.54
(1,878)	1:115:A:THR:H	1:115:A:THR:HG23	12	0.54
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	11	0.54
(1,628)	1:74:A:LEU:HD11	1:74:A:LEU:H	7	0.54
(1,599)	1:70:A:LYS:HD2	1:70:A:LYS:HE3	2	0.54
(1,555)	1:39:A:ALA:H	1:63:A:THR:HG21	13	0.54
(1,441)	1:38:A:LEU:HD21	1:38:A:LEU:HA	11	0.54
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	9	0.54
(1,383)	1:23:A:LEU:HD23	1:33:A:ARG:HA	10	0.54
(1,288)	1:23:A:LEU:HD23	1:33:A:ARG:HA	6	0.54
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD22	18	0.54
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD21	19	0.54
(1,100)	1:48:A:ALA:HB3	1:50:A:SER:H	4	0.54
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	19	0.54
(2,1679)	1:94:A:LEU:HB3	1:94:A:LEU:HD21	7	0.53
(2,1636)	1:83:A:LEU:HB3	1:62:A:THR:HG1	18	0.53
(2,1614)	1:58:A:MET:HE3	1:60:A:ASN:H	1	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1606)	2:1001:A:OLA:H111	1:36:A:ILE:HD12	18	0.53
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG11	1	0.53
(2,1565)	1:19:A:PHE:HZ	2:1001:A:OLA:H32	20	0.53
(2,1521)	1:7:A:PHE:H	1:120:A:ARG:HB2	20	0.53
(2,1511)	1:61:A:LEU:HB2	1:67:A:THR:H	6	0.53
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG13	20	0.53
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	18	0.53
(2,1232)	1:85:A:SER:H	1:81:A:GLU:HB2	6	0.53
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	6	0.53
(2,1006)	1:81:A:GLU:H	1:69:A:HIS:HE1	18	0.53
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	7	0.53
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG22	6	0.53
(2,840)	1:129:A:MET:HE3	1:114:A:GLU:HG3	3	0.53
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE1	7	0.53
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	9	0.53
(2,751)	1:104:A:HIS:HE1	1:82:A:ALA:HB3	17	0.53
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	3	0.53
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	5	0.53
(2,740)	1:31:A:ILE:HD11	1:30:A:TRP:HZ2	8	0.53
(2,734)	1:58:A:MET:HE3	1:100:A:LEU:HD21	13	0.53
(2,732)	1:58:A:MET:HE3	1:67:A:THR:HG1	20	0.53
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG21	15	0.53
(2,604)	1:124:A:TYR:HE2	1:14:A:GLU:HG2	6	0.53
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	2	0.53
(2,571)	1:140:A:TYR:HB2	1:127:A:MET:HB2	17	0.53
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG11	13	0.53
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG23	15	0.53
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	20	0.53
(2,422)	1:74:A:LEU:HD11	1:4:A:PRO:HD2	16	0.53
(2,412)	1:73:A:ALA:HB1	1:55:A:ARG:H	13	0.53
(2,412)	1:73:A:ALA:HB2	1:55:A:ARG:H	14	0.53
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	11	0.53
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG22	13	0.53
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	10	0.53
(2,290)	1:36:A:ILE:HD11	1:36:A:ILE:HA	11	0.53
(2,288)	1:36:A:ILE:HD12	1:37:A:LYS:H	4	0.53
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	11	0.53
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	2	0.53
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	12	0.53
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	12	0.53
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	19	0.53
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD13	15	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	20	0.53
(2,125)	1:35:A:VAL:HG12	1:64:A:LYS:HE3	5	0.53
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	7	0.53
(2,115)	1:8:A:LEU:HD21	1:8:A:LEU:HB2	8	0.53
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	11	0.53
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	12	0.53
(2,115)	1:8:A:LEU:HD21	1:56:A:TYR:HB3	14	0.53
(2,115)	1:8:A:LEU:HD22	1:8:A:LEU:HB2	15	0.53
(2,115)	1:8:A:LEU:HD23	1:8:A:LEU:HB2	16	0.53
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	17	0.53
(2,26)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	2	0.53
(1,2841)	1:36:A:ILE:HD12	2:1001:A:OLA:H10	12	0.53
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	11	0.53
(1,2797)	1:116:A:TYR:HD2	1:118:A:TYR:HH	19	0.53
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG22	18	0.53
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	6	0.53
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	3	0.53
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	17	0.53
(1,1464)	1:8:A:LEU:HD11	1:45:A:PHE:HB2	1	0.53
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	19	0.53
(1,1344)	1:105:A:ILE:HD11	1:105:A:ILE:H	3	0.53
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	5	0.53
(1,1344)	1:105:A:ILE:HD11	1:105:A:ILE:H	15	0.53
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	20	0.53
(1,1262)	1:100:A:LEU:HD22	1:101:A:THR:H	9	0.53
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	18	0.53
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	11	0.53
(1,989)	1:134:A:VAL:HG11	1:22:A:TYR:HB3	19	0.53
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	13	0.53
(1,636)	1:61:A:LEU:HD23	1:66:A:ASP:HB2	12	0.53
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	11	0.53
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD22	9	0.53
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	16	0.53
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	17	0.53
(1,397)	1:35:A:VAL:HG21	1:36:A:ILE:H	10	0.53
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	14	0.53
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	18	0.53
(1,288)	1:23:A:LEU:HD21	1:33:A:ARG:HA	3	0.53
(1,288)	1:23:A:LEU:HD23	1:33:A:ARG:HA	7	0.53
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	20	0.53
(1,130)	1:3:A:LEU:HD11	1:7:A:PHE:HB3	9	0.53
(1,114)	1:50:A:SER:HB3	1:52:A:LYS:HB2	3	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:48:A:ALA:HB3	1:71:A:ASP:HB2	18	0.53
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG22	1	0.53
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	2	0.53
(2,1678)	1:83:A:LEU:HB2	1:67:A:THR:HG22	4	0.52
(2,1652)	1:32:A:MET:HE3	1:35:A:VAL:HG11	2	0.52
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	16	0.52
(2,1606)	2:1001:A:OLA:H111	1:36:A:ILE:HD11	15	0.52
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	9	0.52
(2,1466)	1:98:A:ASN:H	1:95:A:LYS:HD3	13	0.52
(2,1461)	1:136:A:THR:H	1:128:A:LYS:HB3	11	0.52
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	11	0.52
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	16	0.52
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	5	0.52
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	12	0.52
(2,1267)	1:80:A:ASP:H	1:107:A:VAL:HG13	3	0.52
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD11	1	0.52
(2,1098)	1:132:A:LYS:HD3	1:131:A:TRP:HE1	1	0.52
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	20	0.52
(2,936)	1:67:A:THR:H	1:83:A:LEU:HD13	2	0.52
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG21	17	0.52
(2,838)	1:127:A:MET:HE1	1:116:A:TYR:HE2	17	0.52
(2,830)	2:1001:A:OLA:H81	1:36:A:ILE:HA	10	0.52
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	3	0.52
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	19	0.52
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	7	0.52
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	13	0.52
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	16	0.52
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG22	11	0.52
(2,690)	1:141:A:LYS:HD3	1:141:A:LYS:H	17	0.52
(2,677)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	20	0.52
(2,675)	1:139:A:TYR:HA	1:139:A:TYR:HE2	1	0.52
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	15	0.52
(2,623)	1:128:A:LYS:HE3	1:126:A:VAL:HG13	18	0.52
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG12	13	0.52
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	9	0.52
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG12	2	0.52
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	1	0.52
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	12	0.52
(2,533)	1:99:A:THR:HG22	1:95:A:LYS:HE3	4	0.52
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	15	0.52
(2,502)	1:90:A:ILE:HD12	1:90:A:ILE:H	8	0.52
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	3	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	12	0.52
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	2	0.52
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB3	12	0.52
(2,423)	1:3:A:LEU:HD23	1:74:A:LEU:HD13	12	0.52
(2,422)	1:74:A:LEU:HD11	1:4:A:PRO:HD2	9	0.52
(2,378)	1:83:A:LEU:HD13	1:62:A:THR:HG22	19	0.52
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	3	0.52
(2,349)	1:52:A:LYS:HG2	1:52:A:LYS:H	15	0.52
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG23	4	0.52
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	20	0.52
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	7	0.52
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	5	0.52
(2,158)	1:15:A:ARG:HA	1:13:A:LEU:HB3	10	0.52
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD23	1	0.52
(2,107)	1:120:A:ARG:HB2	1:7:A:PHE:HB3	2	0.52
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	11	0.52
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	2	0.52
(2,51)	1:48:A:ALA:HB2	1:56:A:TYR:HB3	16	0.52
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG23	5	0.52
(1,2833)	2:1001:A:OLA:H181	1:36:A:ILE:HA	17	0.52
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	20	0.52
(1,2814)	2:1001:A:OLA:H183	1:19:A:PHE:HE1	17	0.52
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	1	0.52
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	19	0.52
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG22	5	0.52
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	3	0.52
(1,2593)	1:67:A:THR:HG22	1:84:A:ASP:H	20	0.52
(1,2489)	1:13:A:LEU:HD21	1:17:A:GLU:H	4	0.52
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG23	4	0.52
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG22	20	0.52
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	13	0.52
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	19	0.52
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG12	20	0.52
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	13	0.52
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	2	0.52
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD22	14	0.52
(1,1386)	1:83:A:LEU:HD11	1:84:A:ASP:H	15	0.52
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	10	0.52
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	15	0.52
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD22	7	0.52
(1,1223)	1:127:A:MET:HE3	1:116:A:TYR:HD1	8	0.52
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE1	8	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1193)	1:114:A:GLU:HG3	1:131:A:TRP:HE3	18	0.52
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	2	0.52
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE2	6	0.52
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	18	0.52
(1,1111)	1:58:A:MET:HE2	1:43:A:LYS:HE2	19	0.52
(1,878)	1:115:A:THR:H	1:115:A:THR:HG22	18	0.52
(1,754)	1:94:A:LEU:HD11	1:100:A:LEU:HA	13	0.52
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD22	17	0.52
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	20	0.52
(1,441)	1:38:A:LEU:HD23	1:38:A:LEU:HA	9	0.52
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	8	0.52
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD11	13	0.52
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD13	1	0.52
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	5	0.52
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	10	0.52
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB2	20	0.52
(1,97)	1:52:A:LYS:H	1:48:A:ALA:HB3	12	0.52
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	16	0.52
(2,1645)	2:1001:A:OLA:H31	1:140:A:TYR:HH	2	0.51
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	13	0.51
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	11	0.51
(2,1605)	1:36:A:ILE:HD12	2:1001:A:OLA:H121	3	0.51
(2,1540)	1:119:A:ARG:HG2	1:100:A:LEU:H	15	0.51
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	5	0.51
(2,1396)	1:62:A:THR:HG23	1:41:A:VAL:H	14	0.51
(2,1360)	1:52:A:LYS:H	1:52:A:LYS:HG3	7	0.51
(2,1274)	1:105:A:ILE:H	1:105:A:ILE:HG23	8	0.51
(2,1232)	1:65:A:LYS:HB3	1:85:A:SER:H	9	0.51
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	7	0.51
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	3	0.51
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	6	0.51
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	16	0.51
(2,789)	1:26:A:ARG:HD2	1:131:A:TRP:HZ3	18	0.51
(2,784)	1:35:A:VAL:HG22	1:32:A:MET:HE3	7	0.51
(2,760)	1:127:A:MET:HE2	1:140:A:TYR:HH	16	0.51
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG21	2	0.51
(2,732)	1:58:A:MET:HE1	1:67:A:THR:HG1	6	0.51
(2,727)	1:3:A:LEU:HD22	1:7:A:PHE:HA	7	0.51
(2,707)	1:67:A:THR:HG23	1:62:A:THR:HG1	10	0.51
(2,694)	1:141:A:LYS:H	1:141:A:LYS:HE3	14	0.51
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	16	0.51
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	13	0.51
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	3	0.51
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	12	0.51
(2,569)	1:108:A:ASP:H	1:107:A:VAL:HG21	1	0.51
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	6	0.51
(2,538)	1:94:A:LEU:HA	1:100:A:LEU:HD21	4	0.51
(2,533)	1:99:A:THR:HG23	1:96:A:ASP:HB2	2	0.51
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	1	0.51
(2,523)	1:128:A:LYS:HG2	1:129:A:MET:H	2	0.51
(2,497)	1:90:A:ILE:HD13	1:78:A:PHE:HE2	18	0.51
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	15	0.51
(2,494)	1:90:A:ILE:HD13	1:104:A:HIS:HB3	20	0.51
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	14	0.51
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	5	0.51
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD11	7	0.51
(2,349)	1:52:A:LYS:H	1:52:A:LYS:HG3	10	0.51
(2,293)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	2	0.51
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	1	0.51
(2,290)	1:36:A:ILE:HD11	1:36:A:ILE:HA	8	0.51
(2,290)	1:36:A:ILE:HD11	1:36:A:ILE:HA	16	0.51
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG23	15	0.51
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	16	0.51
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	10	0.51
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD21	15	0.51
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD21	19	0.51
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	3	0.51
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	8	0.51
(2,49)	1:47:A:ASN:HB2	1:48:A:ALA:HB2	10	0.51
(2,7)	1:31:A:ILE:HD11	1:34:A:GLN:HB2	8	0.51
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	2	0.51
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	4	0.51
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	3	0.51
(1,2813)	1:127:A:MET:HE1	1:118:A:TYR:HH	2	0.51
(1,2463)	1:111:A:THR:HG21	1:113:A:VAL:H	3	0.51
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG22	7	0.51
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG23	13	0.51
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	3	0.51
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	17	0.51
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	2	0.51
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	6	0.51
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	15	0.51
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG13	18	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	13	0.51
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD21	10	0.51
(1,1464)	1:8:A:LEU:HD13	1:45:A:PHE:HB2	4	0.51
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	3	0.51
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	12	0.51
(1,1344)	1:105:A:ILE:HD11	1:105:A:ILE:H	20	0.51
(1,1262)	1:100:A:LEU:HD21	1:101:A:THR:H	6	0.51
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	4	0.51
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	14	0.51
(1,1226)	1:49:A:ALA:HB3	1:51:A:GLY:H	11	0.51
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE3	10	0.51
(1,1088)	1:61:A:LEU:HD23	1:62:A:THR:H	10	0.51
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	6	0.51
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	11	0.51
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG11	10	0.51
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG12	19	0.51
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	6	0.51
(1,923)	1:125:A:LEU:HD23	1:118:A:TYR:HB2	12	0.51
(1,878)	1:115:A:THR:H	1:115:A:THR:HG23	4	0.51
(1,878)	1:115:A:THR:H	1:115:A:THR:HG23	13	0.51
(1,878)	1:115:A:THR:H	1:115:A:THR:HG22	20	0.51
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG13	7	0.51
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	9	0.51
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG11	6	0.51
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG13	8	0.51
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD11	10	0.51
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD13	12	0.51
(1,629)	1:74:A:LEU:HD13	1:75:A:GLY:H	19	0.51
(1,628)	1:74:A:LEU:HD11	1:74:A:LEU:H	16	0.51
(1,617)	1:73:A:ALA:HB2	1:75:A:GLY:H	1	0.51
(1,617)	1:73:A:ALA:HB3	1:75:A:GLY:H	14	0.51
(1,599)	1:70:A:LYS:HD2	1:70:A:LYS:HE3	20	0.51
(1,591)	1:70:A:LYS:HE3	1:70:A:LYS:HB3	16	0.51
(1,548)	1:62:A:THR:HG22	1:60:A:ASN:HB2	17	0.51
(1,397)	1:35:A:VAL:HG22	1:36:A:ILE:H	2	0.51
(1,397)	1:35:A:VAL:HG21	1:36:A:ILE:H	19	0.51
(1,288)	1:23:A:LEU:HD22	1:33:A:ARG:HA	13	0.51
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD12	9	0.51
(1,120)	1:1:A:LYS:HG3	1:1:A:LYS:HA	1	0.51
(1,114)	1:50:A:SER:HB3	1:52:A:LYS:HB2	19	0.51
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG23	17	0.51
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG22	17	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1679)	2:1001:A:OLA:H172	2:1001:A:OLA:H183	9	0.5
(2,1678)	2:1001:A:OLA:H122	2:1001:A:OLA:H142	9	0.5
(2,1670)	2:1001:A:OLA:H182	2:1001:A:OLA:H21	5	0.5
(2,1614)	1:106:A:LYS:HB2	1:111:A:THR:H	6	0.5
(2,1605)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	19	0.5
(2,1461)	1:136:A:THR:H	1:128:A:LYS:HB3	15	0.5
(2,1439)	1:13:A:LEU:H	1:143:A:GLN:HE21	9	0.5
(2,1360)	1:52:A:LYS:HG2	1:52:A:LYS:H	4	0.5
(2,1313)	1:125:A:LEU:HA	1:124:A:TYR:H	7	0.5
(2,1313)	1:124:A:TYR:H	1:121:A:ASP:HA	20	0.5
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	15	0.5
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD22	8	0.5
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	13	0.5
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	18	0.5
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	12	0.5
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	1	0.5
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	2	0.5
(2,783)	1:127:A:MET:HE3	1:140:A:TYR:HE2	2	0.5
(2,783)	1:127:A:MET:HE2	1:140:A:TYR:HE2	16	0.5
(2,740)	1:31:A:ILE:HD13	1:30:A:TRP:HZ2	14	0.5
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	5	0.5
(2,687)	1:143:A:GLN:HA	1:141:A:LYS:HD2	7	0.5
(2,668)	1:129:A:MET:HE3	1:136:A:THR:HG23	8	0.5
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	17	0.5
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG13	7	0.5
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD21	15	0.5
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	5	0.5
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG22	14	0.5
(2,533)	1:99:A:THR:HG23	1:96:A:ASP:HB2	8	0.5
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	10	0.5
(2,501)	1:90:A:ILE:HD12	1:80:A:ASP:H	11	0.5
(2,494)	1:90:A:ILE:HD13	1:104:A:HIS:HB3	5	0.5
(2,494)	1:90:A:ILE:HD13	1:104:A:HIS:HB3	10	0.5
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	13	0.5
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB3	18	0.5
(2,446)	1:83:A:LEU:HD11	1:60:A:ASN:HD21	9	0.5
(2,437)	1:86:A:THR:HB	1:82:A:ALA:HB2	8	0.5
(2,409)	1:52:A:LYS:HB3	1:71:A:ASP:HB2	7	0.5
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HG23	1	0.5
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	4	0.5
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	13	0.5
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD11	9	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	13	0.5
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	15	0.5
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD11	16	0.5
(2,330)	1:41:A:VAL:HG23	1:43:A:LYS:HE3	3	0.5
(2,320)	1:67:A:THR:HG21	1:60:A:ASN:HD21	18	0.5
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG22	1	0.5
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	11	0.5
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG21	10	0.5
(2,205)	1:23:A:LEU:HD12	1:37:A:LYS:HE3	18	0.5
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	9	0.5
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	7	0.5
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	4	0.5
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	2	0.5
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD3	6	0.5
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	6	0.5
(2,120)	1:8:A:LEU:HD13	1:7:A:PHE:H	18	0.5
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	8	0.5
(2,118)	1:8:A:LEU:HD12	1:8:A:LEU:HA	7	0.5
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	12	0.5
(2,62)	1:0:A:SER:HB3	1:2:A:THR:H	15	0.5
(2,52)	1:49:A:ALA:HB1	1:50:A:SER:HB3	17	0.5
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	7	0.5
(1,2833)	2:1001:A:OLA:H181	1:36:A:ILE:HA	10	0.5
(1,2833)	2:1001:A:OLA:H183	1:36:A:ILE:HA	13	0.5
(1,2833)	2:1001:A:OLA:H183	1:36:A:ILE:HA	15	0.5
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	2	0.5
(1,2814)	2:1001:A:OLA:H182	1:19:A:PHE:HE2	6	0.5
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	14	0.5
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG22	17	0.5
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	1	0.5
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD23	19	0.5
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG23	11	0.5
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	1	0.5
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	12	0.5
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	19	0.5
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD11	1	0.5
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	9	0.5
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD13	12	0.5
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	13	0.5
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	3	0.5
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	10	0.5
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	12	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1292)	1:111:A:THR:HG21	1:112:A:ASP:H	19	0.5
(1,1226)	1:49:A:ALA:HB3	1:51:A:GLY:H	19	0.5
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE3	16	0.5
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE2	9	0.5
(1,1168)	1:32:A:MET:HE1	1:35:A:VAL:H	15	0.5
(1,1168)	1:32:A:MET:HE3	1:35:A:VAL:H	18	0.5
(1,1111)	1:58:A:MET:HE3	1:43:A:LYS:HE2	4	0.5
(1,1088)	1:61:A:LEU:HD23	1:62:A:THR:H	14	0.5
(1,1088)	1:61:A:LEU:HD22	1:62:A:THR:H	15	0.5
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	8	0.5
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG11	18	0.5
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	2	0.5
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	9	0.5
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	19	0.5
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	9	0.5
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	12	0.5
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	4	0.5
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	10	0.5
(1,548)	1:62:A:THR:HG22	1:60:A:ASN:HB2	12	0.5
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG22	19	0.5
(1,397)	1:35:A:VAL:HG22	1:36:A:ILE:H	8	0.5
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD12	16	0.5
(1,212)	1:13:A:LEU:HD23	1:13:A:LEU:HA	12	0.5
(1,137)	1:3:A:LEU:HD22	1:7:A:PHE:HB3	17	0.5
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG21	4	0.5
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	8	0.49
(2,1577)	1:83:A:LEU:HD13	2:1001:A:OLA:H72	14	0.49
(2,1396)	1:63:A:THR:HG21	1:41:A:VAL:H	12	0.49
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	6	0.49
(2,1139)	1:100:A:LEU:H	1:119:A:ARG:HG3	11	0.49
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	15	0.49
(2,1061)	1:118:A:TYR:HD2	1:128:A:LYS:H	6	0.49
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD23	4	0.49
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG13	11	0.49
(2,925)	1:65:A:LYS:HG3	1:67:A:THR:H	9	0.49
(2,849)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	4	0.49
(2,841)	1:129:A:MET:HE1	1:114:A:GLU:HG3	13	0.49
(2,835)	1:20:A:ASP:HA	1:37:A:LYS:HE2	14	0.49
(2,834)	1:68:A:HIS:HE1	1:49:A:ALA:HB2	13	0.49
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	14	0.49
(2,811)	1:89:A:LYS:HE3	1:89:A:LYS:H	11	0.49
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,787)	1:39:A:ALA:HB3	1:40:A:GLY:H	17	0.49
(2,785)	1:32:A:MET:HE3	1:35:A:VAL:HG11	2	0.49
(2,783)	1:127:A:MET:HE1	1:140:A:TYR:HE2	11	0.49
(2,779)	1:119:A:ARG:HA	1:119:A:ARG:HD2	20	0.49
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	16	0.49
(2,734)	1:58:A:MET:HE2	1:100:A:LEU:HD23	14	0.49
(2,732)	1:58:A:MET:HE1	1:67:A:THR:HG1	7	0.49
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	16	0.49
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	19	0.49
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	7	0.49
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	3	0.49
(2,675)	1:139:A:TYR:HA	1:139:A:TYR:HE2	18	0.49
(2,603)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	4	0.49
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG13	4	0.49
(2,543)	1:100:A:LEU:HD22	1:58:A:MET:HG2	9	0.49
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	19	0.49
(2,527)	1:96:A:ASP:H	1:95:A:LYS:HD3	5	0.49
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	3	0.49
(2,494)	1:90:A:ILE:HD12	1:104:A:HIS:HB3	16	0.49
(2,465)	1:87:A:GLN:HG3	1:107:A:VAL:HG12	7	0.49
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB2	11	0.49
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	6	0.49
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB3	5	0.49
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	3	0.49
(2,290)	1:36:A:ILE:HD11	1:36:A:ILE:HA	6	0.49
(2,290)	1:36:A:ILE:HD11	1:36:A:ILE:HA	14	0.49
(2,201)	1:36:A:ILE:H	1:23:A:LEU:HD12	6	0.49
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	19	0.49
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	6	0.49
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD12	3	0.49
(2,162)	1:16:A:ASP:HA	1:13:A:LEU:HD21	8	0.49
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD3	9	0.49
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	2	0.49
(2,119)	1:8:A:LEU:HD11	1:9:A:GLY:H	16	0.49
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	4	0.49
(2,118)	1:8:A:LEU:HD11	1:8:A:LEU:HA	6	0.49
(2,118)	1:8:A:LEU:HD12	1:8:A:LEU:HA	13	0.49
(2,118)	1:8:A:LEU:HD13	1:47:A:ASN:HA	17	0.49
(2,118)	1:8:A:LEU:HD11	1:8:A:LEU:HA	19	0.49
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	16	0.49
(2,76)	1:3:A:LEU:HD12	1:45:A:PHE:HB2	17	0.49
(2,62)	1:0:A:SER:HB3	1:2:A:THR:H	1	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	4	0.49
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	6	0.49
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB3	20	0.49
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	1	0.49
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	15	0.49
(2,51)	1:48:A:ALA:HB3	1:56:A:TYR:HB3	14	0.49
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	6	0.49
(1,2724)	1:2:A:THR:H	1:2:A:THR:HG23	20	0.49
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	17	0.49
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	19	0.49
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG23	16	0.49
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG22	19	0.49
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	12	0.49
(1,1531)	1:70:A:LYS:HG2	1:68:A:HIS:HD2	1	0.49
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG11	10	0.49
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD13	12	0.49
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	3	0.49
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	7	0.49
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	18	0.49
(1,1225)	1:127:A:MET:HE3	1:128:A:LYS:H	18	0.49
(1,1183)	1:35:A:VAL:HB	1:32:A:MET:HE3	18	0.49
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE3	14	0.49
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE3	16	0.49
(1,1111)	1:58:A:MET:HE1	1:43:A:LYS:HE2	2	0.49
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE1	3	0.49
(1,1106)	1:58:A:MET:HE2	1:45:A:PHE:HE1	3	0.49
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG21	15	0.49
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	1	0.49
(1,878)	1:115:A:THR:H	1:115:A:THR:HG23	11	0.49
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	17	0.49
(1,636)	1:61:A:LEU:HD22	1:66:A:ASP:HB2	14	0.49
(1,629)	1:74:A:LEU:HD11	1:75:A:GLY:H	14	0.49
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB2	20	0.49
(1,617)	1:73:A:ALA:HB3	1:75:A:GLY:H	19	0.49
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	16	0.49
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	7	0.49
(1,397)	1:35:A:VAL:HG22	1:36:A:ILE:H	15	0.49
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD13	16	0.49
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD13	17	0.49
(1,173)	1:56:A:TYR:HD2	1:8:A:LEU:HD21	16	0.49
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG22	12	0.49
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG22	16	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1602)	1:32:A:MET:HE2	2:1001:A:OLA:H111	7	0.48
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	3	0.48
(2,1556)	1:35:A:VAL:HG22	1:36:A:ILE:H	5	0.48
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	12	0.48
(2,1556)	1:35:A:VAL:HG21	1:36:A:ILE:H	13	0.48
(2,1555)	1:96:A:ASP:H	1:94:A:LEU:HD21	17	0.48
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	11	0.48
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	4	0.48
(2,929)	1:116:A:TYR:H	1:129:A:MET:HB2	8	0.48
(2,841)	1:129:A:MET:HE2	1:114:A:GLU:HG3	14	0.48
(2,838)	1:127:A:MET:HE2	1:116:A:TYR:HE2	19	0.48
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	15	0.48
(2,825)	1:118:A:TYR:HD1	1:127:A:MET:HG2	2	0.48
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	19	0.48
(2,811)	1:89:A:LYS:H	1:89:A:LYS:HE2	10	0.48
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	9	0.48
(2,740)	1:31:A:ILE:HD13	1:30:A:TRP:HZ2	19	0.48
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	13	0.48
(2,688)	1:141:A:LYS:HD3	1:143:A:GLN:HA	18	0.48
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	4	0.48
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG23	3	0.48
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	9	0.48
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG23	11	0.48
(2,604)	1:124:A:TYR:HE2	1:14:A:GLU:HG2	13	0.48
(2,564)	1:107:A:VAL:HA	1:89:A:LYS:HE2	8	0.48
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG11	18	0.48
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG11	9	0.48
(2,541)	1:100:A:LEU:HD21	1:118:A:TYR:HB2	8	0.48
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	3	0.48
(2,495)	1:90:A:ILE:HD11	1:90:A:ILE:HA	8	0.48
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	16	0.48
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	19	0.48
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	7	0.48
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	6	0.48
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD11	14	0.48
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB1	11	0.48
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	9	0.48
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	14	0.48
(2,293)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	16	0.48
(2,290)	1:36:A:ILE:HD12	1:36:A:ILE:HA	2	0.48
(2,290)	1:36:A:ILE:HD11	1:36:A:ILE:HA	4	0.48
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	12	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	10	0.48
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	11	0.48
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	11	0.48
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD3	11	0.48
(2,132)	1:85:A:SER:H	1:65:A:LYS:HE2	13	0.48
(2,119)	1:8:A:LEU:HD12	1:9:A:GLY:H	18	0.48
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	2	0.48
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	14	0.48
(2,118)	1:8:A:LEU:HD11	1:8:A:LEU:HA	16	0.48
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD23	4	0.48
(2,116)	1:8:A:LEU:HD23	1:9:A:GLY:H	16	0.48
(2,115)	1:8:A:LEU:HD21	1:56:A:TYR:HB3	17	0.48
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	18	0.48
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB1	18	0.48
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	8	0.48
(2,7)	1:31:A:ILE:HD12	1:34:A:GLN:HB2	6	0.48
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	1	0.48
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	3	0.48
(1,2833)	2:1001:A:OLA:H181	1:36:A:ILE:HA	19	0.48
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	12	0.48
(1,2548)	1:112:A:ASP:H	1:106:A:LYS:HD2	12	0.48
(1,2520)	1:143:A:GLN:HE22	1:12:A:LYS:HB2	10	0.48
(1,2243)	1:23:A:LEU:HD21	1:37:A:LYS:H	10	0.48
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	7	0.48
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG22	10	0.48
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	9	0.48
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	11	0.48
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	2	0.48
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	3	0.48
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	8	0.48
(1,1517)	1:80:A:ASP:H	1:79:A:GLN:HG3	7	0.48
(1,1517)	1:80:A:ASP:H	1:79:A:GLN:HG3	16	0.48
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG11	13	0.48
(1,1386)	1:83:A:LEU:HD11	1:84:A:ASP:H	4	0.48
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	16	0.48
(1,1344)	1:105:A:ILE:HD11	1:105:A:ILE:H	19	0.48
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD22	20	0.48
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD11	6	0.48
(1,1223)	1:127:A:MET:HE1	1:116:A:TYR:HD2	17	0.48
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE2	1	0.48
(1,1111)	1:58:A:MET:HE1	1:43:A:LYS:HE2	16	0.48
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	19	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1104)	1:58:A:MET:HE1	1:118:A:TYR:HE1	5	0.48
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	1	0.48
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	5	0.48
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	17	0.48
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	20	0.48
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG23	14	0.48
(1,878)	1:115:A:THR:H	1:115:A:THR:HG22	19	0.48
(1,785)	1:100:A:LEU:HD21	1:45:A:PHE:HE2	12	0.48
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD22	18	0.48
(1,647)	1:79:A:GLN:HG2	1:107:A:VAL:HG11	19	0.48
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	15	0.48
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	1	0.48
(1,617)	1:73:A:ALA:HB2	1:75:A:GLY:H	7	0.48
(1,617)	1:73:A:ALA:HB2	1:75:A:GLY:H	9	0.48
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	18	0.48
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	19	0.48
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	14	0.48
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG23	5	0.48
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	17	0.48
(1,383)	1:23:A:LEU:HD21	1:33:A:ARG:HA	16	0.48
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	4	0.48
(1,212)	1:13:A:LEU:HD23	1:13:A:LEU:HA	9	0.48
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB1	10	0.48
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB2	2	0.48
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	20	0.48
(2,1652)	1:32:A:MET:HE2	2:1001:A:OLA:H131	11	0.47
(2,1602)	2:1001:A:OLA:H111	1:65:A:LYS:HB3	9	0.47
(2,1583)	1:41:A:VAL:HG21	2:1001:A:OLA:H21	9	0.47
(2,1540)	1:119:A:ARG:HG2	1:100:A:LEU:H	4	0.47
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	9	0.47
(2,1495)	1:13:A:LEU:H	1:42:A:THR:HG22	8	0.47
(2,1397)	1:112:A:ASP:H	1:105:A:ILE:HG21	4	0.47
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	6	0.47
(2,1279)	1:80:A:ASP:H	1:89:A:LYS:HB3	1	0.47
(2,1184)	1:61:A:LEU:HD11	1:143:A:GLN:HE22	10	0.47
(2,1184)	1:61:A:LEU:HD12	1:143:A:GLN:HE22	14	0.47
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	17	0.47
(2,1029)	1:105:A:ILE:HD12	1:104:A:HIS:H	19	0.47
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD23	9	0.47
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG11	14	0.47
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	3	0.47
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	8	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,838)	1:127:A:MET:HE2	1:116:A:TYR:HE2	2	0.47
(2,837)	1:58:A:MET:HE3	1:60:A:ASN:HD21	20	0.47
(2,811)	1:89:A:LYS:H	1:89:A:LYS:HE2	4	0.47
(2,810)	1:52:A:LYS:HE2	1:50:A:SER:HB3	18	0.47
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	19	0.47
(2,779)	1:120:A:ARG:HA	1:119:A:ARG:HD2	4	0.47
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD12	2	0.47
(2,732)	1:58:A:MET:HE2	1:67:A:THR:HG1	9	0.47
(2,731)	1:58:A:MET:HE3	1:61:A:LEU:H	18	0.47
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	12	0.47
(2,718)	1:73:A:ALA:HB1	1:0:A:SER:HA	20	0.47
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	1	0.47
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD21	11	0.47
(2,558)	1:105:A:ILE:HD11	1:105:A:ILE:HA	2	0.47
(2,533)	1:99:A:THR:HG23	1:96:A:ASP:HB2	5	0.47
(2,496)	1:90:A:ILE:HD12	1:69:A:HIS:HA	11	0.47
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG21	1	0.47
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	4	0.47
(2,433)	1:81:A:GLU:HG2	1:81:A:GLU:H	4	0.47
(2,433)	1:81:A:GLU:HG2	1:81:A:GLU:H	12	0.47
(2,413)	1:73:A:ALA:HB2	1:54:A:ASP:HB3	1	0.47
(2,412)	1:73:A:ALA:HB3	1:55:A:ARG:H	4	0.47
(2,374)	1:62:A:THR:HG22	1:83:A:LEU:HG	15	0.47
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG11	9	0.47
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	8	0.47
(2,290)	1:36:A:ILE:HD12	1:36:A:ILE:HA	17	0.47
(2,290)	1:36:A:ILE:HD12	1:36:A:ILE:HA	19	0.47
(2,288)	1:36:A:ILE:HD12	1:37:A:LYS:H	6	0.47
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	18	0.47
(2,226)	1:134:A:VAL:HG23	1:25:A:ALA:HA	7	0.47
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD12	8	0.47
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	14	0.47
(2,132)	1:85:A:SER:H	1:65:A:LYS:HE2	19	0.47
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	20	0.47
(2,122)	1:9:A:GLY:HA3	1:142:A:LYS:HE3	6	0.47
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	5	0.47
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	5	0.47
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	11	0.47
(2,118)	1:8:A:LEU:HD12	1:8:A:LEU:HA	18	0.47
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	20	0.47
(2,93)	1:125:A:LEU:HD11	1:127:A:MET:HG3	9	0.47
(2,90)	1:3:A:LEU:HD22	1:7:A:PHE:HB2	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	8	0.47
(2,45)	1:49:A:ALA:HB2	1:48:A:ALA:HA	18	0.47
(1,2841)	1:36:A:ILE:HD11	2:1001:A:OLA:H10	13	0.47
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	6	0.47
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	8	0.47
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	16	0.47
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	11	0.47
(1,2799)	1:83:A:LEU:HD21	1:62:A:THR:HG1	4	0.47
(1,2593)	1:67:A:THR:HG23	1:84:A:ASP:H	5	0.47
(1,2593)	1:67:A:THR:HG21	1:84:A:ASP:H	7	0.47
(1,2593)	1:67:A:THR:HG23	1:84:A:ASP:H	11	0.47
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	18	0.47
(1,2243)	1:23:A:LEU:HD21	1:37:A:LYS:H	6	0.47
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	2	0.47
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG23	16	0.47
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	8	0.47
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG11	17	0.47
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	10	0.47
(1,1580)	1:8:A:LEU:HD13	1:8:A:LEU:H	9	0.47
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	3	0.47
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG11	19	0.47
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD21	17	0.47
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	18	0.47
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	2	0.47
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	18	0.47
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	9	0.47
(1,1245)	1:11:A:PHE:H	1:44:A:LYS:HG2	19	0.47
(1,1240)	1:125:A:LEU:HD23	1:120:A:ARG:HD2	16	0.47
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD21	1	0.47
(1,1225)	1:127:A:MET:HE1	1:128:A:LYS:H	12	0.47
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	17	0.47
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	19	0.47
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE2	20	0.47
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE2	8	0.47
(1,1111)	1:58:A:MET:HE2	1:43:A:LYS:HE2	10	0.47
(1,1104)	1:58:A:MET:HE2	1:118:A:TYR:HE1	7	0.47
(1,1104)	1:58:A:MET:HE3	1:118:A:TYR:HE1	19	0.47
(1,1088)	1:61:A:LEU:HD23	1:62:A:THR:H	12	0.47
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	2	0.47
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	10	0.47
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	7	0.47
(1,878)	1:115:A:THR:H	1:115:A:THR:HG22	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,878)	1:115:A:THR:H	1:115:A:THR:HG23	16	0.47
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	19	0.47
(1,755)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	18	0.47
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	17	0.47
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	6	0.47
(1,617)	1:73:A:ALA:HB3	1:75:A:GLY:H	13	0.47
(1,441)	1:38:A:LEU:HD22	1:38:A:LEU:HA	15	0.47
(1,430)	1:23:A:LEU:HD21	1:37:A:LYS:HG2	6	0.47
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG23	19	0.47
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB1	7	0.47
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD12	15	0.47
(1,195)	1:11:A:PHE:H	1:10:A:THR:HG21	16	0.47
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	10	0.47
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	15	0.47
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG23	20	0.47
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG21	1	0.47
(2,1670)	2:1001:A:OLA:H182	2:1001:A:OLA:H21	15	0.46
(2,1646)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	1	0.46
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	11	0.46
(2,1637)	2:1001:A:OLA:H71	1:62:A:THR:HG1	13	0.46
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	8	0.46
(2,1605)	1:36:A:ILE:HD11	2:1001:A:OLA:H121	2	0.46
(2,1583)	2:1001:A:OLA:H161	2:1001:A:OLA:H21	12	0.46
(2,1394)	1:143:A:GLN:H	1:141:A:LYS:HD3	7	0.46
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	13	0.46
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE2	1	0.46
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	17	0.46
(2,693)	1:12:A:LYS:H	1:141:A:LYS:HD3	18	0.46
(2,675)	1:139:A:TYR:HA	1:139:A:TYR:HE2	5	0.46
(2,635)	1:130:A:SER:HB3	1:128:A:LYS:HD2	4	0.46
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	5	0.46
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG13	10	0.46
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG11	18	0.46
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG11	20	0.46
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	13	0.46
(2,571)	1:106:A:LYS:HB3	1:109:A:ASP:HB2	4	0.46
(2,556)	1:89:A:LYS:HE3	1:105:A:ILE:HD11	3	0.46
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG11	19	0.46
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	16	0.46
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	15	0.46
(2,487)	1:90:A:ILE:HG21	1:92:A:PHE:HB2	6	0.46
(2,487)	1:90:A:ILE:HG23	1:92:A:PHE:HB2	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG22	19	0.46
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB2	16	0.46
(2,446)	1:83:A:LEU:HD13	1:60:A:ASN:HD21	17	0.46
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB2	3	0.46
(2,410)	1:71:A:ASP:HB3	1:48:A:ALA:HB2	8	0.46
(2,409)	1:52:A:LYS:HB3	1:71:A:ASP:HB2	10	0.46
(2,386)	1:35:A:VAL:HG21	1:64:A:LYS:HG2	18	0.46
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	1	0.46
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	17	0.46
(2,349)	1:52:A:LYS:HG2	1:52:A:LYS:H	4	0.46
(2,349)	1:52:A:LYS:H	1:52:A:LYS:HG3	7	0.46
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	5	0.46
(2,290)	1:36:A:ILE:HD12	1:36:A:ILE:HA	15	0.46
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	18	0.46
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	2	0.46
(2,288)	1:36:A:ILE:HD12	1:37:A:LYS:H	8	0.46
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	17	0.46
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG21	1	0.46
(2,247)	1:26:A:ARG:HD3	1:26:A:ARG:H	3	0.46
(2,188)	1:134:A:VAL:HG13	1:21:A:GLU:HG2	10	0.46
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	11	0.46
(2,125)	1:65:A:LYS:HE3	1:67:A:THR:HG22	17	0.46
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	3	0.46
(2,118)	1:8:A:LEU:HD11	1:8:A:LEU:HA	1	0.46
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	8	0.46
(2,118)	1:8:A:LEU:HD13	1:8:A:LEU:HA	10	0.46
(2,118)	1:8:A:LEU:HD12	1:8:A:LEU:HA	12	0.46
(2,49)	1:52:A:LYS:HE3	1:48:A:ALA:HB3	20	0.46
(2,41)	1:54:A:ASP:H	1:53:A:PRO:HG3	15	0.46
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG3	1	0.46
(2,7)	1:31:A:ILE:HD11	1:34:A:GLN:HB2	15	0.46
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	14	0.46
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	1	0.46
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	4	0.46
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	4	0.46
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	9	0.46
(1,2243)	1:23:A:LEU:HD21	1:37:A:LYS:H	7	0.46
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG21	7	0.46
(1,1580)	1:8:A:LEU:HD12	1:8:A:LEU:H	1	0.46
(1,1580)	1:8:A:LEU:HD13	1:8:A:LEU:H	3	0.46
(1,1580)	1:8:A:LEU:HD13	1:8:A:LEU:H	12	0.46
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG11	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	8	0.46
(1,1292)	1:111:A:THR:HG21	1:112:A:ASP:H	13	0.46
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	14	0.46
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	11	0.46
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	1	0.46
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	5	0.46
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	20	0.46
(1,1223)	1:127:A:MET:HE1	1:116:A:TYR:HD2	12	0.46
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	12	0.46
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE3	15	0.46
(1,1111)	1:58:A:MET:HE1	1:43:A:LYS:HE2	5	0.46
(1,1111)	1:58:A:MET:HE1	1:43:A:LYS:HE2	7	0.46
(1,1111)	1:58:A:MET:HE2	1:43:A:LYS:HE2	13	0.46
(1,1104)	1:58:A:MET:HE3	1:118:A:TYR:HE2	10	0.46
(1,1104)	1:58:A:MET:HE2	1:118:A:TYR:HE1	18	0.46
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	17	0.46
(1,1036)	1:124:A:TYR:HE1	1:141:A:LYS:HD2	9	0.46
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	9	0.46
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	20	0.46
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	2	0.46
(1,785)	1:100:A:LEU:HD21	1:45:A:PHE:HE2	7	0.46
(1,753)	1:94:A:LEU:HD11	1:94:A:LEU:HA	13	0.46
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	3	0.46
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD21	9	0.46
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	13	0.46
(1,429)	1:23:A:LEU:HD22	1:37:A:LYS:HG3	17	0.46
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD12	7	0.46
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD13	11	0.46
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	8	0.46
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	18	0.46
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	14	0.46
(1,212)	1:13:A:LEU:HD23	1:13:A:LEU:HA	1	0.46
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	7	0.46
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	9	0.46
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	18	0.45
(2,1614)	1:106:A:LYS:HB2	1:111:A:THR:H	13	0.45
(2,1606)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	2	0.45
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	11	0.45
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	20	0.45
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	3	0.45
(2,1511)	1:61:A:LEU:HB2	1:67:A:THR:H	17	0.45
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG12	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD12	5	0.45
(2,1315)	1:105:A:ILE:HG13	1:113:A:VAL:H	3	0.45
(2,1243)	1:134:A:VAL:H	1:130:A:SER:HB2	10	0.45
(2,1157)	1:26:A:ARG:HD3	1:26:A:ARG:H	19	0.45
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	19	0.45
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	5	0.45
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	1	0.45
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD22	15	0.45
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD22	17	0.45
(2,1019)	1:33:A:ARG:H	1:33:A:ARG:HG3	11	0.45
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	1	0.45
(2,927)	1:38:A:LEU:H	1:38:A:LEU:HB3	5	0.45
(2,925)	1:67:A:THR:H	1:44:A:LYS:HG2	6	0.45
(2,819)	1:36:A:ILE:HG22	2:1001:A:OLA:H82	15	0.45
(2,785)	1:32:A:MET:HE2	2:1001:A:OLA:H131	11	0.45
(2,751)	1:83:A:LEU:HD13	1:104:A:HIS:HE1	20	0.45
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	13	0.45
(2,740)	1:31:A:ILE:HD11	1:30:A:TRP:HZ2	15	0.45
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	6	0.45
(2,694)	1:141:A:LYS:H	1:141:A:LYS:HE3	9	0.45
(2,615)	1:125:A:LEU:HD21	1:120:A:ARG:HA	7	0.45
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	5	0.45
(2,558)	1:105:A:ILE:HD12	1:105:A:ILE:HA	18	0.45
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	11	0.45
(2,544)	1:100:A:LEU:HD23	1:94:A:LEU:HB2	18	0.45
(2,511)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	2	0.45
(2,500)	1:90:A:ILE:HD12	1:88:A:HIS:H	9	0.45
(2,494)	1:90:A:ILE:HD12	1:104:A:HIS:HB3	4	0.45
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	7	0.45
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	10	0.45
(2,461)	1:41:A:VAL:HG21	1:60:A:ASN:HB3	11	0.45
(2,446)	1:83:A:LEU:HD13	1:60:A:ASN:HD21	5	0.45
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB2	2	0.45
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	6	0.45
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	7	0.45
(2,433)	1:81:A:GLU:HG2	1:81:A:GLU:H	13	0.45
(2,421)	1:2:A:THR:HA	1:74:A:LEU:HD13	7	0.45
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB2	12	0.45
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB3	17	0.45
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG13	3	0.45
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	12	0.45
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	2	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB3	10	0.45
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB1	13	0.45
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	18	0.45
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	6	0.45
(2,288)	1:36:A:ILE:HD12	1:37:A:LYS:H	16	0.45
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	2	0.45
(2,164)	1:13:A:LEU:H	1:13:A:LEU:HD11	17	0.45
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	1	0.45
(2,118)	1:8:A:LEU:HD11	1:8:A:LEU:HA	15	0.45
(2,107)	1:120:A:ARG:HB2	1:7:A:PHE:HB3	8	0.45
(2,51)	1:48:A:ALA:HB2	1:56:A:TYR:HB3	17	0.45
(1,2833)	2:1001:A:OLA:H183	1:36:A:ILE:HA	5	0.45
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	7	0.45
(1,2833)	2:1001:A:OLA:H181	1:36:A:ILE:HA	9	0.45
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	19	0.45
(1,2814)	2:1001:A:OLA:H182	1:19:A:PHE:HE1	5	0.45
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	5	0.45
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	8	0.45
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	11	0.45
(1,2767)	1:98:A:ASN:H	1:99:A:THR:HG23	6	0.45
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	10	0.45
(1,2243)	1:23:A:LEU:HD23	1:37:A:LYS:H	13	0.45
(1,2123)	1:82:A:ALA:H	1:81:A:GLU:HG3	8	0.45
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	17	0.45
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG22	4	0.45
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	4	0.45
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	10	0.45
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	1	0.45
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG11	4	0.45
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD11	9	0.45
(1,1476)	1:75:A:GLY:H	1:74:A:LEU:HD21	9	0.45
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	12	0.45
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	11	0.45
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	14	0.45
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	6	0.45
(1,1216)	1:70:A:LYS:HG2	1:68:A:HIS:HD2	8	0.45
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	15	0.45
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD11	19	0.45
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	7	0.45
(1,925)	1:125:A:LEU:HD21	1:7:A:PHE:HA	5	0.45
(1,923)	1:125:A:LEU:HD23	1:118:A:TYR:HB2	8	0.45
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	18	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	14	0.45
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG21	12	0.45
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	17	0.45
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG23	6	0.45
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD11	1	0.45
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	4	0.45
(1,628)	1:74:A:LEU:HD11	1:74:A:LEU:H	11	0.45
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	7	0.45
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	12	0.45
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE1	8	0.45
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	12	0.45
(1,383)	1:23:A:LEU:HD23	1:33:A:ARG:HA	14	0.45
(1,195)	1:11:A:PHE:H	1:10:A:THR:HG21	4	0.45
(1,120)	1:1:A:LYS:HG3	1:1:A:LYS:HA	17	0.45
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB2	9	0.45
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	10	0.45
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	15	0.45
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG23	13	0.45
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG21	18	0.45
(2,1614)	1:58:A:MET:HE2	1:60:A:ASN:H	9	0.44
(2,1581)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	3	0.44
(2,1579)	1:41:A:VAL:HG13	2:1001:A:OLA:H21	15	0.44
(2,1461)	1:136:A:THR:H	1:127:A:MET:HG2	3	0.44
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	5	0.44
(2,1168)	1:128:A:LYS:HE3	1:135:A:SER:H	3	0.44
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	9	0.44
(2,1019)	1:33:A:ARG:H	1:33:A:ARG:HG3	13	0.44
(2,1019)	1:33:A:ARG:H	1:33:A:ARG:HG3	19	0.44
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	14	0.44
(2,837)	1:58:A:MET:HE1	1:60:A:ASN:HD21	14	0.44
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	10	0.44
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	16	0.44
(2,819)	1:36:A:ILE:HG22	2:1001:A:OLA:H82	5	0.44
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	14	0.44
(2,787)	1:39:A:ALA:HB1	1:40:A:GLY:H	8	0.44
(2,787)	1:39:A:ALA:HB3	1:40:A:GLY:H	16	0.44
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	6	0.44
(2,740)	1:31:A:ILE:HD13	1:30:A:TRP:HZ2	20	0.44
(2,697)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	19	0.44
(2,635)	1:130:A:SER:HB3	1:128:A:LYS:HD2	13	0.44
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG23	16	0.44
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG12	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,621)	1:139:A:TYR:HD2	1:126:A:VAL:HG12	13	0.44
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD23	19	0.44
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	20	0.44
(2,556)	1:105:A:ILE:HD12	1:89:A:LYS:HE2	6	0.44
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	4	0.44
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	8	0.44
(2,511)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	19	0.44
(2,494)	1:90:A:ILE:HD12	1:104:A:HIS:HB3	6	0.44
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	2	0.44
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	17	0.44
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG23	12	0.44
(2,448)	1:84:A:ASP:HA	2:1001:A:OLA:H121	8	0.44
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	18	0.44
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	15	0.44
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG13	16	0.44
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	8	0.44
(2,331)	1:44:A:LYS:HE3	1:44:A:LYS:HA	20	0.44
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	1	0.44
(2,263)	1:30:A:TRP:HA	1:30:A:TRP:HE3	2	0.44
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB2	14	0.44
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG21	7	0.44
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	4	0.44
(2,169)	1:15:A:ARG:HD2	1:139:A:TYR:HD1	9	0.44
(2,160)	1:13:A:LEU:HD22	1:41:A:VAL:H	20	0.44
(2,120)	1:8:A:LEU:HD11	1:7:A:PHE:H	17	0.44
(2,119)	1:8:A:LEU:HD12	1:9:A:GLY:H	3	0.44
(2,118)	1:8:A:LEU:HD12	1:8:A:LEU:HA	3	0.44
(2,118)	1:8:A:LEU:HD12	1:8:A:LEU:HA	9	0.44
(2,116)	1:8:A:LEU:HD23	1:9:A:GLY:H	3	0.44
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD23	5	0.44
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD21	13	0.44
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	15	0.44
(2,41)	1:54:A:ASP:H	1:53:A:PRO:HG3	16	0.44
(1,2836)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	14	0.44
(1,2814)	2:1001:A:OLA:H183	1:19:A:PHE:HE1	10	0.44
(1,2809)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	14	0.44
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	13	0.44
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	15	0.44
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	16	0.44
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	18	0.44
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	13	0.44
(1,2489)	1:13:A:LEU:HD21	1:17:A:GLU:H	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	3	0.44
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	5	0.44
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	8	0.44
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG22	9	0.44
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG21	14	0.44
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	11	0.44
(1,1580)	1:8:A:LEU:HD13	1:8:A:LEU:H	18	0.44
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	10	0.44
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD11	11	0.44
(1,1344)	1:105:A:ILE:HD13	1:105:A:ILE:H	17	0.44
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	14	0.44
(1,1292)	1:111:A:THR:HG22	1:112:A:ASP:H	7	0.44
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	3	0.44
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	8	0.44
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	17	0.44
(1,1226)	1:49:A:ALA:HB2	1:51:A:GLY:H	9	0.44
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	3	0.44
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE3	4	0.44
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	11	0.44
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE3	13	0.44
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	11	0.44
(1,1111)	1:58:A:MET:HE3	1:43:A:LYS:HE2	8	0.44
(1,1097)	1:136:A:THR:HG21	1:129:A:MET:HB3	13	0.44
(1,925)	1:125:A:LEU:HD22	1:7:A:PHE:HA	17	0.44
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	5	0.44
(1,878)	1:115:A:THR:H	1:115:A:THR:HG22	9	0.44
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	5	0.44
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	14	0.44
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	7	0.44
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD21	2	0.44
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB3	14	0.44
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	2	0.44
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD12	19	0.44
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	10	0.44
(1,628)	1:74:A:LEU:HD11	1:74:A:LEU:H	13	0.44
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB3	6	0.44
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB2	18	0.44
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	5	0.44
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG23	6	0.44
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	4	0.44
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	11	0.44
(1,195)	1:11:A:PHE:H	1:10:A:THR:HG22	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	11	0.44
(1,13)	1:31:A:ILE:HD13	1:31:A:ILE:H	4	0.44
(1,13)	1:31:A:ILE:HD13	1:31:A:ILE:H	14	0.44
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	4	0.44
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG23	5	0.44
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	2	0.44
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG21	5	0.44
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	12	0.44
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	15	0.44
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	19	0.43
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	14	0.43
(2,1605)	1:36:A:ILE:HD13	2:1001:A:OLA:H121	16	0.43
(2,1579)	2:1001:A:OLA:H22	1:41:A:VAL:HG11	5	0.43
(2,1540)	1:94:A:LEU:HG	1:100:A:LEU:H	6	0.43
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	6	0.43
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	12	0.43
(2,1511)	1:61:A:LEU:HB2	1:67:A:THR:H	7	0.43
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD11	8	0.43
(2,1459)	1:10:A:THR:HG23	1:45:A:PHE:H	5	0.43
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	18	0.43
(2,1144)	1:105:A:ILE:H	1:113:A:VAL:HB	10	0.43
(2,1141)	1:120:A:ARG:HD2	1:126:A:VAL:H	14	0.43
(2,1098)	1:132:A:LYS:HD3	1:131:A:TRP:HE1	4	0.43
(2,1019)	1:33:A:ARG:H	1:33:A:ARG:HG3	2	0.43
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG13	6	0.43
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG13	16	0.43
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG21	14	0.43
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	17	0.43
(2,782)	1:127:A:MET:HE2	1:116:A:TYR:HA	15	0.43
(2,760)	1:118:A:TYR:H	1:127:A:MET:HE2	1	0.43
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	3	0.43
(2,687)	1:141:A:LYS:HD2	1:141:A:LYS:HA	18	0.43
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG11	15	0.43
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG13	2	0.43
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD23	10	0.43
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG22	18	0.43
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	1	0.43
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG11	18	0.43
(2,541)	1:100:A:LEU:HD23	1:118:A:TYR:HB2	5	0.43
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	8	0.43
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG22	7	0.43
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG21	6	0.43
(2,482)	1:90:A:ILE:HG22	1:78:A:PHE:HD1	2	0.43
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	7	0.43
(2,410)	1:71:A:ASP:HB3	1:55:A:ARG:HB3	16	0.43
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	4	0.43
(2,350)	1:52:A:LYS:H	1:52:A:LYS:HD2	15	0.43
(2,263)	1:30:A:TRP:HA	1:30:A:TRP:HE3	3	0.43
(2,229)	1:25:A:ALA:HB2	1:132:A:LYS:HE2	8	0.43
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG23	4	0.43
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	6	0.43
(2,178)	1:134:A:VAL:HG13	1:18:A:ASN:HB2	3	0.43
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	8	0.43
(2,121)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	11	0.43
(2,120)	1:8:A:LEU:HD12	1:7:A:PHE:H	6	0.43
(2,119)	1:8:A:LEU:HD11	1:9:A:GLY:H	15	0.43
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	17	0.43
(2,83)	1:120:A:ARG:HD2	1:125:A:LEU:HD12	4	0.43
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	18	0.43
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB3	17	0.43
(2,49)	1:47:A:ASN:HB2	1:48:A:ALA:HB2	15	0.43
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	17	0.43
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD23	11	0.43
(1,2841)	1:36:A:ILE:HD12	2:1001:A:OLA:H10	1	0.43
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	14	0.43
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	14	0.43
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	7	0.43
(1,2807)	1:118:A:TYR:HD2	1:118:A:TYR:HH	10	0.43
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	17	0.43
(1,2807)	1:118:A:TYR:HD1	1:118:A:TYR:HH	20	0.43
(1,2463)	1:111:A:THR:HG21	1:113:A:VAL:H	17	0.43
(1,2243)	1:23:A:LEU:HD23	1:37:A:LYS:H	18	0.43
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	6	0.43
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	15	0.43
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	16	0.43
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	2	0.43
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	5	0.43
(1,1580)	1:8:A:LEU:HD13	1:8:A:LEU:H	7	0.43
(1,1580)	1:8:A:LEU:HD13	1:8:A:LEU:H	13	0.43
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	14	0.43
(1,1580)	1:8:A:LEU:HD12	1:8:A:LEU:H	15	0.43
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	15	0.43
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD13	17	0.43
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	18	0.43
(1,1386)	1:83:A:LEU:HD11	1:84:A:ASP:H	17	0.43
(1,1240)	1:125:A:LEU:HD23	1:120:A:ARG:HD2	15	0.43
(1,1225)	1:127:A:MET:HE3	1:128:A:LYS:H	17	0.43
(1,1169)	1:32:A:MET:H	1:32:A:MET:HE1	8	0.43
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE2	17	0.43
(1,1112)	1:58:A:MET:HE1	1:43:A:LYS:HE3	5	0.43
(1,1105)	1:58:A:MET:HE1	1:92:A:PHE:HE2	8	0.43
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD21	6	0.43
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	4	0.43
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG11	9	0.43
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	8	0.43
(1,785)	1:100:A:LEU:HD23	1:45:A:PHE:HE2	16	0.43
(1,629)	1:74:A:LEU:HD13	1:75:A:GLY:H	20	0.43
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	10	0.43
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	9	0.43
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG23	9	0.43
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE1	3	0.43
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE1	19	0.43
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD11	19	0.43
(1,137)	1:3:A:LEU:HD21	1:7:A:PHE:HB3	20	0.43
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	8	0.43
(1,13)	1:31:A:ILE:HD12	1:31:A:ILE:H	13	0.43
(1,13)	1:31:A:ILE:HD13	1:31:A:ILE:H	19	0.43
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	11	0.43
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG22	2	0.43
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	4	0.42
(2,1590)	2:1001:A:OLA:H32	1:116:A:TYR:HD2	20	0.42
(2,1564)	2:1001:A:OLA:H81	1:36:A:ILE:HG21	20	0.42
(2,1480)	1:49:A:ALA:HB2	1:71:A:ASP:H	18	0.42
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD22	3	0.42
(2,1471)	1:101:A:THR:HG21	1:93:A:ASP:H	11	0.42
(2,1305)	1:116:A:TYR:H	1:127:A:MET:HG2	13	0.42
(2,1267)	1:80:A:ASP:H	1:107:A:VAL:HG12	8	0.42
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	7	0.42
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD13	19	0.42
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	3	0.42
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG22	3	0.42
(2,848)	1:76:A:GLU:H	1:91:A:THR:HG21	13	0.42
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	2	0.42
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,814)	1:60:A:ASN:HD21	1:83:A:LEU:HD23	20	0.42
(2,787)	1:127:A:MET:HE2	1:117:A:GLU:H	1	0.42
(2,787)	1:127:A:MET:HE2	1:117:A:GLU:H	5	0.42
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	2	0.42
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	15	0.42
(2,727)	1:3:A:LEU:HD23	1:7:A:PHE:HA	11	0.42
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	1	0.42
(2,680)	1:140:A:TYR:HE1	1:43:A:LYS:HG2	6	0.42
(2,653)	1:132:A:LYS:HG2	1:132:A:LYS:HE3	10	0.42
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG21	18	0.42
(2,617)	1:125:A:LEU:HD23	1:127:A:MET:H	9	0.42
(2,610)	1:125:A:LEU:HD22	1:125:A:LEU:H	12	0.42
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	18	0.42
(2,605)	1:14:A:GLU:HB3	1:124:A:TYR:HE2	1	0.42
(2,556)	1:89:A:LYS:HE3	1:105:A:ILE:HD13	17	0.42
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG13	13	0.42
(2,543)	1:74:A:LEU:HG	1:100:A:LEU:HD22	11	0.42
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	12	0.42
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	20	0.42
(2,495)	1:90:A:ILE:HD12	1:82:A:ALA:HA	6	0.42
(2,494)	1:90:A:ILE:HD11	1:104:A:HIS:HB3	14	0.42
(2,456)	1:85:A:SER:HA	1:65:A:LYS:HB3	14	0.42
(2,451)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	8	0.42
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	19	0.42
(2,410)	1:71:A:ASP:HB3	1:55:A:ARG:HB3	7	0.42
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	16	0.42
(2,366)	1:61:A:LEU:HA	1:61:A:LEU:HD13	10	0.42
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	19	0.42
(2,226)	1:134:A:VAL:HG22	1:25:A:ALA:HA	4	0.42
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	9	0.42
(2,158)	1:41:A:VAL:HA	1:13:A:LEU:HB3	8	0.42
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	15	0.42
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG23	6	0.42
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD21	5	0.42
(2,51)	1:48:A:ALA:HB3	1:56:A:TYR:HB3	10	0.42
(2,49)	1:48:A:ALA:HB3	1:55:A:ARG:HD2	5	0.42
(2,45)	1:49:A:ALA:HB1	1:48:A:ALA:HA	4	0.42
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG22	6	0.42
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG23	15	0.42
(1,2833)	2:1001:A:OLA:H182	1:36:A:ILE:HA	18	0.42
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	6	0.42
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD21	14	0.42
(1,2489)	1:13:A:LEU:HD22	1:17:A:GLU:H	10	0.42
(1,2296)	1:94:A:LEU:H	1:100:A:LEU:HD11	14	0.42
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	1	0.42
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG22	3	0.42
(1,1984)	1:115:A:THR:H	1:115:A:THR:HG21	15	0.42
(1,1627)	1:126:A:VAL:H	1:126:A:VAL:HG12	10	0.42
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	13	0.42
(1,1580)	1:8:A:LEU:HD12	1:8:A:LEU:H	6	0.42
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	20	0.42
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	15	0.42
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	13	0.42
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	15	0.42
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	2	0.42
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	7	0.42
(1,1344)	1:105:A:ILE:HD12	1:105:A:ILE:H	6	0.42
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD13	17	0.42
(1,1225)	1:127:A:MET:HE3	1:128:A:LYS:H	11	0.42
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD13	8	0.42
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	15	0.42
(1,1105)	1:58:A:MET:HE2	1:92:A:PHE:HE2	7	0.42
(1,1097)	1:136:A:THR:HG22	1:129:A:MET:HB3	17	0.42
(1,1097)	1:136:A:THR:HG22	1:129:A:MET:HB3	19	0.42
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG22	18	0.42
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	11	0.42
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG11	6	0.42
(1,933)	1:137:A:SER:HB2	1:126:A:VAL:HG13	4	0.42
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	16	0.42
(1,878)	1:115:A:THR:H	1:115:A:THR:HG22	3	0.42
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	6	0.42
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	7	0.42
(1,703)	1:24:A:LYS:HG2	1:21:A:GLU:HA	12	0.42
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	11	0.42
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	14	0.42
(1,687)	1:86:A:THR:HG21	1:87:A:GLN:H	1	0.42
(1,629)	1:74:A:LEU:HD13	1:75:A:GLY:H	9	0.42
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG23	16	0.42
(1,418)	1:32:A:MET:HG2	1:36:A:ILE:HD11	15	0.42
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE2	9	0.42
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE2	20	0.42
(1,13)	1:31:A:ILE:HD11	1:31:A:ILE:H	8	0.42
(1,13)	1:31:A:ILE:HD13	1:31:A:ILE:H	20	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG23	5	0.42
(2,1652)	1:32:A:MET:HE3	2:1001:A:OLA:H131	1	0.41
(2,1651)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	12	0.41
(2,1580)	1:129:A:MET:HE3	2:1001:A:OLA:H182	12	0.41
(2,1568)	2:1001:A:OLA:H82	2:1001:A:OLA:H181	9	0.41
(2,1394)	1:143:A:GLN:H	1:141:A:LYS:HD3	4	0.41
(2,1279)	1:80:A:ASP:H	1:89:A:LYS:HB3	5	0.41
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	6	0.41
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	2	0.41
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	7	0.41
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	7	0.41
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD23	1	0.41
(2,1006)	1:81:A:GLU:H	1:87:A:GLN:HE22	20	0.41
(2,838)	1:127:A:MET:HE1	1:116:A:TYR:HE2	16	0.41
(2,826)	1:65:A:LYS:HB2	1:83:A:LEU:HD13	13	0.41
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	17	0.41
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	18	0.41
(2,802)	1:62:A:THR:HA	1:41:A:VAL:HG13	19	0.41
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	1	0.41
(2,653)	1:132:A:LYS:HG3	1:132:A:LYS:HE3	3	0.41
(2,653)	1:132:A:LYS:HG2	1:132:A:LYS:HE3	7	0.41
(2,653)	1:132:A:LYS:HG3	1:132:A:LYS:HE3	14	0.41
(2,635)	1:128:A:LYS:HD3	1:130:A:SER:HB3	20	0.41
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD21	2	0.41
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	1	0.41
(2,610)	1:125:A:LEU:HD21	1:125:A:LEU:H	16	0.41
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	10	0.41
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG23	16	0.41
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	14	0.41
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG11	15	0.41
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	20	0.41
(2,534)	1:99:A:THR:HG21	1:95:A:LYS:HD2	6	0.41
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD21	19	0.41
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	19	0.41
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	5	0.41
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	11	0.41
(2,487)	1:90:A:ILE:HG23	1:92:A:PHE:HB2	4	0.41
(2,469)	1:88:A:HIS:HD2	1:82:A:ALA:HB3	17	0.41
(2,461)	1:86:A:THR:HG21	1:84:A:ASP:HB3	8	0.41
(2,433)	1:81:A:GLU:HG2	1:81:A:GLU:H	15	0.41
(2,419)	1:74:A:LEU:HD13	1:56:A:TYR:HD1	6	0.41
(2,374)	1:62:A:THR:HG22	2:1001:A:OLA:H82	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,350)	1:33:A:ARG:HG2	1:34:A:GLN:H	8	0.41
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	3	0.41
(2,226)	1:134:A:VAL:HG22	1:25:A:ALA:HA	1	0.41
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	15	0.41
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	18	0.41
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	9	0.41
(2,155)	1:12:A:LYS:HE2	1:12:A:LYS:HA	11	0.41
(2,144)	1:126:A:VAL:HG22	1:124:A:TYR:HD2	10	0.41
(2,139)	1:14:A:GLU:HG2	1:124:A:TYR:HD2	19	0.41
(2,120)	1:8:A:LEU:HD11	1:7:A:PHE:H	14	0.41
(2,117)	1:8:A:LEU:HD13	1:5:A:ASP:HB3	13	0.41
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	4	0.41
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG23	13	0.41
(1,2833)	2:1001:A:OLA:H183	1:36:A:ILE:HA	12	0.41
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	12	0.41
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	6	0.41
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	7	0.41
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H182	9	0.41
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG22	19	0.41
(1,1580)	1:8:A:LEU:HD12	1:8:A:LEU:H	16	0.41
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	7	0.41
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	2	0.41
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD13	3	0.41
(1,1461)	1:55:A:ARG:HG2	1:56:A:TYR:H	9	0.41
(1,1386)	1:83:A:LEU:HD11	1:84:A:ASP:H	5	0.41
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	15	0.41
(1,1240)	1:125:A:LEU:HD21	1:120:A:ARG:HD2	14	0.41
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	12	0.41
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD22	10	0.41
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	4	0.41
(1,1193)	1:114:A:GLU:HG3	1:131:A:TRP:HE3	6	0.41
(1,1171)	1:32:A:MET:HE3	1:33:A:ARG:H	5	0.41
(1,1168)	1:32:A:MET:HE3	1:35:A:VAL:H	13	0.41
(1,1112)	1:58:A:MET:HE3	1:43:A:LYS:HE3	4	0.41
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	10	0.41
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	16	0.41
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD23	7	0.41
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	3	0.41
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG11	19	0.41
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	15	0.41
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	1	0.41
(1,878)	1:115:A:THR:H	1:115:A:THR:HG21	15	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD22	13	0.41
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG13	4	0.41
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	3	0.41
(1,557)	1:63:A:THR:HG22	1:40:A:GLY:HA2	7	0.41
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	13	0.41
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE2	2	0.41
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE3	4	0.41
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE2	12	0.41
(1,195)	1:11:A:PHE:H	1:10:A:THR:HG23	14	0.41
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB3	16	0.41
(1,101)	1:49:A:ALA:H	1:48:A:ALA:HB2	4	0.41
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB2	13	0.41
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB3	16	0.41
(1,13)	1:31:A:ILE:HD12	1:31:A:ILE:H	3	0.41
(1,13)	1:31:A:ILE:HD11	1:31:A:ILE:H	16	0.41
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG22	14	0.41
(2,1670)	2:1001:A:OLA:H181	2:1001:A:OLA:H21	11	0.4
(2,1652)	1:32:A:MET:HE2	1:35:A:VAL:HG13	16	0.4
(2,1641)	2:1001:A:OLA:H31	1:140:A:TYR:HH	2	0.4
(2,1511)	1:61:A:LEU:HB2	1:67:A:THR:H	5	0.4
(2,1480)	1:46:A:ARG:HG3	1:71:A:ASP:H	12	0.4
(2,1461)	1:136:A:THR:H	1:128:A:LYS:HB3	2	0.4
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	12	0.4
(2,1325)	1:130:A:SER:H	1:128:A:LYS:HG2	1	0.4
(2,1279)	1:80:A:ASP:H	1:89:A:LYS:HB3	8	0.4
(2,1279)	1:80:A:ASP:H	1:89:A:LYS:HB3	16	0.4
(2,1279)	1:80:A:ASP:H	1:89:A:LYS:HB3	18	0.4
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	8	0.4
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	1	0.4
(2,1098)	1:132:A:LYS:HD3	1:131:A:TRP:HE1	17	0.4
(2,1061)	1:118:A:TYR:HD1	1:128:A:LYS:H	1	0.4
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD21	11	0.4
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG12	12	0.4
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG22	15	0.4
(2,904)	1:106:A:LYS:H	1:109:A:ASP:HB3	4	0.4
(2,849)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	19	0.4
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	13	0.4
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	5	0.4
(2,786)	1:32:A:MET:HE3	1:36:A:ILE:HA	5	0.4
(2,779)	1:120:A:ARG:HA	1:119:A:ARG:HD2	15	0.4
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	4	0.4
(2,684)	1:125:A:LEU:HD13	1:140:A:TYR:HE2	16	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,653)	1:132:A:LYS:HG3	1:132:A:LYS:HE3	12	0.4
(2,635)	1:128:A:LYS:HD3	1:130:A:SER:HB3	7	0.4
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG21	12	0.4
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	4	0.4
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	3	0.4
(2,610)	1:125:A:LEU:HD21	1:125:A:LEU:H	15	0.4
(2,603)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	19	0.4
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG23	12	0.4
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD13	3	0.4
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG11	6	0.4
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG13	17	0.4
(2,541)	1:100:A:LEU:HD22	1:118:A:TYR:HB2	3	0.4
(2,533)	1:99:A:THR:HG23	1:96:A:ASP:HB2	17	0.4
(2,501)	1:90:A:ILE:HD12	1:80:A:ASP:H	10	0.4
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	1	0.4
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB1	13	0.4
(2,413)	1:73:A:ALA:HB2	1:55:A:ARG:HD2	11	0.4
(2,412)	1:73:A:ALA:HB3	1:55:A:ARG:H	18	0.4
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG21	11	0.4
(2,350)	1:33:A:ARG:HG2	1:34:A:GLN:H	18	0.4
(2,326)	1:140:A:TYR:HE2	1:43:A:LYS:HE3	6	0.4
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG21	9	0.4
(2,290)	1:36:A:ILE:HD12	1:36:A:ILE:HA	9	0.4
(2,288)	1:36:A:ILE:HD11	1:37:A:LYS:H	3	0.4
(2,288)	1:36:A:ILE:HD12	1:37:A:LYS:H	11	0.4
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG22	7	0.4
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	13	0.4
(2,170)	1:15:A:ARG:HD2	1:15:A:ARG:H	7	0.4
(2,162)	1:13:A:LEU:HD23	1:140:A:TYR:HA	6	0.4
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	5	0.4
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG23	2	0.4
(2,61)	1:0:A:SER:HB3	1:1:A:LYS:HG2	9	0.4
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	1	0.4
(2,41)	1:54:A:ASP:H	1:53:A:PRO:HG3	2	0.4
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	19	0.4
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	4	0.4
(2,23)	1:34:A:GLN:HG3	1:34:A:GLN:H	3	0.4
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	4	0.4
(1,2814)	2:1001:A:OLA:H182	1:19:A:PHE:HE1	15	0.4
(1,2314)	1:81:A:GLU:H	1:87:A:GLN:HE21	11	0.4
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	4	0.4
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG22	18	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	17	0.4
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	20	0.4
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG13	9	0.4
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD13	1	0.4
(1,1292)	1:111:A:THR:HG21	1:112:A:ASP:H	11	0.4
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	15	0.4
(1,1111)	1:58:A:MET:HE2	1:43:A:LYS:HE2	17	0.4
(1,1105)	1:58:A:MET:HE2	1:92:A:PHE:HE2	2	0.4
(1,1105)	1:58:A:MET:HE2	1:92:A:PHE:HE2	3	0.4
(1,1034)	1:124:A:TYR:HE2	1:141:A:LYS:HB3	9	0.4
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG23	12	0.4
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	11	0.4
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG12	3	0.4
(1,924)	1:125:A:LEU:HD21	1:140:A:TYR:HB3	17	0.4
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	14	0.4
(1,730)	1:90:A:ILE:HD12	1:92:A:PHE:HE1	13	0.4
(1,729)	1:90:A:ILE:HD11	1:78:A:PHE:HZ	10	0.4
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	15	0.4
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	18	0.4
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD12	20	0.4
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	8	0.4
(1,620)	1:73:A:ALA:HB1	1:76:A:GLU:HB3	12	0.4
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG21	9	0.4
(1,448)	1:41:A:VAL:HG22	1:140:A:TYR:HE1	8	0.4
(1,441)	1:38:A:LEU:HD22	1:38:A:LEU:HA	16	0.4
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE1	8	0.4
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE3	10	0.4
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE3	16	0.4
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE1	17	0.4
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB1	18	0.4
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	16	0.4
(1,13)	1:31:A:ILE:HD12	1:31:A:ILE:H	1	0.4
(1,13)	1:31:A:ILE:HD12	1:31:A:ILE:H	6	0.4
(1,13)	1:31:A:ILE:HD11	1:31:A:ILE:H	15	0.4
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	6	0.4
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG22	13	0.4
(2,1679)	1:94:A:LEU:HB3	1:94:A:LEU:HD11	13	0.39
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	4	0.39
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	1	0.39
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	18	0.39
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	20	0.39
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	5	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1488)	1:81:A:GLU:H	1:87:A:GLN:HE21	10	0.39
(2,1471)	1:101:A:THR:HG22	1:93:A:ASP:H	2	0.39
(2,1459)	1:10:A:THR:HG22	1:45:A:PHE:H	4	0.39
(2,1360)	1:52:A:LYS:HG2	1:52:A:LYS:H	3	0.39
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	10	0.39
(2,1301)	1:125:A:LEU:HD13	1:141:A:LYS:H	9	0.39
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	9	0.39
(2,1202)	1:77:A:GLU:H	1:73:A:ALA:HB1	19	0.39
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD12	13	0.39
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	12	0.39
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	3	0.39
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG12	8	0.39
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	9	0.39
(2,841)	1:116:A:TYR:HB3	1:129:A:MET:HE1	12	0.39
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	4	0.39
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	11	0.39
(2,819)	1:36:A:ILE:HG23	2:1001:A:OLA:H82	10	0.39
(2,811)	1:89:A:LYS:H	1:89:A:LYS:HE2	9	0.39
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	11	0.39
(2,785)	1:32:A:MET:HE3	2:1001:A:OLA:H131	1	0.39
(2,752)	1:69:A:HIS:HE1	1:67:A:THR:HG21	1	0.39
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD21	10	0.39
(2,706)	1:41:A:VAL:HG21	1:62:A:THR:HG1	8	0.39
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	6	0.39
(2,617)	1:125:A:LEU:HD21	1:127:A:MET:H	7	0.39
(2,610)	1:125:A:LEU:HD21	1:125:A:LEU:H	2	0.39
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	8	0.39
(2,597)	1:118:A:TYR:HD2	1:127:A:MET:HG3	16	0.39
(2,564)	1:88:A:HIS:HB2	1:107:A:VAL:HA	20	0.39
(2,555)	1:89:A:LYS:HE2	1:105:A:ILE:HG21	17	0.39
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	7	0.39
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	12	0.39
(2,534)	1:119:A:ARG:HG2	1:99:A:THR:HG21	7	0.39
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD21	1	0.39
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD23	12	0.39
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD21	18	0.39
(2,496)	1:90:A:ILE:HD11	1:69:A:HIS:HA	9	0.39
(2,447)	1:84:A:ASP:HA	1:65:A:LYS:HD2	5	0.39
(2,446)	1:83:A:LEU:HD13	1:60:A:ASN:HD21	7	0.39
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB2	19	0.39
(2,412)	1:73:A:ALA:HB1	1:55:A:ARG:H	6	0.39
(2,412)	1:73:A:ALA:HB3	1:55:A:ARG:H	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,400)	1:83:A:LEU:HD12	1:65:A:LYS:HG2	17	0.39
(2,394)	1:65:A:LYS:HE2	1:65:A:LYS:HA	6	0.39
(2,393)	1:89:A:LYS:HE3	1:105:A:ILE:HG22	2	0.39
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	11	0.39
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG12	7	0.39
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	5	0.39
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	18	0.39
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	18	0.39
(2,229)	1:131:A:TRP:HB2	1:25:A:ALA:HB3	10	0.39
(2,226)	1:134:A:VAL:HG23	1:25:A:ALA:HA	17	0.39
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	18	0.39
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	11	0.39
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	14	0.39
(2,116)	1:8:A:LEU:HD22	1:9:A:GLY:H	15	0.39
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	18	0.39
(2,56)	1:63:A:THR:HG23	1:40:A:GLY:HA2	20	0.39
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	20	0.39
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD13	16	0.39
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	9	0.39
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	9	0.39
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	11	0.39
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H181	13	0.39
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	14	0.39
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	20	0.39
(1,2314)	1:81:A:GLU:H	1:87:A:GLN:HE21	1	0.39
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG21	1	0.39
(1,1580)	1:8:A:LEU:HD11	1:8:A:LEU:H	8	0.39
(1,1580)	1:8:A:LEU:HD12	1:8:A:LEU:H	19	0.39
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	14	0.39
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD11	16	0.39
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	1	0.39
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	16	0.39
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	16	0.39
(1,1225)	1:127:A:MET:HE3	1:128:A:LYS:H	16	0.39
(1,1217)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	5	0.39
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	7	0.39
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE3	20	0.39
(1,1088)	1:61:A:LEU:HD22	1:62:A:THR:H	6	0.39
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	4	0.39
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	8	0.39
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG23	6	0.39
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	15	0.39
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	16	0.39
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	13	0.39
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	8	0.39
(1,617)	1:73:A:ALA:HB2	1:75:A:GLY:H	5	0.39
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD12	13	0.39
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	11	0.39
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD12	3	0.39
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD11	8	0.39
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB1	11	0.39
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB1	13	0.39
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	19	0.39
(1,13)	1:31:A:ILE:HD12	1:31:A:ILE:H	17	0.39
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG22	8	0.39
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	11	0.39
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	6	0.38
(2,1556)	1:35:A:VAL:HG21	1:36:A:ILE:H	16	0.38
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	19	0.38
(2,1521)	1:7:A:PHE:H	1:120:A:ARG:HB2	16	0.38
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	1	0.38
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD13	10	0.38
(2,1168)	1:56:A:TYR:H	1:55:A:ARG:HD2	5	0.38
(2,1125)	1:118:A:TYR:H	1:95:A:LYS:HD3	18	0.38
(2,1085)	1:12:A:LYS:HE2	1:143:A:GLN:HE22	14	0.38
(2,925)	1:65:A:LYS:HG3	1:67:A:THR:H	5	0.38
(2,838)	1:127:A:MET:HE2	1:60:A:ASN:HD21	12	0.38
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	3	0.38
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	15	0.38
(2,786)	1:32:A:MET:HE1	1:36:A:ILE:HA	12	0.38
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE2	6	0.38
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	16	0.38
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	6	0.38
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	8	0.38
(2,706)	1:41:A:VAL:HG22	1:62:A:THR:HG1	15	0.38
(2,665)	1:136:A:THR:HG21	1:19:A:PHE:HE1	19	0.38
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD23	3	0.38
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	20	0.38
(2,596)	1:100:A:LEU:HG	1:118:A:TYR:HD2	19	0.38
(2,580)	1:111:A:THR:HG23	1:110:A:PRO:HG2	17	0.38
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG11	14	0.38
(2,541)	1:100:A:LEU:HD23	1:118:A:TYR:HB2	10	0.38
(2,535)	1:99:A:THR:HG22	1:95:A:LYS:HB3	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,518)	1:95:A:LYS:H	1:94:A:LEU:HD11	10	0.38
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	2	0.38
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	1	0.38
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	9	0.38
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	18	0.38
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	20	0.38
(2,482)	1:90:A:ILE:HG21	1:78:A:PHE:HD1	1	0.38
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	9	0.38
(2,448)	2:1001:A:OLA:H151	1:84:A:ASP:HA	16	0.38
(2,446)	1:83:A:LEU:HD12	1:60:A:ASN:HD21	2	0.38
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB2	9	0.38
(2,436)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	18	0.38
(2,422)	1:74:A:LEU:HD13	1:4:A:PRO:HD2	1	0.38
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB1	3	0.38
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG22	17	0.38
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	9	0.38
(2,290)	1:36:A:ILE:HD13	1:36:A:ILE:HA	20	0.38
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG22	20	0.38
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD12	10	0.38
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	20	0.38
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	17	0.38
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	10	0.38
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	11	0.38
(2,121)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	7	0.38
(2,119)	1:8:A:LEU:HD13	1:46:A:ARG:H	10	0.38
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD23	18	0.38
(2,112)	1:8:A:LEU:HD22	1:47:A:ASN:HD21	9	0.38
(2,107)	1:120:A:ARG:HB2	1:7:A:PHE:HB3	10	0.38
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD11	3	0.38
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	3	0.38
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	12	0.38
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	14	0.38
(2,26)	1:94:A:LEU:HD12	1:4:A:PRO:HG3	20	0.38
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	5	0.38
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	8	0.38
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	13	0.38
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	15	0.38
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	16	0.38
(1,2828)	2:1001:A:OLA:H10	1:32:A:MET:HE3	5	0.38
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H181	15	0.38
(1,2809)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	7	0.38
(1,2326)	1:74:A:LEU:HD11	1:2:A:THR:H	8	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD21	4	0.38
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD23	6	0.38
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG22	6	0.38
(1,1510)	1:114:A:GLU:H	1:113:A:VAL:HG13	3	0.38
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD13	13	0.38
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	1	0.38
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD13	19	0.38
(1,1226)	1:49:A:ALA:HB1	1:51:A:GLY:H	6	0.38
(1,1223)	1:127:A:MET:HE3	1:116:A:TYR:HD2	13	0.38
(1,1193)	1:114:A:GLU:HG3	1:131:A:TRP:HE3	16	0.38
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD12	20	0.38
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE2	3	0.38
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE1	4	0.38
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD22	9	0.38
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG11	20	0.38
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG11	18	0.38
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	7	0.38
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG23	19	0.38
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	12	0.38
(1,785)	1:100:A:LEU:HD22	1:45:A:PHE:HE2	17	0.38
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	1	0.38
(1,753)	1:94:A:LEU:HD11	1:94:A:LEU:HA	5	0.38
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	6	0.38
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB2	17	0.38
(1,617)	1:73:A:ALA:HB2	1:75:A:GLY:H	3	0.38
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	17	0.38
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD13	10	0.38
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG22	17	0.38
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE2	1	0.38
(1,375)	1:36:A:ILE:HD12	1:32:A:MET:HG3	7	0.38
(1,111)	1:48:A:ALA:HB1	1:71:A:ASP:HB2	5	0.38
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB2	11	0.38
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	7	0.38
(2,1652)	1:32:A:MET:HE2	1:35:A:VAL:HG13	14	0.37
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	7	0.37
(2,1618)	1:36:A:ILE:HA	2:1001:A:OLA:H131	18	0.37
(2,1411)	1:13:A:LEU:H	1:143:A:GLN:HE22	12	0.37
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	7	0.37
(2,1267)	1:80:A:ASP:H	1:107:A:VAL:HG11	6	0.37
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD12	4	0.37
(2,1112)	1:143:A:GLN:HE21	1:141:A:LYS:HG3	16	0.37
(2,1102)	1:58:A:MET:H	1:70:A:LYS:HG2	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,936)	1:67:A:THR:H	1:83:A:LEU:HD13	1	0.37
(2,880)	1:128:A:LYS:HE3	1:128:A:LYS:HB2	6	0.37
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	20	0.37
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	5	0.37
(2,787)	1:39:A:ALA:HB3	1:40:A:GLY:H	11	0.37
(2,785)	1:32:A:MET:HE2	1:35:A:VAL:HG13	16	0.37
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE3	12	0.37
(2,757)	1:58:A:MET:HE3	1:43:A:LYS:HB3	3	0.37
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG23	10	0.37
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG22	19	0.37
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG23	20	0.37
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	4	0.37
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	10	0.37
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	16	0.37
(2,683)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	19	0.37
(2,683)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	20	0.37
(2,653)	1:132:A:LYS:HG3	1:132:A:LYS:HE3	2	0.37
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	6	0.37
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	13	0.37
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG21	20	0.37
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG11	13	0.37
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD22	8	0.37
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG21	6	0.37
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG12	6	0.37
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD12	5	0.37
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG21	20	0.37
(2,501)	1:90:A:ILE:HD11	1:80:A:ASP:H	9	0.37
(2,500)	1:90:A:ILE:HD11	1:88:A:HIS:H	19	0.37
(2,416)	1:77:A:GLU:H	1:73:A:ALA:HB1	15	0.37
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG21	2	0.37
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	15	0.37
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG12	10	0.37
(2,350)	1:33:A:ARG:HG2	1:34:A:GLN:H	2	0.37
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	17	0.37
(2,301)	1:24:A:LYS:H	1:24:A:LYS:HE3	15	0.37
(2,297)	1:37:A:LYS:HG3	1:19:A:PHE:HD2	12	0.37
(2,278)	1:35:A:VAL:HG23	2:1001:A:OLA:H10	3	0.37
(2,183)	1:24:A:LYS:HE2	1:21:A:GLU:HA	16	0.37
(2,143)	1:42:A:THR:HG22	1:140:A:TYR:HD1	3	0.37
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	3	0.37
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	14	0.37
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	1	0.37
(2,98)	1:8:A:LEU:HD22	1:5:A:ASP:HA	5	0.37
(2,98)	1:8:A:LEU:HD23	1:5:A:ASP:HA	19	0.37
(2,55)	1:50:A:SER:HB2	1:48:A:ALA:HB1	9	0.37
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	15	0.37
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	16	0.37
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	1	0.37
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	10	0.37
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	17	0.37
(1,2836)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	7	0.37
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	10	0.37
(1,2832)	1:118:A:TYR:HD2	1:118:A:TYR:HH	18	0.37
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	20	0.37
(1,2826)	1:127:A:MET:HE3	1:118:A:TYR:HH	18	0.37
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H182	17	0.37
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	20	0.37
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	7	0.37
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG13	3	0.37
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG23	6	0.37
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG21	8	0.37
(1,1982)	1:8:A:LEU:HD13	1:47:A:ASN:HD22	14	0.37
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	8	0.37
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD13	13	0.37
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	17	0.37
(1,1223)	1:127:A:MET:HE1	1:116:A:TYR:HD2	19	0.37
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	2	0.37
(1,1105)	1:58:A:MET:HE2	1:92:A:PHE:HE2	4	0.37
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	13	0.37
(1,1097)	1:136:A:THR:HG22	1:129:A:MET:HB3	14	0.37
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	13	0.37
(1,989)	1:134:A:VAL:HG13	1:22:A:TYR:HB3	13	0.37
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG13	13	0.37
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG12	16	0.37
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG13	7	0.37
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB1	8	0.37
(1,629)	1:74:A:LEU:HD11	1:75:A:GLY:H	18	0.37
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	1	0.37
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	4	0.37
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG23	10	0.37
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG22	14	0.37
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	16	0.37
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE3	14	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:23:A:LEU:HD21	1:33:A:ARG:HA	19	0.37
(1,181)	1:45:A:PHE:H	1:8:A:LEU:HD23	6	0.37
(1,137)	1:3:A:LEU:HD22	1:7:A:PHE:HB3	16	0.37
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	3	0.37
(1,100)	1:48:A:ALA:HB2	1:50:A:SER:H	11	0.37
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	17	0.37
(1,9)	1:30:A:TRP:HZ3	1:31:A:ILE:HG23	19	0.37
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	2	0.36
(2,1665)	1:22:A:TYR:HD1	2:1001:A:OLA:H181	7	0.36
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	17	0.36
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	16	0.36
(2,1614)	1:58:A:MET:HE1	1:60:A:ASN:H	4	0.36
(2,1606)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	4	0.36
(2,1593)	1:84:A:ASP:HA	2:1001:A:OLA:H112	3	0.36
(2,1556)	1:35:A:VAL:HG21	1:36:A:ILE:H	6	0.36
(2,1553)	1:136:A:THR:H	1:129:A:MET:HE1	11	0.36
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	11	0.36
(2,1394)	1:143:A:GLN:H	1:141:A:LYS:HD3	8	0.36
(2,1312)	1:128:A:LYS:HG3	1:130:A:SER:H	6	0.36
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	16	0.36
(2,1232)	1:85:A:SER:H	1:81:A:GLU:HG2	15	0.36
(2,1216)	1:36:A:ILE:HB	1:34:A:GLN:HE22	12	0.36
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	20	0.36
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	3	0.36
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	11	0.36
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	4	0.36
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	8	0.36
(2,1112)	1:143:A:GLN:HE21	1:141:A:LYS:HG3	18	0.36
(2,1027)	1:39:A:ALA:H	1:38:A:LEU:HD23	20	0.36
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG12	18	0.36
(2,1006)	1:81:A:GLU:H	1:87:A:GLN:HE22	3	0.36
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG21	20	0.36
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB1	6	0.36
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD2	10	0.36
(2,840)	1:129:A:MET:HE3	1:114:A:GLU:HG3	6	0.36
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	15	0.36
(2,808)	1:78:A:PHE:H	1:77:A:GLU:HG2	13	0.36
(2,750)	1:104:A:HIS:HB3	1:104:A:HIS:HE1	12	0.36
(2,740)	1:31:A:ILE:HD11	1:30:A:TRP:HZ2	16	0.36
(2,697)	1:65:A:LYS:HE2	1:83:A:LEU:HA	7	0.36
(2,679)	1:140:A:TYR:HE1	1:42:A:THR:H	10	0.36
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG13	20	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	9	0.36
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	10	0.36
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	11	0.36
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	10	0.36
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG21	10	0.36
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	4	0.36
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	1	0.36
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	3	0.36
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	11	0.36
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG22	14	0.36
(2,488)	1:102:A:GLU:HB3	1:90:A:ILE:HG21	20	0.36
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG23	13	0.36
(2,461)	1:41:A:VAL:HG22	1:60:A:ASN:HB3	13	0.36
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB3	6	0.36
(2,445)	1:66:A:ASP:HA	1:83:A:LEU:HD22	11	0.36
(2,421)	1:2:A:THR:HA	1:74:A:LEU:HD13	11	0.36
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD11	13	0.36
(2,374)	2:1001:A:OLA:H81	1:62:A:THR:HG22	19	0.36
(2,372)	1:62:A:THR:HG23	1:42:A:THR:H	12	0.36
(2,331)	1:44:A:LYS:HE3	1:44:A:LYS:HA	2	0.36
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	3	0.36
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	18	0.36
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD2	18	0.36
(2,125)	1:65:A:LYS:HE3	1:67:A:THR:HG22	1	0.36
(2,122)	1:9:A:GLY:HA3	1:142:A:LYS:HE3	11	0.36
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	7	0.36
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD13	13	0.36
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	7	0.36
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	18	0.36
(1,2841)	1:36:A:ILE:HD12	2:1001:A:OLA:H10	10	0.36
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG23	3	0.36
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	7	0.36
(1,2832)	1:118:A:TYR:HD1	1:118:A:TYR:HH	17	0.36
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	4	0.36
(1,2314)	1:81:A:GLU:H	1:87:A:GLN:HE21	2	0.36
(1,1762)	1:8:A:LEU:HD13	1:47:A:ASN:HD21	17	0.36
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG22	5	0.36
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD13	14	0.36
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	19	0.36
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	4	0.36
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	5	0.36
(1,1277)	1:127:A:MET:HE3	1:118:A:TYR:HH	1	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	16	0.36
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD21	19	0.36
(1,1173)	1:125:A:LEU:HD21	1:120:A:ARG:HD3	5	0.36
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	18	0.36
(1,1168)	1:32:A:MET:HE3	1:35:A:VAL:H	6	0.36
(1,1105)	1:58:A:MET:HE2	1:92:A:PHE:HE2	6	0.36
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	17	0.36
(1,1081)	1:0:A:SER:HA	1:74:A:LEU:HD21	15	0.36
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG23	20	0.36
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	14	0.36
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG11	15	0.36
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	20	0.36
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	15	0.36
(1,805)	1:101:A:THR:HG23	1:102:A:GLU:H	3	0.36
(1,805)	1:101:A:THR:HG22	1:102:A:GLU:H	15	0.36
(1,805)	1:101:A:THR:HG23	1:102:A:GLU:H	20	0.36
(1,743)	1:93:A:ASP:HB2	1:91:A:THR:HG22	11	0.36
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	4	0.36
(1,687)	1:86:A:THR:HG21	1:87:A:GLN:H	12	0.36
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	7	0.36
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	18	0.36
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	7	0.36
(1,620)	1:73:A:ALA:HB1	1:76:A:GLU:HB3	16	0.36
(1,616)	1:73:A:ALA:HB1	1:76:A:GLU:H	14	0.36
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	2	0.36
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	15	0.36
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	6	0.36
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB3	2	0.36
(1,97)	1:52:A:LYS:H	1:48:A:ALA:HB3	1	0.36
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB2	10	0.36
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	13	0.36
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	10	0.36
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG23	19	0.36
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	9	0.35
(2,1540)	1:119:A:ARG:HG2	1:100:A:LEU:H	3	0.35
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	19	0.35
(2,1360)	1:52:A:LYS:HG2	1:52:A:LYS:H	2	0.35
(2,1325)	1:129:A:MET:HE2	1:130:A:SER:H	4	0.35
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD11	8	0.35
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	10	0.35
(2,1040)	1:34:A:GLN:HE21	1:35:A:VAL:HG21	19	0.35
(2,1019)	1:33:A:ARG:H	1:33:A:ARG:HG3	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG22	10	0.35
(2,787)	1:39:A:ALA:HB1	1:40:A:GLY:H	4	0.35
(2,785)	1:32:A:MET:HE2	1:35:A:VAL:HG13	14	0.35
(2,727)	1:7:A:PHE:HA	1:125:A:LEU:HD11	13	0.35
(2,677)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	10	0.35
(2,665)	1:136:A:THR:HG21	1:19:A:PHE:HE1	14	0.35
(2,652)	1:132:A:LYS:HG2	1:132:A:LYS:HE2	8	0.35
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD23	9	0.35
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	6	0.35
(2,610)	1:125:A:LEU:HD22	1:125:A:LEU:H	8	0.35
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	14	0.35
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	1	0.35
(2,564)	1:88:A:HIS:HB2	1:107:A:VAL:HA	6	0.35
(2,556)	1:89:A:LYS:HE3	1:105:A:ILE:HD13	5	0.35
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG22	2	0.35
(2,533)	1:99:A:THR:HG22	1:96:A:ASP:HB2	18	0.35
(2,527)	1:96:A:ASP:H	1:95:A:LYS:HD3	9	0.35
(2,526)	1:95:A:LYS:HG2	1:99:A:THR:HB	14	0.35
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	14	0.35
(2,495)	1:90:A:ILE:HD13	1:82:A:ALA:HA	10	0.35
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	2	0.35
(2,416)	1:77:A:GLU:H	1:73:A:ALA:HB1	16	0.35
(2,410)	1:71:A:ASP:HB3	1:48:A:ALA:HB3	9	0.35
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	2	0.35
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	4	0.35
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	7	0.35
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	10	0.35
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	13	0.35
(2,331)	1:44:A:LYS:HE3	1:44:A:LYS:HA	1	0.35
(2,284)	1:35:A:VAL:HB	1:36:A:ILE:HG23	3	0.35
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	20	0.35
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	11	0.35
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	20	0.35
(2,162)	1:13:A:LEU:HD22	1:140:A:TYR:HA	4	0.35
(2,160)	1:13:A:LEU:HD22	1:41:A:VAL:H	15	0.35
(2,147)	1:12:A:LYS:HE3	1:12:A:LYS:HB2	19	0.35
(2,125)	1:65:A:LYS:HE3	1:67:A:THR:HG21	8	0.35
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	2	0.35
(2,107)	1:3:A:LEU:HG	1:7:A:PHE:HB3	14	0.35
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD22	1	0.35
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	11	0.35
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	5	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	7	0.35
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	9	0.35
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	10	0.35
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	11	0.35
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	13	0.35
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	19	0.35
(1,2243)	1:23:A:LEU:HD23	1:37:A:LYS:H	8	0.35
(1,2243)	1:23:A:LEU:HD22	1:37:A:LYS:H	17	0.35
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG22	15	0.35
(1,1459)	1:55:A:ARG:H	1:55:A:ARG:HD3	14	0.35
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD11	4	0.35
(1,1279)	1:40:A:GLY:H	1:39:A:ALA:HA	7	0.35
(1,1226)	1:49:A:ALA:HB3	1:51:A:GLY:H	14	0.35
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	2	0.35
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	10	0.35
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	14	0.35
(1,1222)	1:127:A:MET:HE1	1:118:A:TYR:HD1	15	0.35
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	11	0.35
(1,1168)	1:32:A:MET:HE1	1:35:A:VAL:H	11	0.35
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	18	0.35
(1,1160)	1:43:A:LYS:HD3	1:125:A:LEU:HD11	9	0.35
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	9	0.35
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	18	0.35
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	9	0.35
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	16	0.35
(1,1105)	1:58:A:MET:HE1	1:92:A:PHE:HE2	12	0.35
(1,1104)	1:58:A:MET:HE3	1:118:A:TYR:HE1	17	0.35
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	5	0.35
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	10	0.35
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG11	6	0.35
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	10	0.35
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG13	17	0.35
(1,925)	1:125:A:LEU:HD22	1:7:A:PHE:HA	4	0.35
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG22	1	0.35
(1,805)	1:101:A:THR:HG22	1:102:A:GLU:H	1	0.35
(1,805)	1:101:A:THR:HG22	1:102:A:GLU:H	8	0.35
(1,805)	1:101:A:THR:HG23	1:102:A:GLU:H	13	0.35
(1,792)	1:100:A:LEU:HD11	1:118:A:TYR:HD2	12	0.35
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	20	0.35
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB1	16	0.35
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB1	19	0.35
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD11	9	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:74:A:LEU:HD13	1:75:A:GLY:H	17	0.35
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	8	0.35
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	12	0.35
(1,544)	1:65:A:LYS:H	1:62:A:THR:HG23	10	0.35
(1,429)	1:23:A:LEU:HD21	1:37:A:LYS:HG3	6	0.35
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	8	0.35
(1,120)	1:1:A:LYS:HG3	1:1:A:LYS:HA	14	0.35
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB3	17	0.35
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB3	20	0.35
(2,1679)	2:1001:A:OLA:H172	2:1001:A:OLA:H181	1	0.34
(2,1679)	2:1001:A:OLA:H172	2:1001:A:OLA:H183	19	0.34
(2,1658)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	14	0.34
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	1	0.34
(2,1637)	2:1001:A:OLA:H71	1:62:A:THR:HG1	19	0.34
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	9	0.34
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	11	0.34
(2,1613)	1:102:A:GLU:HG3	1:118:A:TYR:HE2	15	0.34
(2,1599)	1:61:A:LEU:HD11	1:44:A:LYS:HG2	5	0.34
(2,1579)	1:41:A:VAL:HG12	2:1001:A:OLA:H21	9	0.34
(2,1556)	1:35:A:VAL:HG21	1:36:A:ILE:H	10	0.34
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	14	0.34
(2,1553)	1:136:A:THR:H	1:129:A:MET:HE2	4	0.34
(2,1539)	1:125:A:LEU:HA	1:120:A:ARG:H	14	0.34
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	13	0.34
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	1	0.34
(2,1332)	1:75:A:GLY:H	1:91:A:THR:HG22	5	0.34
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	6	0.34
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	18	0.34
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	11	0.34
(2,1139)	1:100:A:LEU:H	1:119:A:ARG:HB3	10	0.34
(2,1112)	1:143:A:GLN:HE21	1:141:A:LYS:HG3	15	0.34
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	8	0.34
(2,1020)	1:120:A:ARG:H	1:118:A:TYR:HB3	4	0.34
(2,1019)	1:33:A:ARG:H	1:33:A:ARG:HG3	9	0.34
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG21	18	0.34
(2,843)	1:17:A:GLU:HG3	1:139:A:TYR:HD1	15	0.34
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	7	0.34
(2,811)	1:89:A:LYS:H	1:89:A:LYS:HE2	12	0.34
(2,783)	1:127:A:MET:HE3	1:140:A:TYR:HE2	10	0.34
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE3	19	0.34
(2,780)	1:37:A:LYS:HD2	1:34:A:GLN:HE22	16	0.34
(2,750)	1:104:A:HIS:HB3	1:104:A:HIS:HE1	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD12	13	0.34
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	1	0.34
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD22	6	0.34
(2,675)	1:126:A:VAL:HA	1:139:A:TYR:HE2	14	0.34
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	8	0.34
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	15	0.34
(2,610)	1:125:A:LEU:HD21	1:125:A:LEU:H	7	0.34
(2,610)	1:125:A:LEU:HD21	1:125:A:LEU:H	13	0.34
(2,610)	1:125:A:LEU:HD22	1:125:A:LEU:H	14	0.34
(2,591)	1:118:A:TYR:HA	1:127:A:MET:HG2	7	0.34
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD13	15	0.34
(2,543)	1:100:A:LEU:HD23	1:74:A:LEU:HB2	3	0.34
(2,541)	1:100:A:LEU:HD21	1:118:A:TYR:HB2	12	0.34
(2,533)	1:99:A:THR:HG21	1:96:A:ASP:HB2	14	0.34
(2,526)	1:13:A:LEU:HA	1:12:A:LYS:HG3	7	0.34
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	4	0.34
(2,511)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	20	0.34
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG21	8	0.34
(2,491)	1:77:A:GLU:HA	1:90:A:ILE:HG23	13	0.34
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	8	0.34
(2,446)	1:83:A:LEU:HD11	1:60:A:ASN:HD21	14	0.34
(2,400)	1:83:A:LEU:HD11	1:65:A:LYS:HG2	15	0.34
(2,392)	1:1:A:LYS:HA	1:1:A:LYS:HE3	19	0.34
(2,350)	1:52:A:LYS:H	1:52:A:LYS:HD2	7	0.34
(2,349)	1:52:A:LYS:HG2	1:52:A:LYS:H	3	0.34
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	11	0.34
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	20	0.34
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	10	0.34
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	10	0.34
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	6	0.34
(2,228)	1:25:A:ALA:HB1	1:26:A:ARG:HA	7	0.34
(2,228)	1:25:A:ALA:HB1	1:26:A:ARG:HA	17	0.34
(2,158)	1:15:A:ARG:HA	1:13:A:LEU:HB3	7	0.34
(2,154)	1:13:A:LEU:H	1:12:A:LYS:HE3	13	0.34
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	6	0.34
(2,91)	1:125:A:LEU:HB3	1:125:A:LEU:HD11	1	0.34
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD21	16	0.34
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	13	0.34
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	6	0.34
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	7	0.34
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	6	0.34
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	18	0.34
(1,2841)	1:36:A:ILE:HD12	2:1001:A:OLA:H10	5	0.34
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	3	0.34
(1,2813)	1:127:A:MET:HE1	1:118:A:TYR:HH	13	0.34
(1,2656)	1:111:A:THR:H	1:112:A:ASP:HB3	10	0.34
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	8	0.34
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD13	6	0.34
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD11	12	0.34
(1,1479)	1:46:A:ARG:HA	1:47:A:ASN:HB3	12	0.34
(1,1456)	1:103:A:THR:HG21	1:104:A:HIS:H	11	0.34
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	14	0.34
(1,1278)	1:113:A:VAL:H	1:113:A:VAL:HG13	19	0.34
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG22	9	0.34
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	17	0.34
(1,1230)	1:15:A:ARG:H	1:13:A:LEU:HD13	16	0.34
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB1	10	0.34
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB1	12	0.34
(1,1222)	1:127:A:MET:HE2	1:118:A:TYR:HD1	7	0.34
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE3	5	0.34
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE3	6	0.34
(1,1148)	1:37:A:LYS:H	1:36:A:ILE:HG23	7	0.34
(1,1110)	1:59:A:GLU:HA	1:58:A:MET:HE2	5	0.34
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	5	0.34
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	5	0.34
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	9	0.34
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	12	0.34
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	3	0.34
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG23	16	0.34
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG22	19	0.34
(1,989)	1:134:A:VAL:HG11	1:22:A:TYR:HB3	18	0.34
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	20	0.34
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	7	0.34
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	12	0.34
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG23	5	0.34
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	2	0.34
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	4	0.34
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	6	0.34
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	10	0.34
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	12	0.34
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	15	0.34
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	18	0.34
(1,805)	1:101:A:THR:HG22	1:102:A:GLU:H	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,805)	1:101:A:THR:HG23	1:102:A:GLU:H	16	0.34
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	18	0.34
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	19	0.34
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD21	20	0.34
(1,752)	1:94:A:LEU:HD13	1:7:A:PHE:HD2	13	0.34
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	8	0.34
(1,628)	1:74:A:LEU:HD13	1:74:A:LEU:H	6	0.34
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB3	4	0.34
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG22	4	0.34
(1,397)	1:35:A:VAL:HG23	1:36:A:ILE:H	1	0.34
(1,230)	1:40:A:GLY:HA3	1:13:A:LEU:HD12	8	0.34
(1,218)	1:13:A:LEU:HD21	1:139:A:TYR:H	8	0.34
(1,187)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	6	0.34
(1,132)	1:72:A:TRP:HZ3	1:3:A:LEU:HD12	17	0.34
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	7	0.34
(1,130)	1:3:A:LEU:HD11	1:7:A:PHE:HB3	18	0.34
(1,107)	1:63:A:THR:HG22	1:40:A:GLY:H	7	0.34
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	19	0.34
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB3	7	0.34
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB1	18	0.34
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG23	5	0.34
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG22	15	0.34
(2,1679)	2:1001:A:OLA:H172	2:1001:A:OLA:H181	6	0.33
(2,1670)	2:1001:A:OLA:H82	2:1001:A:OLA:H183	12	0.33
(2,1670)	2:1001:A:OLA:H183	2:1001:A:OLA:H21	17	0.33
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H183	19	0.33
(2,1627)	2:1001:A:OLA:H122	1:84:A:ASP:HB3	6	0.33
(2,1623)	2:1001:A:OLA:H81	1:36:A:ILE:HA	10	0.33
(2,1601)	2:1001:A:OLA:H22	2:1001:A:OLA:H183	9	0.33
(2,1596)	2:1001:A:OLA:H31	2:1001:A:OLA:H181	10	0.33
(2,1593)	1:84:A:ASP:HA	2:1001:A:OLA:H112	18	0.33
(2,1556)	1:35:A:VAL:HG22	1:36:A:ILE:H	2	0.33
(2,1544)	1:134:A:VAL:HG13	1:21:A:GLU:H	8	0.33
(2,1540)	1:94:A:LEU:HG	1:100:A:LEU:H	11	0.33
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	17	0.33
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	15	0.33
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	17	0.33
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD11	12	0.33
(2,1168)	1:56:A:TYR:H	1:55:A:ARG:HD2	9	0.33
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD12	6	0.33
(2,1098)	1:132:A:LYS:HD3	1:131:A:TRP:HE1	9	0.33
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	17	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	13	0.33
(2,925)	1:65:A:LYS:HG3	1:67:A:THR:H	2	0.33
(2,834)	1:68:A:HIS:HE1	1:49:A:ALA:HB3	9	0.33
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	11	0.33
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	2	0.33
(2,751)	1:104:A:HIS:HE1	1:82:A:ALA:HB3	3	0.33
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	12	0.33
(2,744)	1:78:A:PHE:HE1	1:72:A:TRP:HZ3	19	0.33
(2,740)	1:31:A:ILE:HD12	1:30:A:TRP:HZ2	17	0.33
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG23	9	0.33
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	14	0.33
(2,706)	1:41:A:VAL:HG21	1:62:A:THR:HG1	18	0.33
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	15	0.33
(2,677)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	17	0.33
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	12	0.33
(2,675)	1:126:A:VAL:HA	1:139:A:TYR:HE2	19	0.33
(2,668)	1:129:A:MET:HE2	1:136:A:THR:HG23	13	0.33
(2,652)	1:132:A:LYS:HG2	1:132:A:LYS:HE2	11	0.33
(2,632)	1:128:A:LYS:HB3	1:128:A:LYS:HE2	8	0.33
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	5	0.33
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG12	2	0.33
(2,544)	1:100:A:LEU:HD21	1:58:A:MET:HG3	2	0.33
(2,539)	1:118:A:TYR:HD2	1:100:A:LEU:HD21	12	0.33
(2,534)	1:99:A:THR:HG22	1:95:A:LYS:HD3	1	0.33
(2,482)	1:90:A:ILE:HG23	1:78:A:PHE:HD1	12	0.33
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB1	9	0.33
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	6	0.33
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	20	0.33
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	14	0.33
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	8	0.33
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	9	0.33
(2,209)	1:23:A:LEU:HD11	1:36:A:ILE:HG23	17	0.33
(2,183)	1:21:A:GLU:HA	1:24:A:LYS:HE3	11	0.33
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	17	0.33
(2,160)	1:13:A:LEU:HD22	1:41:A:VAL:H	18	0.33
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG23	9	0.33
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	12	0.33
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	11	0.33
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD13	12	0.33
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	10	0.33
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	17	0.33
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	20	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,24)	1:32:A:MET:HG3	1:31:A:ILE:HG21	13	0.33
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	2	0.33
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	6	0.33
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H182	10	0.33
(1,2813)	1:127:A:MET:HE1	1:118:A:TYR:HH	10	0.33
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H181	5	0.33
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	6	0.33
(1,2331)	1:60:A:ASN:HB3	1:67:A:THR:H	18	0.33
(1,1590)	1:2:A:THR:H	1:2:A:THR:HG23	20	0.33
(1,1386)	1:83:A:LEU:HD11	1:84:A:ASP:H	7	0.33
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG11	2	0.33
(1,1297)	1:8:A:LEU:HD21	1:8:A:LEU:H	13	0.33
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	17	0.33
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	7	0.33
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	7	0.33
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	15	0.33
(1,1088)	1:61:A:LEU:HD22	1:62:A:THR:H	16	0.33
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	14	0.33
(1,925)	1:125:A:LEU:HD21	1:7:A:PHE:HA	1	0.33
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	11	0.33
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	3	0.33
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	5	0.33
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	13	0.33
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	14	0.33
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	20	0.33
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD12	17	0.33
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	7	0.33
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD21	17	0.33
(1,771)	1:99:A:THR:H	1:99:A:THR:HG21	4	0.33
(1,752)	1:94:A:LEU:HD11	1:7:A:PHE:HD2	15	0.33
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	5	0.33
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	10	0.33
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	20	0.33
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	4	0.33
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	12	0.33
(1,426)	1:37:A:LYS:HG3	1:37:A:LYS:H	11	0.33
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	11	0.33
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG22	15	0.33
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	20	0.33
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB1	17	0.33
(1,137)	1:3:A:LEU:HD21	1:7:A:PHE:HB3	13	0.33
(1,111)	1:48:A:ALA:HB2	1:71:A:ASP:HB2	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB2	17	0.33
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	5	0.33
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB2	18	0.33
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB3	13	0.33
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB2	15	0.33
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	7	0.33
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	18	0.33
(2,1678)	1:10:A:THR:HG23	1:44:A:LYS:HG2	7	0.32
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	16	0.32
(2,1670)	2:1001:A:OLA:H181	2:1001:A:OLA:H21	20	0.32
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	5	0.32
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	15	0.32
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	5	0.32
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	3	0.32
(2,1619)	1:84:A:ASP:HB3	2:1001:A:OLA:H131	17	0.32
(2,1556)	1:35:A:VAL:HG22	1:36:A:ILE:H	8	0.32
(2,1556)	1:35:A:VAL:HG21	1:36:A:ILE:H	19	0.32
(2,1540)	1:119:A:ARG:HG2	1:100:A:LEU:H	5	0.32
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	13	0.32
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	17	0.32
(2,1478)	1:45:A:PHE:HD1	1:11:A:PHE:H	20	0.32
(2,1328)	1:34:A:GLN:HB2	1:36:A:ILE:H	10	0.32
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	4	0.32
(2,1203)	1:112:A:ASP:H	1:106:A:LYS:HB3	1	0.32
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	1	0.32
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	8	0.32
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	19	0.32
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	8	0.32
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	13	0.32
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	20	0.32
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD12	9	0.32
(2,1098)	1:132:A:LYS:HD2	1:131:A:TRP:HE1	10	0.32
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	12	0.32
(2,1018)	1:68:A:HIS:H	1:61:A:LEU:HD21	17	0.32
(2,967)	1:88:A:HIS:H	1:82:A:ALA:HB1	1	0.32
(2,849)	1:124:A:TYR:HE2	1:141:A:LYS:HE2	17	0.32
(2,821)	1:14:A:GLU:HB2	1:141:A:LYS:HG3	13	0.32
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	4	0.32
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	8	0.32
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	10	0.32
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	14	0.32
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD22	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,706)	1:41:A:VAL:HG23	1:62:A:THR:HG1	5	0.32
(2,692)	1:12:A:LYS:H	1:141:A:LYS:HD2	11	0.32
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	2	0.32
(2,675)	1:139:A:TYR:HA	1:139:A:TYR:HE2	11	0.32
(2,674)	1:16:A:ASP:HA	1:139:A:TYR:HE1	18	0.32
(2,652)	1:132:A:LYS:HG2	1:132:A:LYS:HE2	6	0.32
(2,623)	1:128:A:LYS:HE3	1:126:A:VAL:HG11	17	0.32
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD21	16	0.32
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	4	0.32
(2,610)	1:125:A:LEU:HD23	1:125:A:LEU:H	17	0.32
(2,603)	1:124:A:TYR:HE2	1:141:A:LYS:HE2	17	0.32
(2,596)	1:118:A:TYR:HD1	1:125:A:LEU:HG	18	0.32
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	8	0.32
(2,544)	1:100:A:LEU:HD21	1:58:A:MET:HG3	19	0.32
(2,541)	1:100:A:LEU:HD21	1:118:A:TYR:HB2	18	0.32
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD22	5	0.32
(2,500)	1:90:A:ILE:HD13	1:88:A:HIS:H	11	0.32
(2,450)	1:84:A:ASP:HA	1:82:A:ALA:HB1	19	0.32
(2,447)	1:84:A:ASP:HA	2:1001:A:OLA:H82	18	0.32
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB3	20	0.32
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	16	0.32
(2,388)	1:63:A:THR:HB	1:64:A:LYS:HD2	8	0.32
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	10	0.32
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	9	0.32
(2,288)	1:36:A:ILE:HD12	1:37:A:LYS:H	14	0.32
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	15	0.32
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	12	0.32
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	18	0.32
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	20	0.32
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD23	8	0.32
(2,76)	1:3:A:LEU:HD12	1:45:A:PHE:HB2	14	0.32
(2,37)	1:53:A:PRO:HA	1:53:A:PRO:HG2	3	0.32
(2,23)	1:34:A:GLN:HG3	1:30:A:TRP:HZ2	8	0.32
(1,2826)	1:127:A:MET:HE1	1:118:A:TYR:HH	2	0.32
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	10	0.32
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	8	0.32
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD21	17	0.32
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	12	0.32
(1,2059)	1:143:A:GLN:H	1:142:A:LYS:HG2	1	0.32
(1,2040)	1:48:A:ALA:HB3	1:50:A:SER:H	4	0.32
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG22	5	0.32
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1386)	1:83:A:LEU:HD12	1:84:A:ASP:H	13	0.32
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	11	0.32
(1,1297)	1:8:A:LEU:HD21	1:8:A:LEU:H	15	0.32
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	18	0.32
(1,1259)	1:125:A:LEU:HA	1:125:A:LEU:HD12	17	0.32
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	2	0.32
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	6	0.32
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB2	17	0.32
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	18	0.32
(1,1112)	1:58:A:MET:HE1	1:43:A:LYS:HE3	14	0.32
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	11	0.32
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG23	8	0.32
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG11	4	0.32
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG21	3	0.32
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	1	0.32
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	8	0.32
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	9	0.32
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	16	0.32
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD13	14	0.32
(1,805)	1:101:A:THR:HG23	1:102:A:GLU:H	14	0.32
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	14	0.32
(1,771)	1:99:A:THR:H	1:99:A:THR:HG21	20	0.32
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	17	0.32
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB3	18	0.32
(1,429)	1:23:A:LEU:HD23	1:37:A:LYS:HG3	2	0.32
(1,426)	1:37:A:LYS:HG3	1:37:A:LYS:H	15	0.32
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG21	1	0.32
(1,397)	1:35:A:VAL:HG21	1:36:A:ILE:H	3	0.32
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	18	0.32
(1,283)	1:19:A:PHE:HZ	1:23:A:LEU:HD13	7	0.32
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	3	0.32
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB3	10	0.32
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB1	11	0.32
(1,100)	1:48:A:ALA:HB1	1:50:A:SER:H	6	0.32
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	2	0.32
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	11	0.32
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	12	0.32
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	8	0.32
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	11	0.32
(2,1637)	1:65:A:LYS:HG3	1:62:A:THR:HG1	4	0.31
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	8	0.31
(2,1614)	1:58:A:MET:HE3	1:60:A:ASN:H	12	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1613)	1:102:A:GLU:HG3	1:118:A:TYR:HE2	17	0.31
(2,1581)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	5	0.31
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	7	0.31
(2,1556)	1:35:A:VAL:HG22	1:36:A:ILE:H	15	0.31
(2,1537)	1:41:A:VAL:H	1:13:A:LEU:HD11	5	0.31
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG13	6	0.31
(2,1480)	1:46:A:ARG:HG3	1:71:A:ASP:H	8	0.31
(2,1478)	1:45:A:PHE:HD1	1:11:A:PHE:H	14	0.31
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	11	0.31
(2,1442)	1:64:A:LYS:HG3	1:64:A:LYS:H	6	0.31
(2,1390)	1:54:A:ASP:H	1:53:A:PRO:HG3	15	0.31
(2,1306)	1:72:A:TRP:H	1:55:A:ARG:HG3	8	0.31
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	5	0.31
(2,1112)	1:143:A:GLN:HE21	1:61:A:LEU:HD23	19	0.31
(2,975)	1:136:A:THR:H	1:128:A:LYS:HG3	6	0.31
(2,929)	1:116:A:TYR:H	1:103:A:THR:HG23	16	0.31
(2,894)	1:64:A:LYS:HG3	1:64:A:LYS:H	6	0.31
(2,893)	1:64:A:LYS:HG3	2:1001:A:OLA:H9	11	0.31
(2,888)	1:59:A:GLU:HG2	1:68:A:HIS:HD2	14	0.31
(2,878)	1:132:A:LYS:HG3	1:132:A:LYS:H	2	0.31
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	13	0.31
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	7	0.31
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	2	0.31
(2,780)	1:109:A:ASP:H	1:106:A:LYS:HD2	14	0.31
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	13	0.31
(2,694)	1:141:A:LYS:H	1:141:A:LYS:HE3	5	0.31
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	12	0.31
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	15	0.31
(2,652)	1:132:A:LYS:HG2	1:132:A:LYS:HE2	15	0.31
(2,632)	1:128:A:LYS:HB3	1:128:A:LYS:HE2	3	0.31
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG23	10	0.31
(2,545)	1:100:A:LEU:HD22	1:94:A:LEU:HD21	13	0.31
(2,544)	1:100:A:LEU:HD23	1:58:A:MET:HG3	14	0.31
(2,518)	1:95:A:LYS:H	1:94:A:LEU:HD13	7	0.31
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD23	4	0.31
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	14	0.31
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	15	0.31
(2,487)	1:90:A:ILE:HG23	1:92:A:PHE:HB2	18	0.31
(2,478)	1:88:A:HIS:HB2	1:90:A:ILE:HG13	20	0.31
(2,433)	1:85:A:SER:H	1:81:A:GLU:HG2	5	0.31
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB3	5	0.31
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG21	8	0.31
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG21	17	0.31
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	1	0.31
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	1	0.31
(2,228)	1:25:A:ALA:HB1	1:26:A:ARG:HA	4	0.31
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	6	0.31
(2,178)	1:134:A:VAL:HG13	1:18:A:ASN:HB2	9	0.31
(2,178)	1:134:A:VAL:HG13	1:18:A:ASN:HB2	17	0.31
(2,155)	1:12:A:LYS:HE2	1:12:A:LYS:HA	6	0.31
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	18	0.31
(2,125)	1:65:A:LYS:HE3	1:67:A:THR:HG23	2	0.31
(2,91)	1:125:A:LEU:HB3	1:125:A:LEU:HD11	5	0.31
(2,86)	1:125:A:LEU:HD11	1:45:A:PHE:HE1	16	0.31
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD12	6	0.31
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	14	0.31
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	8	0.31
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	9	0.31
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	13	0.31
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	14	0.31
(2,33)	1:52:A:LYS:HG3	1:53:A:PRO:HD3	12	0.31
(2,3)	1:89:A:LYS:H	1:105:A:ILE:HG23	19	0.31
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	17	0.31
(1,2818)	1:83:A:LEU:HD23	1:62:A:THR:HG1	11	0.31
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H181	5	0.31
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	18	0.31
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	11	0.31
(1,2789)	2:1001:A:OLA:H181	1:36:A:ILE:HA	17	0.31
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	20	0.31
(1,2326)	1:74:A:LEU:HD12	1:2:A:THR:H	20	0.31
(1,2243)	1:23:A:LEU:HD23	1:37:A:LYS:H	9	0.31
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG21	2	0.31
(1,2029)	1:114:A:GLU:H	1:103:A:THR:HG23	8	0.31
(1,1456)	1:103:A:THR:HG21	1:104:A:HIS:H	8	0.31
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	2	0.31
(1,1297)	1:8:A:LEU:HD23	1:8:A:LEU:H	5	0.31
(1,1222)	1:127:A:MET:HE1	1:118:A:TYR:HD1	9	0.31
(1,1105)	1:58:A:MET:HE1	1:92:A:PHE:HE2	1	0.31
(1,1105)	1:58:A:MET:HE1	1:92:A:PHE:HE2	20	0.31
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	11	0.31
(1,1033)	1:141:A:LYS:HG3	1:141:A:LYS:HA	13	0.31
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	13	0.31
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG21	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	1	0.31
(1,952)	1:129:A:MET:HB2	1:136:A:THR:HG23	17	0.31
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG13	14	0.31
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	3	0.31
(1,923)	1:125:A:LEU:HD21	1:118:A:TYR:HB2	19	0.31
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	7	0.31
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	17	0.31
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	11	0.31
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD11	11	0.31
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	7	0.31
(1,805)	1:101:A:THR:HG22	1:102:A:GLU:H	10	0.31
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD22	10	0.31
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	10	0.31
(1,743)	1:93:A:ASP:HB2	1:91:A:THR:HG22	2	0.31
(1,729)	1:90:A:ILE:HD13	1:78:A:PHE:HZ	14	0.31
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	12	0.31
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB2	11	0.31
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	15	0.31
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB2	19	0.31
(1,383)	1:23:A:LEU:HD23	1:33:A:ARG:HA	6	0.31
(1,310)	1:25:A:ALA:HB1	1:134:A:VAL:HB	17	0.31
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	13	0.31
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE1	16	0.31
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	9	0.31
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	10	0.31
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	8	0.3
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	14	0.3
(2,1670)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	14	0.3
(2,1637)	2:1001:A:OLA:H71	1:62:A:THR:HG1	16	0.3
(2,1636)	1:65:A:LYS:HG2	1:62:A:THR:HG1	2	0.3
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	15	0.3
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	12	0.3
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	14	0.3
(2,1583)	1:41:A:VAL:HG23	2:1001:A:OLA:H21	13	0.3
(2,1560)	1:11:A:PHE:H	1:44:A:LYS:HG3	9	0.3
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	15	0.3
(2,1521)	1:7:A:PHE:H	1:120:A:ARG:HB2	8	0.3
(2,1487)	1:67:A:THR:HG22	1:65:A:LYS:H	3	0.3
(2,1487)	1:67:A:THR:HG22	1:65:A:LYS:H	18	0.3
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD11	2	0.3
(2,1471)	1:101:A:THR:HG21	1:93:A:ASP:H	9	0.3
(2,1232)	1:65:A:LYS:HB3	1:85:A:SER:H	19	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	3	0.3
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD12	5	0.3
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	20	0.3
(2,1168)	1:56:A:TYR:H	1:55:A:ARG:HD2	10	0.3
(2,1102)	1:58:A:MET:H	1:70:A:LYS:HG2	3	0.3
(2,1029)	1:113:A:VAL:HG13	1:104:A:HIS:H	15	0.3
(2,979)	1:132:A:LYS:HG2	1:131:A:TRP:HE1	11	0.3
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	6	0.3
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	7	0.3
(2,814)	1:60:A:ASN:HD21	1:83:A:LEU:HD21	16	0.3
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	12	0.3
(2,787)	1:39:A:ALA:HB2	1:40:A:GLY:H	20	0.3
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	15	0.3
(2,750)	1:104:A:HIS:HB3	1:104:A:HIS:HE1	19	0.3
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG23	7	0.3
(2,727)	1:3:A:LEU:HD22	1:7:A:PHE:HA	12	0.3
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	11	0.3
(2,684)	1:125:A:LEU:HD13	1:140:A:TYR:HE2	20	0.3
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	16	0.3
(2,596)	1:118:A:TYR:HD1	1:125:A:LEU:HG	17	0.3
(2,580)	1:111:A:THR:HG22	1:110:A:PRO:HG2	7	0.3
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG22	17	0.3
(2,551)	1:135:A:SER:H	1:134:A:VAL:HG13	16	0.3
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	4	0.3
(2,479)	1:90:A:ILE:HG21	1:78:A:PHE:H	6	0.3
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HB2	11	0.3
(2,448)	2:1001:A:OLA:H151	1:84:A:ASP:HA	1	0.3
(2,441)	1:141:A:LYS:H	1:141:A:LYS:HG3	2	0.3
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB2	8	0.3
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG21	5	0.3
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	20	0.3
(2,355)	1:57:A:ASP:HA	1:48:A:ALA:HB2	4	0.3
(2,349)	1:52:A:LYS:HG2	1:52:A:LYS:H	2	0.3
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	2	0.3
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	16	0.3
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	13	0.3
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	10	0.3
(2,224)	1:36:A:ILE:HG13	1:37:A:LYS:H	19	0.3
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	5	0.3
(2,183)	1:21:A:GLU:HA	1:24:A:LYS:HE3	20	0.3
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	16	0.3
(2,158)	1:15:A:ARG:HA	1:13:A:LEU:HB3	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	13	0.3
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	15	0.3
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD22	1	0.3
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	20	0.3
(2,85)	1:125:A:LEU:HD12	1:118:A:TYR:HE1	3	0.3
(2,66)	1:12:A:LYS:HG3	1:141:A:LYS:HG3	20	0.3
(2,3)	1:89:A:LYS:H	1:105:A:ILE:HG21	7	0.3
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG23	6	0.3
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG22	17	0.3
(1,2828)	2:1001:A:OLA:H10	1:32:A:MET:HE1	9	0.3
(1,2828)	2:1001:A:OLA:H10	1:32:A:MET:HE3	12	0.3
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	14	0.3
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	2	0.3
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG13	8	0.3
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG12	10	0.3
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG11	13	0.3
(1,2600)	1:15:A:ARG:HG2	1:15:A:ARG:H	9	0.3
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	10	0.3
(1,2326)	1:74:A:LEU:HD11	1:2:A:THR:H	4	0.3
(1,2326)	1:74:A:LEU:HD13	1:2:A:THR:H	14	0.3
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	18	0.3
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD22	13	0.3
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	4	0.3
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	14	0.3
(1,1456)	1:103:A:THR:HG22	1:104:A:HIS:H	19	0.3
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	20	0.3
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	17	0.3
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	2	0.3
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	2	0.3
(1,1297)	1:8:A:LEU:HD21	1:8:A:LEU:H	9	0.3
(1,1292)	1:111:A:THR:HG23	1:112:A:ASP:H	4	0.3
(1,1259)	1:125:A:LEU:HA	1:125:A:LEU:HD13	4	0.3
(1,1223)	1:127:A:MET:HE3	1:116:A:TYR:HD2	14	0.3
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE2	12	0.3
(1,1105)	1:58:A:MET:HE3	1:92:A:PHE:HE2	9	0.3
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	15	0.3
(1,1062)	1:68:A:HIS:HE1	1:70:A:LYS:HE3	5	0.3
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	7	0.3
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG22	15	0.3
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	12	0.3
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	14	0.3
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	7	0.3
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG13	3	0.3
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG12	2	0.3
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	8	0.3
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	19	0.3
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	19	0.3
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	3	0.3
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG22	5	0.3
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	17	0.3
(1,793)	1:100:A:LEU:HD11	1:118:A:TYR:HB3	18	0.3
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	12	0.3
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	19	0.3
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	19	0.3
(1,755)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	19	0.3
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG23	1	0.3
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	18	0.3
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB3	2	0.3
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	15	0.3
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG11	14	0.3
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	1	0.3
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB3	20	0.3
(1,449)	1:61:A:LEU:HB2	1:42:A:THR:HB	1	0.3
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE1	14	0.3
(1,383)	1:23:A:LEU:HD21	1:33:A:ARG:HA	3	0.3
(1,383)	1:23:A:LEU:HD23	1:33:A:ARG:HA	7	0.3
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	5	0.3
(1,307)	1:25:A:ALA:HB1	1:27:A:GLY:H	7	0.3
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	8	0.3
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	10	0.3
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	16	0.3
(1,137)	1:3:A:LEU:HD22	1:7:A:PHE:HB3	19	0.3
(1,100)	1:48:A:ALA:HB2	1:50:A:SER:H	19	0.3
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB2	19	0.3
(1,17)	1:31:A:ILE:HD13	1:31:A:ILE:HA	18	0.3
(3,43)	1:55:A:ARG:H	1:53:A:PRO:O	14	0.29
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	14	0.29
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	8	0.29
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	5	0.29
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	9	0.29
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	12	0.29
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	17	0.29
(2,1511)	1:61:A:LEU:HB2	1:67:A:THR:H	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1397)	1:113:A:VAL:HG13	1:112:A:ASP:H	9	0.29
(2,1390)	1:54:A:ASP:H	1:53:A:PRO:HG3	16	0.29
(2,1275)	1:3:A:LEU:HD21	1:7:A:PHE:H	17	0.29
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB3	12	0.29
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	7	0.29
(2,1080)	1:102:A:GLU:H	1:92:A:PHE:HD2	16	0.29
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	9	0.29
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD21	9	0.29
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	10	0.29
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	12	0.29
(2,967)	1:88:A:HIS:H	1:82:A:ALA:HB1	17	0.29
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	11	0.29
(2,838)	1:127:A:MET:HE3	1:116:A:TYR:HE2	5	0.29
(2,837)	1:58:A:MET:HE3	1:60:A:ASN:HD21	12	0.29
(2,820)	1:43:A:LYS:HE2	1:127:A:MET:HG3	3	0.29
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	9	0.29
(2,803)	1:1:A:LYS:HA	1:-2:A:HIS:HB3	11	0.29
(2,789)	1:26:A:ARG:HD3	1:131:A:TRP:HZ3	17	0.29
(2,787)	1:39:A:ALA:HB3	1:40:A:GLY:H	9	0.29
(2,783)	1:127:A:MET:HE3	1:140:A:TYR:HE2	19	0.29
(2,782)	1:127:A:MET:HA	1:127:A:MET:HE2	4	0.29
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	3	0.29
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	7	0.29
(2,759)	1:32:A:MET:HE2	2:1001:A:OLA:H121	15	0.29
(2,757)	1:58:A:MET:HE3	1:43:A:LYS:HD2	19	0.29
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	3	0.29
(2,750)	1:104:A:HIS:HB3	1:104:A:HIS:HE1	18	0.29
(2,744)	1:45:A:PHE:HD2	1:72:A:TRP:HZ3	18	0.29
(2,732)	1:58:A:MET:HE3	1:67:A:THR:HG1	1	0.29
(2,727)	1:3:A:LEU:HD23	1:7:A:PHE:HA	15	0.29
(2,727)	1:3:A:LEU:HD23	1:7:A:PHE:HA	18	0.29
(2,720)	1:14:A:GLU:H	1:124:A:TYR:HE2	2	0.29
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD22	18	0.29
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD22	19	0.29
(2,677)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	7	0.29
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	9	0.29
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD21	13	0.29
(2,610)	1:125:A:LEU:HD22	1:125:A:LEU:H	19	0.29
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	6	0.29
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG23	11	0.29
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG22	5	0.29
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG23	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG23	19	0.29
(2,525)	1:95:A:LYS:HG3	1:95:A:LYS:HE3	20	0.29
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	12	0.29
(2,501)	1:90:A:ILE:HD11	1:80:A:ASP:H	6	0.29
(2,501)	1:90:A:ILE:HD11	1:80:A:ASP:H	12	0.29
(2,488)	1:90:A:ILE:HG23	1:102:A:GLU:HB2	1	0.29
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG23	3	0.29
(2,446)	1:83:A:LEU:HD11	1:60:A:ASN:HD21	13	0.29
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB3	10	0.29
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB2	14	0.29
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB3	18	0.29
(2,380)	1:65:A:LYS:HB2	2:1001:A:OLA:H10	11	0.29
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	19	0.29
(2,249)	1:26:A:ARG:HD2	1:131:A:TRP:HZ2	7	0.29
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	6	0.29
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	13	0.29
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	8	0.29
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	15	0.29
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	13	0.29
(2,224)	1:36:A:ILE:HG13	1:37:A:LYS:H	12	0.29
(2,160)	1:13:A:LEU:HD23	1:41:A:VAL:H	4	0.29
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD3	4	0.29
(2,98)	1:8:A:LEU:HD23	1:5:A:ASP:HA	15	0.29
(2,51)	1:48:A:ALA:HB2	1:56:A:TYR:HB3	2	0.29
(2,33)	1:52:A:LYS:HG2	1:53:A:PRO:HD3	13	0.29
(2,33)	1:52:A:LYS:HG2	1:53:A:PRO:HD3	20	0.29
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	13	0.29
(2,26)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	18	0.29
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	6	0.29
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG23	15	0.29
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG22	14	0.29
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	16	0.29
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	18	0.29
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	4	0.29
(1,2789)	2:1001:A:OLA:H181	1:36:A:ILE:HA	10	0.29
(1,2789)	2:1001:A:OLA:H183	1:36:A:ILE:HA	15	0.29
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG13	4	0.29
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	4	0.29
(1,2390)	1:74:A:LEU:HD13	1:3:A:LEU:H	12	0.29
(1,2326)	1:74:A:LEU:HD11	1:2:A:THR:H	10	0.29
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	7	0.29
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG22	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	17	0.29
(1,1972)	1:21:A:GLU:H	1:21:A:GLU:HG2	5	0.29
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	10	0.29
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	11	0.29
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	3	0.29
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	12	0.29
(1,1249)	1:3:A:LEU:HD23	1:3:A:LEU:H	12	0.29
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG22	19	0.29
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB2	19	0.29
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD13	8	0.29
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	15	0.29
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	10	0.29
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	6	0.29
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	10	0.29
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	16	0.29
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	7	0.29
(1,833)	1:110:A:PRO:HB2	1:110:A:PRO:HD3	17	0.29
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG23	20	0.29
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	4	0.29
(1,793)	1:100:A:LEU:HD11	1:118:A:TYR:HB3	5	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	2	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	7	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	8	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	9	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	11	0.29
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	12	0.29
(1,752)	1:94:A:LEU:HD11	1:7:A:PHE:HD2	4	0.29
(1,752)	1:94:A:LEU:HD13	1:7:A:PHE:HD2	5	0.29
(1,729)	1:90:A:ILE:HD13	1:78:A:PHE:HZ	19	0.29
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	18	0.29
(1,687)	1:86:A:THR:HG21	1:87:A:GLN:H	7	0.29
(1,687)	1:86:A:THR:HG21	1:87:A:GLN:H	9	0.29
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	11	0.29
(1,636)	1:61:A:LEU:HD21	1:66:A:ASP:HB2	9	0.29
(1,636)	1:61:A:LEU:HD21	1:66:A:ASP:HB2	11	0.29
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	6	0.29
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB3	3	0.29
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD13	6	0.29
(1,307)	1:25:A:ALA:HB1	1:27:A:GLY:H	3	0.29
(1,307)	1:25:A:ALA:HB1	1:27:A:GLY:H	17	0.29
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	20	0.29
(1,193)	1:10:A:THR:HA	1:10:A:THR:HG21	4	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:3:A:LEU:HD22	1:7:A:PHE:HB3	9	0.29
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	5	0.29
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB3	15	0.29
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB2	18	0.29
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	8	0.28
(2,1679)	2:1001:A:OLA:H41	2:1001:A:OLA:H181	8	0.28
(2,1660)	2:1001:A:OLA:H81	1:36:A:ILE:HA	17	0.28
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	2	0.28
(2,1653)	1:32:A:MET:HE2	2:1001:A:OLA:H121	15	0.28
(2,1652)	2:1001:A:OLA:H142	1:32:A:MET:HE3	20	0.28
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	18	0.28
(2,1601)	2:1001:A:OLA:H22	2:1001:A:OLA:H182	13	0.28
(2,1332)	1:75:A:GLY:H	1:74:A:LEU:HD22	8	0.28
(2,1325)	1:129:A:MET:HE2	1:130:A:SER:H	12	0.28
(2,1325)	1:129:A:MET:HE1	1:130:A:SER:H	19	0.28
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB2	2	0.28
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	3	0.28
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	14	0.28
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD13	11	0.28
(2,1112)	1:143:A:GLN:HE21	1:141:A:LYS:HG3	11	0.28
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	1	0.28
(2,875)	1:-5:A:HIS:HA	1:-5:A:HIS:HB2	6	0.28
(2,849)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	13	0.28
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	1	0.28
(2,811)	1:89:A:LYS:H	1:89:A:LYS:HE2	15	0.28
(2,805)	1:0:A:SER:HA	1:-1:A:GLY:HA3	6	0.28
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	20	0.28
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	19	0.28
(2,759)	1:32:A:MET:HE3	2:1001:A:OLA:H121	12	0.28
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	4	0.28
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	7	0.28
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	10	0.28
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	17	0.28
(2,727)	1:3:A:LEU:HD23	1:7:A:PHE:HA	6	0.28
(2,720)	1:124:A:TYR:HE2	1:141:A:LYS:H	7	0.28
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	20	0.28
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	11	0.28
(2,677)	1:139:A:TYR:HE2	1:121:A:ASP:HB3	3	0.28
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	12	0.28
(2,632)	1:128:A:LYS:HB3	1:128:A:LYS:HE2	12	0.28
(2,625)	1:127:A:MET:H	1:126:A:VAL:HG22	10	0.28
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	2	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG12	1	0.28
(2,620)	1:140:A:TYR:HD2	1:126:A:VAL:HG13	3	0.28
(2,603)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	13	0.28
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG22	20	0.28
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	7	0.28
(2,511)	1:92:A:PHE:HB3	1:100:A:LEU:HD11	10	0.28
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	7	0.28
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	10	0.28
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG23	14	0.28
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG22	15	0.28
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	19	0.28
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG23	20	0.28
(2,482)	1:90:A:ILE:HG23	1:78:A:PHE:HD1	3	0.28
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG22	14	0.28
(2,479)	1:90:A:ILE:HG22	1:78:A:PHE:H	17	0.28
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	1	0.28
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	13	0.28
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	19	0.28
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	13	0.28
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	15	0.28
(2,313)	1:129:A:MET:HE1	1:22:A:TYR:HD1	11	0.28
(2,309)	1:65:A:LYS:H	1:83:A:LEU:HD23	16	0.28
(2,301)	1:37:A:LYS:H	1:37:A:LYS:HE3	16	0.28
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG23	17	0.28
(2,249)	1:26:A:ARG:HD2	1:131:A:TRP:HZ2	17	0.28
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	14	0.28
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	19	0.28
(2,228)	1:25:A:ALA:HB1	1:26:A:ARG:HA	3	0.28
(2,209)	1:23:A:LEU:HD12	1:36:A:ILE:HG21	9	0.28
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD12	2	0.28
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	18	0.28
(2,154)	1:12:A:LYS:HE2	1:13:A:LEU:H	17	0.28
(2,120)	1:8:A:LEU:HD11	1:7:A:PHE:H	2	0.28
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD23	2	0.28
(2,112)	1:8:A:LEU:HD21	1:47:A:ASN:HD21	20	0.28
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	14	0.28
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	14	0.28
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	17	0.28
(2,61)	1:73:A:ALA:HB1	1:0:A:SER:HB3	18	0.28
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	3	0.28
(1,2839)	2:1001:A:OLA:H183	1:19:A:PHE:HE1	17	0.28
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	2	0.28
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H181	12	0.28
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	14	0.28
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H182	19	0.28
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	5	0.28
(1,2789)	2:1001:A:OLA:H183	1:36:A:ILE:HA	13	0.28
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG11	15	0.28
(1,2041)	1:52:A:LYS:H	1:48:A:ALA:HB3	12	0.28
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	16	0.28
(1,1488)	1:23:A:LEU:H	1:23:A:LEU:HD12	7	0.28
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	19	0.28
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	4	0.28
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	10	0.28
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	4	0.28
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	7	0.28
(1,1297)	1:8:A:LEU:HD23	1:8:A:LEU:H	8	0.28
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	14	0.28
(1,1297)	1:8:A:LEU:HD21	1:8:A:LEU:H	19	0.28
(1,1249)	1:3:A:LEU:HD22	1:3:A:LEU:H	15	0.28
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE1	12	0.28
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	16	0.28
(1,1112)	1:58:A:MET:HE3	1:43:A:LYS:HE3	12	0.28
(1,1088)	1:61:A:LEU:HD21	1:62:A:THR:H	7	0.28
(1,1064)	1:36:A:ILE:HD12	1:36:A:ILE:HA	13	0.28
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	14	0.28
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	20	0.28
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG12	2	0.28
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG12	12	0.28
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	1	0.28
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	11	0.28
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	13	0.28
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD12	16	0.28
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	2	0.28
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	16	0.28
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	17	0.28
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	7	0.28
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	18	0.28
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD22	15	0.28
(1,772)	1:118:A:TYR:H	1:99:A:THR:HG22	6	0.28
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	13	0.28
(1,771)	1:99:A:THR:H	1:99:A:THR:HG21	18	0.28
(1,729)	1:90:A:ILE:HD11	1:78:A:PHE:HZ	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,729)	1:90:A:ILE:HD11	1:78:A:PHE:HZ	5	0.28
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	3	0.28
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB3	3	0.28
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	7	0.28
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	15	0.28
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	3	0.28
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	6	0.28
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB3	10	0.28
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	13	0.28
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	14	0.28
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB2	10	0.28
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB1	14	0.28
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB1	15	0.28
(1,568)	1:65:A:LYS:HG3	1:66:A:ASP:H	10	0.28
(1,548)	1:62:A:THR:HG22	1:60:A:ASN:HB2	11	0.28
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	3	0.28
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	17	0.28
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	11	0.28
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB2	19	0.28
(1,191)	1:10:A:THR:HB	1:143:A:GLN:H	14	0.28
(1,173)	1:56:A:TYR:HD2	1:8:A:LEU:HD21	17	0.28
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB1	6	0.28
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB1	15	0.28
(1,36)	1:31:A:ILE:HG12	1:31:A:ILE:HA	5	0.28
(3,65)	1:88:A:HIS:H	1:80:A:ASP:O	10	0.27
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	7	0.27
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	9	0.27
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	20	0.27
(2,1636)	1:65:A:LYS:HG2	1:62:A:THR:HG1	11	0.27
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	19	0.27
(2,1580)	1:129:A:MET:HE1	2:1001:A:OLA:H181	14	0.27
(2,1559)	1:72:A:TRP:H	1:48:A:ALA:HB1	13	0.27
(2,1540)	1:94:A:LEU:HG	1:100:A:LEU:H	16	0.27
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	2	0.27
(2,1332)	1:75:A:GLY:H	1:74:A:LEU:HD23	1	0.27
(2,1325)	1:129:A:MET:HE2	1:130:A:SER:H	8	0.27
(2,1193)	1:42:A:THR:HG23	1:61:A:LEU:H	1	0.27
(2,1187)	1:38:A:LEU:H	1:38:A:LEU:HD11	7	0.27
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	17	0.27
(2,1100)	1:65:A:LYS:HB3	1:84:A:ASP:H	11	0.27
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	12	0.27
(2,984)	1:49:A:ALA:HB2	1:51:A:GLY:H	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	7	0.27
(2,834)	1:68:A:HIS:HE1	1:70:A:LYS:HD2	12	0.27
(2,832)	1:80:A:ASP:HA	1:81:A:GLU:HB2	8	0.27
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	10	0.27
(2,789)	1:26:A:ARG:HD2	1:131:A:TRP:HZ3	13	0.27
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	20	0.27
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD22	1	0.27
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	2	0.27
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	3	0.27
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD21	16	0.27
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	1	0.27
(2,683)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	4	0.27
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	7	0.27
(2,660)	1:128:A:LYS:HE3	1:135:A:SER:HB3	1	0.27
(2,621)	1:139:A:TYR:HE2	1:126:A:VAL:HG13	11	0.27
(2,618)	1:121:A:ASP:H	1:125:A:LEU:HD22	12	0.27
(2,596)	1:118:A:TYR:HD1	1:125:A:LEU:HG	8	0.27
(2,528)	1:141:A:LYS:HE3	1:141:A:LYS:HA	18	0.27
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	3	0.27
(2,498)	1:90:A:ILE:HD12	1:78:A:PHE:HD2	17	0.27
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG22	4	0.27
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	5	0.27
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG22	6	0.27
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG23	17	0.27
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG22	18	0.27
(2,479)	1:90:A:ILE:HG22	1:78:A:PHE:H	2	0.27
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG22	10	0.27
(2,442)	1:83:A:LEU:H	1:83:A:LEU:HD21	20	0.27
(2,416)	1:77:A:GLU:H	1:73:A:ALA:HB3	6	0.27
(2,412)	1:73:A:ALA:HB2	1:55:A:ARG:H	15	0.27
(2,402)	1:66:A:ASP:HA	1:62:A:THR:HG21	5	0.27
(2,372)	1:62:A:THR:HG23	1:42:A:THR:H	14	0.27
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	17	0.27
(2,308)	1:35:A:VAL:HA	1:38:A:LEU:HD11	7	0.27
(2,286)	2:1001:A:OLA:H61	1:36:A:ILE:HG23	9	0.27
(2,247)	1:26:A:ARG:HD3	1:131:A:TRP:HE3	13	0.27
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	2	0.27
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	5	0.27
(2,226)	1:134:A:VAL:HG23	1:25:A:ALA:HA	15	0.27
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD1	8	0.27
(2,209)	1:23:A:LEU:HD12	1:36:A:ILE:HG22	12	0.27
(2,205)	1:23:A:LEU:HD11	1:37:A:LYS:HE3	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD11	16	0.27
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG12	17	0.27
(2,170)	1:15:A:ARG:HD3	1:15:A:ARG:H	15	0.27
(2,158)	1:41:A:VAL:HA	1:13:A:LEU:HB3	3	0.27
(2,154)	1:13:A:LEU:H	1:12:A:LYS:HE3	15	0.27
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	2	0.27
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	15	0.27
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD22	9	0.27
(2,84)	1:3:A:LEU:HD21	1:7:A:PHE:H	13	0.27
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD11	10	0.27
(2,61)	1:73:A:ALA:HB2	1:0:A:SER:HB3	3	0.27
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD22	2	0.27
(2,53)	1:33:A:ARG:HD3	1:30:A:TRP:HA	7	0.27
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	20	0.27
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	5	0.27
(2,33)	1:52:A:LYS:HG2	1:53:A:PRO:HD3	19	0.27
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	4	0.27
(2,23)	1:34:A:GLN:HG3	1:30:A:TRP:HZ2	17	0.27
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG22	4	0.27
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG11	9	0.27
(1,2742)	1:79:A:GLN:HE21	1:107:A:VAL:HG23	2	0.27
(1,2490)	1:41:A:VAL:H	1:13:A:LEU:HB3	10	0.27
(1,2489)	1:13:A:LEU:HD22	1:17:A:GLU:H	19	0.27
(1,2243)	1:23:A:LEU:HD23	1:37:A:LYS:H	4	0.27
(1,1386)	1:83:A:LEU:HD11	1:84:A:ASP:H	6	0.27
(1,1369)	1:70:A:LYS:HD2	1:70:A:LYS:H	8	0.27
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	11	0.27
(1,1297)	1:8:A:LEU:HD22	1:8:A:LEU:H	1	0.27
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	5	0.27
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	8	0.27
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE1	14	0.27
(1,1106)	1:58:A:MET:HE2	1:45:A:PHE:HE1	8	0.27
(1,1105)	1:58:A:MET:HE2	1:92:A:PHE:HE2	18	0.27
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG23	8	0.27
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	10	0.27
(1,1064)	1:36:A:ILE:HD11	1:36:A:ILE:HA	11	0.27
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	6	0.27
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	5	0.27
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	12	0.27
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	13	0.27
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	19	0.27
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG12	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	15	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	2	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	4	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	5	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	6	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	9	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	12	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	14	0.27
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	15	0.27
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	12	0.27
(1,805)	1:101:A:THR:HG23	1:102:A:GLU:H	2	0.27
(1,805)	1:101:A:THR:HG21	1:102:A:GLU:H	5	0.27
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD21	3	0.27
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD22	5	0.27
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	3	0.27
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	5	0.27
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	1	0.27
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB3	11	0.27
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	2	0.27
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB1	9	0.27
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB2	16	0.27
(1,616)	1:73:A:ALA:HB1	1:76:A:GLU:H	19	0.27
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	5	0.27
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	15	0.27
(1,441)	1:38:A:LEU:HD22	1:38:A:LEU:HA	17	0.27
(1,440)	1:38:A:LEU:H	1:38:A:LEU:HD11	7	0.27
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG23	3	0.27
(1,383)	1:23:A:LEU:HD22	1:33:A:ARG:HA	13	0.27
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD11	13	0.27
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	9	0.27
(1,193)	1:10:A:THR:HA	1:10:A:THR:HG21	16	0.27
(1,187)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	19	0.27
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	12	0.27
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB2	3	0.27
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	9	0.26
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	4	0.26
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	16	0.26
(2,1653)	1:32:A:MET:HE3	2:1001:A:OLA:H121	12	0.26
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	1	0.26
(2,1619)	2:1001:A:OLA:H141	1:84:A:ASP:HB3	8	0.26
(2,1591)	1:41:A:VAL:HG12	2:1001:A:OLA:H72	14	0.26
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1555)	1:96:A:ASP:H	1:94:A:LEU:HD22	10	0.26
(2,1544)	1:134:A:VAL:HG12	1:21:A:GLU:H	18	0.26
(2,1353)	1:45:A:PHE:H	1:58:A:MET:HE2	3	0.26
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB1	18	0.26
(2,1243)	1:134:A:VAL:H	1:135:A:SER:HB3	2	0.26
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	16	0.26
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	6	0.26
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	10	0.26
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	15	0.26
(2,1098)	1:132:A:LYS:HD3	1:131:A:TRP:HE1	18	0.26
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HB2	13	0.26
(2,1075)	1:94:A:LEU:HD21	1:93:A:ASP:H	1	0.26
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	14	0.26
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	4	0.26
(2,928)	1:88:A:HIS:HB2	1:90:A:ILE:H	20	0.26
(2,878)	1:132:A:LYS:HG3	1:132:A:LYS:H	15	0.26
(2,878)	1:132:A:LYS:HG3	1:132:A:LYS:H	19	0.26
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	8	0.26
(2,841)	1:129:A:MET:HE1	1:114:A:GLU:HG3	17	0.26
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	18	0.26
(2,787)	1:39:A:ALA:HB1	1:40:A:GLY:H	19	0.26
(2,785)	2:1001:A:OLA:H142	1:32:A:MET:HE3	20	0.26
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	1	0.26
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	9	0.26
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG23	18	0.26
(2,727)	1:3:A:LEU:HD23	1:7:A:PHE:HA	3	0.26
(2,697)	1:65:A:LYS:HE2	1:83:A:LEU:HA	3	0.26
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	10	0.26
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB2	19	0.26
(2,568)	1:114:A:GLU:HA	1:113:A:VAL:HG22	8	0.26
(2,567)	1:88:A:HIS:HB2	1:107:A:VAL:HG13	8	0.26
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG12	19	0.26
(2,500)	1:90:A:ILE:HD12	1:88:A:HIS:H	6	0.26
(2,498)	1:90:A:ILE:HD11	1:78:A:PHE:HD2	16	0.26
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG23	1	0.26
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	13	0.26
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	16	0.26
(2,479)	1:90:A:ILE:HG21	1:78:A:PHE:H	1	0.26
(2,479)	1:90:A:ILE:HG23	1:78:A:PHE:H	7	0.26
(2,479)	1:90:A:ILE:HG23	1:78:A:PHE:H	9	0.26
(2,420)	1:74:A:LEU:HD12	1:55:A:ARG:HA	3	0.26
(2,400)	1:83:A:LEU:HD11	1:65:A:LYS:HG2	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	7	0.26
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	9	0.26
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	11	0.26
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	20	0.26
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	10	0.26
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	2	0.26
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	4	0.26
(2,218)	1:23:A:LEU:HD23	1:23:A:LEU:HB2	5	0.26
(2,218)	1:23:A:LEU:HD22	1:23:A:LEU:HB2	8	0.26
(2,218)	1:23:A:LEU:HD22	1:23:A:LEU:HB2	11	0.26
(2,218)	1:23:A:LEU:HD22	1:23:A:LEU:HB2	13	0.26
(2,218)	1:23:A:LEU:HD23	1:23:A:LEU:HB2	15	0.26
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	17	0.26
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	19	0.26
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	8	0.26
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	4	0.26
(2,144)	1:124:A:TYR:HD2	1:141:A:LYS:HG3	7	0.26
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD11	20	0.26
(2,65)	1:12:A:LYS:HE2	1:12:A:LYS:HG3	17	0.26
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	6	0.26
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	19	0.26
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	4	0.26
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	4	0.26
(1,2839)	2:1001:A:OLA:H182	1:19:A:PHE:HE2	6	0.26
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG22	15	0.26
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	11	0.26
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	11	0.26
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	18	0.26
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	1	0.26
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	3	0.26
(1,2789)	2:1001:A:OLA:H181	1:36:A:ILE:HA	19	0.26
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG12	11	0.26
(1,2314)	1:81:A:GLU:H	1:87:A:GLN:HE21	8	0.26
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG21	10	0.26
(1,1603)	1:86:A:THR:HG22	1:86:A:THR:H	17	0.26
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	19	0.26
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	13	0.26
(1,1249)	1:3:A:LEU:HD23	1:3:A:LEU:H	17	0.26
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB2	9	0.26
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB1	13	0.26
(1,1223)	1:127:A:MET:HE2	1:116:A:TYR:HD1	9	0.26
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE2	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	2	0.26
(1,1112)	1:58:A:MET:HE2	1:43:A:LYS:HE3	20	0.26
(1,1111)	1:58:A:MET:HE3	1:43:A:LYS:HE2	3	0.26
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE1	19	0.26
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	7	0.26
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG21	3	0.26
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG21	17	0.26
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	14	0.26
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	2	0.26
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	12	0.26
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	3	0.26
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	18	0.26
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	20	0.26
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	9	0.26
(1,793)	1:100:A:LEU:HD12	1:118:A:TYR:HB3	19	0.26
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	20	0.26
(1,703)	1:24:A:LYS:HG2	1:21:A:GLU:HA	2	0.26
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD23	5	0.26
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB3	9	0.26
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	13	0.26
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	1	0.26
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	6	0.26
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	8	0.26
(1,441)	1:38:A:LEU:HD22	1:38:A:LEU:HA	8	0.26
(1,384)	1:36:A:ILE:HD12	1:33:A:ARG:HA	7	0.26
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	2	0.26
(1,130)	1:3:A:LEU:HD11	1:7:A:PHE:HB3	15	0.26
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB3	14	0.26
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB3	4	0.26
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	7	0.25
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	16	0.25
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	3	0.25
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	13	0.25
(2,1670)	2:1001:A:OLA:H183	2:1001:A:OLA:H21	10	0.25
(2,1660)	2:1001:A:OLA:H82	1:36:A:ILE:HA	16	0.25
(2,1652)	1:32:A:MET:HE1	2:1001:A:OLA:H131	4	0.25
(2,1652)	1:32:A:MET:HE2	2:1001:A:OLA:H131	15	0.25
(2,1647)	1:36:A:ILE:HD13	2:1001:A:OLA:H131	5	0.25
(2,1635)	2:1001:A:OLA:H81	1:62:A:THR:HG1	1	0.25
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	4	0.25
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	2	0.25
(2,1579)	1:41:A:VAL:HG12	2:1001:A:OLA:H21	4	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1478)	1:45:A:PHE:HD1	1:11:A:PHE:H	4	0.25
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD12	17	0.25
(2,1390)	1:54:A:ASP:H	1:53:A:PRO:HG3	2	0.25
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	19	0.25
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	20	0.25
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD12	6	0.25
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	4	0.25
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD11	19	0.25
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD12	2	0.25
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD12	7	0.25
(2,1079)	1:89:A:LYS:H	1:79:A:GLN:HB3	5	0.25
(2,1075)	1:94:A:LEU:HD23	1:93:A:ASP:H	12	0.25
(2,1029)	1:113:A:VAL:HG11	1:104:A:HIS:H	5	0.25
(2,1017)	1:8:A:LEU:HD11	1:9:A:GLY:H	19	0.25
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	20	0.25
(2,990)	1:132:A:LYS:HG3	1:132:A:LYS:H	2	0.25
(2,888)	1:59:A:GLU:HG2	1:68:A:HIS:HD2	19	0.25
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB1	20	0.25
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	10	0.25
(2,819)	1:36:A:ILE:HG21	2:1001:A:OLA:H82	8	0.25
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	13	0.25
(2,789)	1:26:A:ARG:HD3	1:131:A:TRP:HZ3	7	0.25
(2,760)	1:118:A:TYR:H	1:127:A:MET:HE2	6	0.25
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	15	0.25
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	8	0.25
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	3	0.25
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	11	0.25
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	3	0.25
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	2	0.25
(2,580)	1:111:A:THR:HG21	1:110:A:PRO:HG2	19	0.25
(2,535)	1:99:A:THR:HG22	1:95:A:LYS:HB3	8	0.25
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	20	0.25
(2,524)	1:95:A:LYS:H	1:95:A:LYS:HG3	7	0.25
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	2	0.25
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	6	0.25
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	20	0.25
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	13	0.25
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	14	0.25
(2,498)	1:90:A:ILE:HD12	1:78:A:PHE:HD2	11	0.25
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	11	0.25
(2,482)	1:90:A:ILE:HG22	1:78:A:PHE:HD1	5	0.25
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG23	15	0.25
(2,479)	1:90:A:ILE:HG22	1:78:A:PHE:H	16	0.25
(2,479)	1:90:A:ILE:HG22	1:78:A:PHE:H	20	0.25
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB2	11	0.25
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	20	0.25
(2,435)	1:104:A:HIS:HB2	1:82:A:ALA:HB1	7	0.25
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB1	1	0.25
(2,393)	1:105:A:ILE:HD12	1:89:A:LYS:HE2	11	0.25
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	20	0.25
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG21	20	0.25
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG21	12	0.25
(2,326)	1:140:A:TYR:HE2	1:43:A:LYS:HE3	16	0.25
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	3	0.25
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	5	0.25
(2,247)	1:26:A:ARG:HD2	1:26:A:ARG:H	11	0.25
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	19	0.25
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	19	0.25
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	16	0.25
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	19	0.25
(2,219)	1:23:A:LEU:HD23	1:36:A:ILE:HB	6	0.25
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	1	0.25
(2,218)	1:23:A:LEU:HD23	1:23:A:LEU:HB2	6	0.25
(2,218)	1:23:A:LEU:HD23	1:23:A:LEU:HB2	7	0.25
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	9	0.25
(2,218)	1:23:A:LEU:HD22	1:23:A:LEU:HB2	10	0.25
(2,218)	1:23:A:LEU:HD23	1:23:A:LEU:HB2	12	0.25
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	16	0.25
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	18	0.25
(2,218)	1:23:A:LEU:HD22	1:23:A:LEU:HB2	20	0.25
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG22	13	0.25
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	1	0.25
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	4	0.25
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	15	0.25
(2,158)	1:15:A:ARG:HA	1:13:A:LEU:HB3	2	0.25
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	18	0.25
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD22	19	0.25
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	4	0.25
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	18	0.25
(2,86)	1:125:A:LEU:HD11	1:45:A:PHE:HE1	12	0.25
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD23	7	0.25
(1,2819)	1:116:A:TYR:HD2	1:118:A:TYR:HH	19	0.25
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	8	0.25
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	14	0.25
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	16	0.25
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG12	2	0.25
(1,2692)	1:124:A:TYR:H	1:126:A:VAL:HG21	14	0.25
(1,2590)	1:6:A:LYS:HG2	1:7:A:PHE:H	3	0.25
(1,2559)	1:85:A:SER:H	1:65:A:LYS:HE2	16	0.25
(1,2497)	1:78:A:PHE:H	1:77:A:GLU:HG2	13	0.25
(1,2123)	1:82:A:ALA:H	1:81:A:GLU:HG3	9	0.25
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG23	8	0.25
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	7	0.25
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	18	0.25
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	8	0.25
(1,1386)	1:83:A:LEU:HD12	1:84:A:ASP:H	9	0.25
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	16	0.25
(1,1297)	1:8:A:LEU:HD23	1:8:A:LEU:H	20	0.25
(1,1222)	1:127:A:MET:HE1	1:118:A:TYR:HD1	14	0.25
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	12	0.25
(1,1171)	1:32:A:MET:HE3	1:33:A:ARG:H	10	0.25
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE3	1	0.25
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE1	16	0.25
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	1	0.25
(1,1064)	1:36:A:ILE:HD11	1:36:A:ILE:HA	8	0.25
(1,1064)	1:36:A:ILE:HD11	1:36:A:ILE:HA	16	0.25
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	15	0.25
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG21	6	0.25
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	7	0.25
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	13	0.25
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	6	0.25
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	18	0.25
(1,987)	1:135:A:SER:H	1:134:A:VAL:HG13	16	0.25
(1,854)	1:110:A:PRO:HB2	1:110:A:PRO:HD2	10	0.25
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD12	1	0.25
(1,785)	1:100:A:LEU:HD23	1:45:A:PHE:HE2	10	0.25
(1,771)	1:99:A:THR:H	1:99:A:THR:HG22	17	0.25
(1,729)	1:90:A:ILE:HD12	1:78:A:PHE:HZ	2	0.25
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	4	0.25
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	2	0.25
(1,678)	1:60:A:ASN:HB3	1:83:A:LEU:HD21	19	0.25
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB3	5	0.25
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	6	0.25
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB1	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	17	0.25
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD13	13	0.25
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	11	0.25
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	7	0.25
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	13	0.25
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	13	0.25
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	19	0.25
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD11	1	0.25
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	1	0.25
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	19	0.25
(1,227)	1:41:A:VAL:H	1:13:A:LEU:HD11	5	0.25
(1,193)	1:10:A:THR:HA	1:10:A:THR:HG22	5	0.25
(1,193)	1:10:A:THR:HA	1:10:A:THR:HG23	14	0.25
(1,187)	1:8:A:LEU:HD13	1:47:A:ASN:HD22	17	0.25
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB1	4	0.25
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB2	16	0.25
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	19	0.25
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	4	0.24
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	13	0.24
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	20	0.24
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	5	0.24
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	12	0.24
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	18	0.24
(2,1678)	1:10:A:THR:HG21	1:44:A:LYS:HG2	3	0.24
(2,1678)	1:10:A:THR:HG21	1:44:A:LYS:HG2	17	0.24
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	6	0.24
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H131	20	0.24
(2,1613)	1:102:A:GLU:HG3	1:118:A:TYR:HE2	18	0.24
(2,1568)	2:1001:A:OLA:H82	2:1001:A:OLA:H183	13	0.24
(2,1553)	1:136:A:THR:H	1:129:A:MET:HE1	6	0.24
(2,1540)	1:119:A:ARG:HG2	1:100:A:LEU:H	8	0.24
(2,1475)	1:65:A:LYS:H	1:83:A:LEU:HD11	1	0.24
(2,1466)	1:98:A:ASN:H	1:94:A:LEU:HG	16	0.24
(2,1411)	1:13:A:LEU:H	1:143:A:GLN:HE22	14	0.24
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	17	0.24
(2,1279)	1:80:A:ASP:H	1:89:A:LYS:HB3	14	0.24
(2,1243)	1:134:A:VAL:H	1:130:A:SER:HB2	15	0.24
(2,1153)	1:80:A:ASP:H	1:88:A:HIS:HB3	12	0.24
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD11	14	0.24
(2,1080)	1:102:A:GLU:H	1:92:A:PHE:HD2	17	0.24
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	17	0.24
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD22	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,930)	1:134:A:VAL:H	1:25:A:ALA:HB3	17	0.24
(2,878)	1:132:A:LYS:HG3	1:132:A:LYS:H	20	0.24
(2,875)	1:-5:A:HIS:HA	1:-5:A:HIS:HB2	3	0.24
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	4	0.24
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	10	0.24
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	14	0.24
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	17	0.24
(2,849)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	18	0.24
(2,808)	1:78:A:PHE:H	1:77:A:GLU:HG2	14	0.24
(2,805)	1:-1:A:GLY:HA2	1:0:A:SER:HA	7	0.24
(2,787)	1:39:A:ALA:HB1	1:40:A:GLY:H	15	0.24
(2,782)	1:127:A:MET:HE3	1:116:A:TYR:HA	7	0.24
(2,759)	1:32:A:MET:HE1	2:1001:A:OLA:H121	9	0.24
(2,751)	1:104:A:HIS:HE1	1:82:A:ALA:HB1	16	0.24
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	11	0.24
(2,750)	1:104:A:HIS:HB3	1:104:A:HIS:HE1	16	0.24
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	9	0.24
(2,694)	1:141:A:LYS:H	1:141:A:LYS:HE3	1	0.24
(2,632)	1:128:A:LYS:HE3	1:128:A:LYS:HB3	11	0.24
(2,632)	1:128:A:LYS:HB3	1:128:A:LYS:HE2	19	0.24
(2,603)	1:124:A:TYR:HE2	1:141:A:LYS:HE3	18	0.24
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG23	3	0.24
(2,551)	1:114:A:GLU:H	1:103:A:THR:HG22	3	0.24
(2,544)	1:100:A:LEU:HD21	1:94:A:LEU:HB2	3	0.24
(2,544)	1:100:A:LEU:HD21	1:58:A:MET:HG3	11	0.24
(2,534)	1:99:A:THR:HG21	1:95:A:LYS:HD3	15	0.24
(2,528)	1:141:A:LYS:HE2	1:141:A:LYS:HA	8	0.24
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	2	0.24
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG22	3	0.24
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG22	8	0.24
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	9	0.24
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	5	0.24
(2,479)	1:90:A:ILE:H	1:90:A:ILE:HG23	4	0.24
(2,479)	1:90:A:ILE:HG23	1:78:A:PHE:H	11	0.24
(2,479)	1:90:A:ILE:HG23	1:78:A:PHE:H	18	0.24
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB2	5	0.24
(2,400)	1:83:A:LEU:HD12	1:65:A:LYS:HG2	7	0.24
(2,392)	1:1:A:LYS:HE2	1:1:A:LYS:HA	1	0.24
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	5	0.24
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	16	0.24
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	8	0.24
(2,249)	1:26:A:ARG:HD2	1:131:A:TRP:HZ2	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,247)	1:26:A:ARG:HD2	1:26:A:ARG:H	18	0.24
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	1	0.24
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	4	0.24
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	9	0.24
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	16	0.24
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	8	0.24
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	11	0.24
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	14	0.24
(2,218)	1:23:A:LEU:HD21	1:23:A:LEU:HB2	3	0.24
(2,218)	1:23:A:LEU:HD23	1:23:A:LEU:HB2	14	0.24
(2,213)	1:23:A:LEU:HD21	1:19:A:PHE:HD2	5	0.24
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	4	0.24
(2,158)	1:41:A:VAL:HA	1:13:A:LEU:HB3	16	0.24
(2,155)	1:12:A:LYS:HE2	1:12:A:LYS:HA	8	0.24
(2,155)	1:12:A:LYS:HE2	1:12:A:LYS:HA	17	0.24
(2,153)	1:12:A:LYS:H	1:12:A:LYS:HD3	10	0.24
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	8	0.24
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	13	0.24
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	18	0.24
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD21	20	0.24
(2,85)	1:125:A:LEU:HD11	1:118:A:TYR:HE1	13	0.24
(2,84)	1:3:A:LEU:HD22	1:7:A:PHE:H	16	0.24
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	14	0.24
(1,2813)	1:127:A:MET:HE3	1:118:A:TYR:HH	4	0.24
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	1	0.24
(1,2789)	2:1001:A:OLA:H183	1:36:A:ILE:HA	5	0.24
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG11	12	0.24
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG11	14	0.24
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG11	18	0.24
(1,2325)	1:90:A:ILE:H	1:77:A:GLU:HG2	18	0.24
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	15	0.24
(1,2132)	1:69:A:HIS:H	1:68:A:HIS:HD2	8	0.24
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	11	0.24
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	11	0.24
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	12	0.24
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	17	0.24
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	7	0.24
(1,1603)	1:86:A:THR:HG21	1:86:A:THR:H	8	0.24
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	16	0.24
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	2	0.24
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	11	0.24
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	20	0.24
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD13	13	0.24
(1,1262)	1:100:A:LEU:HD23	1:101:A:THR:H	13	0.24
(1,1233)	1:15:A:ARG:HG2	1:139:A:TYR:H	9	0.24
(1,1231)	1:72:A:TRP:HZ3	1:74:A:LEU:HD23	9	0.24
(1,1228)	1:139:A:TYR:HE2	1:126:A:VAL:HG23	2	0.24
(1,1225)	1:127:A:MET:HE2	1:128:A:LYS:H	13	0.24
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	3	0.24
(1,1222)	1:127:A:MET:HE3	1:118:A:TYR:HD1	12	0.24
(1,1194)	1:139:A:TYR:HE2	1:126:A:VAL:HG23	2	0.24
(1,1168)	1:32:A:MET:HE2	1:35:A:VAL:H	20	0.24
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE3	20	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	1	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	2	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	3	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	4	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	5	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	6	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	7	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	8	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	9	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	10	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	11	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	13	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	14	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	16	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	17	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	18	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	19	0.24
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	20	0.24
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	3	0.24
(1,1064)	1:36:A:ILE:HD11	1:36:A:ILE:HA	6	0.24
(1,1064)	1:36:A:ILE:HD11	1:36:A:ILE:HA	14	0.24
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	5	0.24
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	12	0.24
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	16	0.24
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	18	0.24
(1,992)	1:135:A:SER:H	1:135:A:SER:HB3	11	0.24
(1,932)	1:137:A:SER:HA	1:126:A:VAL:HG13	9	0.24
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG22	18	0.24
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	15	0.24
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:101:A:THR:HG21	1:95:A:LYS:HB3	6	0.24
(1,752)	1:94:A:LEU:HD12	1:7:A:PHE:HD2	12	0.24
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	16	0.24
(1,678)	1:60:A:ASN:HB3	1:83:A:LEU:HD21	8	0.24
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	1	0.24
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB2	4	0.24
(1,616)	1:73:A:ALA:HB1	1:76:A:GLU:H	11	0.24
(1,616)	1:73:A:ALA:HB3	1:76:A:GLU:H	13	0.24
(1,616)	1:73:A:ALA:HB2	1:76:A:GLU:H	17	0.24
(1,310)	1:25:A:ALA:HB3	1:134:A:VAL:HB	1	0.24
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	14	0.24
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB2	16	0.24
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB2	2	0.24
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB2	8	0.24
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB1	7	0.24
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB1	19	0.24
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG22	6	0.24
(1,7)	1:106:A:LYS:H	1:105:A:ILE:HG23	2	0.24
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	3	0.23
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	5	0.23
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	12	0.23
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	18	0.23
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	2	0.23
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	6	0.23
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	15	0.23
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	17	0.23
(2,1679)	2:1001:A:OLA:H62	1:36:A:ILE:HG21	18	0.23
(2,1665)	1:22:A:TYR:HD1	2:1001:A:OLA:H182	17	0.23
(2,1652)	1:32:A:MET:HE2	2:1001:A:OLA:H131	8	0.23
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	2	0.23
(2,1619)	2:1001:A:OLA:H141	1:84:A:ASP:HB3	14	0.23
(2,1617)	1:36:A:ILE:HA	2:1001:A:OLA:H71	19	0.23
(2,1614)	1:64:A:LYS:H	2:1001:A:OLA:H81	5	0.23
(2,1591)	1:41:A:VAL:HG12	2:1001:A:OLA:H72	12	0.23
(2,1544)	1:134:A:VAL:HG13	1:21:A:GLU:H	2	0.23
(2,1544)	1:134:A:VAL:HG13	1:21:A:GLU:H	10	0.23
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	16	0.23
(2,1520)	1:126:A:VAL:HG21	1:119:A:ARG:H	10	0.23
(2,1432)	1:34:A:GLN:HE22	1:35:A:VAL:H	1	0.23
(2,1411)	1:13:A:LEU:H	1:143:A:GLN:HE22	3	0.23
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	1	0.23
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	17	0.23
(2,1376)	1:59:A:GLU:H	1:61:A:LEU:HD12	12	0.23
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	2	0.23
(2,1332)	1:75:A:GLY:H	1:74:A:LEU:HD22	3	0.23
(2,1232)	1:65:A:LYS:HB3	1:85:A:SER:H	4	0.23
(2,1222)	1:118:A:TYR:HD1	1:119:A:ARG:H	16	0.23
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	13	0.23
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD11	10	0.23
(2,1112)	1:143:A:GLN:HE21	1:61:A:LEU:HD11	5	0.23
(2,1102)	1:58:A:MET:H	1:70:A:LYS:HG2	6	0.23
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD21	11	0.23
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	11	0.23
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	8	0.23
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	15	0.23
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	16	0.23
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG11	9	0.23
(2,917)	1:86:A:THR:H	1:82:A:ALA:HB3	7	0.23
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	12	0.23
(2,837)	1:58:A:MET:HE1	1:60:A:ASN:HD21	7	0.23
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	13	0.23
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	17	0.23
(2,837)	1:58:A:MET:HE1	1:60:A:ASN:HD21	18	0.23
(2,835)	1:20:A:ASP:HA	1:37:A:LYS:HE2	3	0.23
(2,820)	1:41:A:VAL:HG21	1:43:A:LYS:HE2	20	0.23
(2,785)	1:32:A:MET:HE1	2:1001:A:OLA:H131	4	0.23
(2,759)	1:32:A:MET:HE2	2:1001:A:OLA:H121	18	0.23
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	5	0.23
(2,750)	1:104:A:HIS:HB2	1:104:A:HIS:HE1	8	0.23
(2,737)	1:30:A:TRP:HH2	1:31:A:ILE:HG23	11	0.23
(2,720)	1:124:A:TYR:HE2	1:141:A:LYS:H	11	0.23
(2,718)	1:73:A:ALA:HB1	1:0:A:SER:HA	10	0.23
(2,692)	1:142:A:LYS:H	1:141:A:LYS:HD2	18	0.23
(2,684)	1:125:A:LEU:HD13	1:140:A:TYR:HE2	7	0.23
(2,683)	1:41:A:VAL:HG23	1:140:A:TYR:HE1	1	0.23
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	6	0.23
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	10	0.23
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	12	0.23
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	17	0.23
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB3	2	0.23
(2,632)	1:128:A:LYS:HB3	1:128:A:LYS:HE2	2	0.23
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	9	0.23
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG23	2	0.23
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD12	1	0.23
(2,543)	1:100:A:LEU:HD21	1:74:A:LEU:HB2	10	0.23
(2,541)	1:100:A:LEU:HD22	1:118:A:TYR:HB2	20	0.23
(2,533)	1:95:A:LYS:HE2	1:99:A:THR:HG23	3	0.23
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG22	3	0.23
(2,518)	1:95:A:LYS:H	1:94:A:LEU:HD12	17	0.23
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD22	9	0.23
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	19	0.23
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	10	0.23
(2,433)	1:85:A:SER:H	1:81:A:GLU:HG2	7	0.23
(2,392)	1:64:A:LYS:HA	1:64:A:LYS:HE2	17	0.23
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	12	0.23
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	6	0.23
(2,250)	1:26:A:ARG:HD2	1:131:A:TRP:HD1	1	0.23
(2,228)	1:25:A:ALA:HB2	1:26:A:ARG:HA	14	0.23
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	20	0.23
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD2	1	0.23
(2,209)	1:23:A:LEU:HD12	1:36:A:ILE:HG22	1	0.23
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG22	8	0.23
(2,188)	1:134:A:VAL:HG11	1:21:A:GLU:HG2	5	0.23
(2,178)	1:134:A:VAL:HG12	1:18:A:ASN:HB2	1	0.23
(2,149)	1:12:A:LYS:HB3	1:13:A:LEU:HA	8	0.23
(2,144)	1:124:A:TYR:HD2	1:141:A:LYS:HG3	13	0.23
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	7	0.23
(2,84)	1:3:A:LEU:HD21	1:7:A:PHE:H	2	0.23
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	18	0.23
(2,65)	1:12:A:LYS:HE3	1:12:A:LYS:HG3	19	0.23
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	5	0.23
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	12	0.23
(2,58)	1:0:A:SER:HB3	1:74:A:LEU:HD21	6	0.23
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	8	0.23
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	15	0.23
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	20	0.23
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	1	0.23
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG23	10	0.23
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	7	0.23
(1,2789)	2:1001:A:OLA:H181	1:36:A:ILE:HA	9	0.23
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	3	0.23
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	17	0.23
(1,2413)	1:23:A:LEU:HD22	1:33:A:ARG:H	1	0.23
(1,2314)	1:81:A:GLU:H	1:87:A:GLN:HE21	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	1	0.23
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG21	20	0.23
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG21	9	0.23
(1,2000)	1:8:A:LEU:HD21	1:47:A:ASN:HD21	14	0.23
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	2	0.23
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	1	0.23
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	12	0.23
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	13	0.23
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	16	0.23
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	17	0.23
(1,1516)	1:79:A:GLN:HG2	1:79:A:GLN:HE22	18	0.23
(1,1456)	1:103:A:THR:HG22	1:104:A:HIS:H	9	0.23
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG13	19	0.23
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	6	0.23
(1,1361)	1:70:A:LYS:HE3	1:68:A:HIS:HD2	17	0.23
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD13	9	0.23
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	14	0.23
(1,1173)	1:125:A:LEU:HD23	1:120:A:ARG:HD3	4	0.23
(1,1171)	1:32:A:MET:HE3	1:33:A:ARG:H	6	0.23
(1,1171)	1:32:A:MET:HE2	1:33:A:ARG:H	20	0.23
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE3	9	0.23
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE3	9	0.23
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	12	0.23
(1,1125)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	15	0.23
(1,1104)	1:58:A:MET:HE3	1:118:A:TYR:HE2	13	0.23
(1,1064)	1:36:A:ILE:HD11	1:36:A:ILE:HA	4	0.23
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	12	0.23
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	2	0.23
(1,968)	1:130:A:SER:HB2	1:131:A:TRP:H	2	0.23
(1,952)	1:129:A:MET:HB2	1:136:A:THR:HG22	13	0.23
(1,925)	1:125:A:LEU:HD21	1:7:A:PHE:HA	14	0.23
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG23	7	0.23
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG22	16	0.23
(1,843)	1:108:A:ASP:HB2	1:108:A:ASP:H	4	0.23
(1,843)	1:108:A:ASP:HB2	1:108:A:ASP:H	6	0.23
(1,843)	1:108:A:ASP:HB2	1:108:A:ASP:H	20	0.23
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG23	13	0.23
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	8	0.23
(1,729)	1:90:A:ILE:HD13	1:78:A:PHE:HZ	16	0.23
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG21	2	0.23
(1,687)	1:86:A:THR:HG23	1:87:A:GLN:H	16	0.23
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB3	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB1	8	0.23
(1,616)	1:73:A:ALA:HB2	1:76:A:GLU:H	4	0.23
(1,616)	1:73:A:ALA:HB3	1:76:A:GLU:H	9	0.23
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	18	0.23
(1,524)	1:66:A:ASP:HB2	1:66:A:ASP:H	2	0.23
(1,466)	1:44:A:LYS:HE3	1:44:A:LYS:HB3	17	0.23
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD11	18	0.23
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD13	4	0.23
(1,310)	1:25:A:ALA:HB1	1:134:A:VAL:HB	15	0.23
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	8	0.23
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB2	14	0.23
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG23	15	0.23
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	6	0.22
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	15	0.22
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	10	0.22
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	11	0.22
(2,1679)	2:1001:A:OLA:H61	1:36:A:ILE:HG21	11	0.22
(2,1653)	1:32:A:MET:HE1	2:1001:A:OLA:H121	9	0.22
(2,1652)	1:32:A:MET:HE2	2:1001:A:OLA:H131	19	0.22
(2,1646)	1:36:A:ILE:HD11	2:1001:A:OLA:H82	7	0.22
(2,1644)	2:1001:A:OLA:H82	2:1001:A:OLA:H9	9	0.22
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	1	0.22
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	11	0.22
(2,1636)	1:65:A:LYS:HG2	1:62:A:THR:HG1	6	0.22
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	2	0.22
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	19	0.22
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	7	0.22
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	15	0.22
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	20	0.22
(2,1553)	1:136:A:THR:H	1:128:A:LYS:HG2	19	0.22
(2,1544)	1:134:A:VAL:HG11	1:21:A:GLU:H	16	0.22
(2,1471)	1:101:A:THR:HG23	1:93:A:ASP:H	5	0.22
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	10	0.22
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	11	0.22
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	10	0.22
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	15	0.22
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	9	0.22
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	12	0.22
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	15	0.22
(2,1168)	1:56:A:TYR:H	1:55:A:ARG:HD2	4	0.22
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	14	0.22
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1125)	1:118:A:TYR:H	1:119:A:ARG:HG2	15	0.22
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	18	0.22
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	5	0.22
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	8	0.22
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	11	0.22
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	16	0.22
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD21	3	0.22
(2,928)	1:90:A:ILE:H	1:89:A:LYS:HE3	15	0.22
(2,928)	1:104:A:HIS:HB3	1:90:A:ILE:H	17	0.22
(2,888)	1:59:A:GLU:HG3	1:68:A:HIS:HD2	5	0.22
(2,888)	1:59:A:GLU:HG2	1:68:A:HIS:HD2	8	0.22
(2,878)	1:132:A:LYS:HG3	1:132:A:LYS:H	11	0.22
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	9	0.22
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	15	0.22
(2,837)	1:58:A:MET:HE1	1:60:A:ASN:HD21	3	0.22
(2,837)	1:58:A:MET:HE3	1:60:A:ASN:HD21	8	0.22
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	11	0.22
(2,814)	1:60:A:ASN:HD21	1:83:A:LEU:HD23	3	0.22
(2,811)	1:89:A:LYS:HE3	1:89:A:LYS:H	20	0.22
(2,803)	1:-5:A:HIS:HA	1:-2:A:HIS:HB2	12	0.22
(2,785)	1:32:A:MET:HE2	2:1001:A:OLA:H131	15	0.22
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD21	12	0.22
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	12	0.22
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	2	0.22
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	16	0.22
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	20	0.22
(2,661)	1:128:A:LYS:HE3	1:135:A:SER:HB2	1	0.22
(2,661)	1:128:A:LYS:HE2	1:135:A:SER:HB2	18	0.22
(2,612)	1:125:A:LEU:HD21	1:125:A:LEU:HB3	16	0.22
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	19	0.22
(2,609)	1:11:A:PHE:HD2	1:125:A:LEU:HG	4	0.22
(2,596)	1:100:A:LEU:HG	1:118:A:TYR:HD2	2	0.22
(2,580)	1:111:A:THR:HG22	1:110:A:PRO:HG2	14	0.22
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD13	19	0.22
(2,555)	1:89:A:LYS:HE3	1:105:A:ILE:HG21	3	0.22
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	16	0.22
(2,551)	1:114:A:GLU:H	1:103:A:THR:HG22	10	0.22
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG21	4	0.22
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	18	0.22
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	7	0.22
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	20	0.22
(2,500)	1:90:A:ILE:HD13	1:88:A:HIS:H	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,498)	1:90:A:ILE:HD13	1:78:A:PHE:HD2	12	0.22
(2,482)	1:90:A:ILE:HG22	1:78:A:PHE:HD1	20	0.22
(2,481)	1:88:A:HIS:HE1	1:90:A:ILE:HG21	19	0.22
(2,473)	1:87:A:GLN:HA	1:88:A:HIS:HB3	10	0.22
(2,457)	1:86:A:THR:HB	1:87:A:GLN:HG2	8	0.22
(2,422)	1:74:A:LEU:HD11	1:4:A:PRO:HD2	17	0.22
(2,405)	1:66:A:ASP:HA	1:61:A:LEU:HB2	7	0.22
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG22	10	0.22
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG2	12	0.22
(2,319)	1:42:A:THR:HB	1:61:A:LEU:HD11	6	0.22
(2,299)	1:37:A:LYS:HG3	1:38:A:LEU:HD21	11	0.22
(2,267)	1:32:A:MET:HG2	1:31:A:ILE:HG21	18	0.22
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	2	0.22
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	8	0.22
(2,231)	1:25:A:ALA:HB1	1:134:A:VAL:HG21	10	0.22
(2,228)	1:25:A:ALA:HB3	1:26:A:ARG:HA	20	0.22
(2,226)	1:134:A:VAL:HG21	1:25:A:ALA:HA	20	0.22
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	6	0.22
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	10	0.22
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD2	13	0.22
(2,212)	1:23:A:LEU:HD23	1:26:A:ARG:H	12	0.22
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	16	0.22
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	15	0.22
(2,144)	1:126:A:VAL:HG22	1:124:A:TYR:HD2	6	0.22
(2,132)	1:85:A:SER:H	1:65:A:LYS:HE2	3	0.22
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	1	0.22
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG23	20	0.22
(2,119)	1:8:A:LEU:HD13	1:9:A:GLY:H	4	0.22
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD23	6	0.22
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	3	0.22
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD3	10	0.22
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	17	0.22
(2,65)	1:1:A:LYS:HG2	1:1:A:LYS:HE3	20	0.22
(2,23)	1:34:A:GLN:HG3	1:30:A:TRP:HZ2	15	0.22
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG23	1	0.22
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	3	0.22
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	13	0.22
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	20	0.22
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	1	0.22
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	2	0.22
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	6	0.22
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	18	0.22
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	16	0.22
(1,2836)	2:1001:A:OLA:H181	1:36:A:ILE:HD12	13	0.22
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	4	0.22
(1,2813)	1:127:A:MET:HE1	1:118:A:TYR:HH	9	0.22
(1,2809)	2:1001:A:OLA:H181	1:36:A:ILE:HD12	13	0.22
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H181	15	0.22
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	1	0.22
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	5	0.22
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	8	0.22
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	15	0.22
(1,2489)	1:13:A:LEU:HD22	1:17:A:GLU:H	6	0.22
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	8	0.22
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG23	17	0.22
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	1	0.22
(1,1981)	1:8:A:LEU:HD22	1:47:A:ASN:H	13	0.22
(1,1603)	1:86:A:THR:HG21	1:86:A:THR:H	11	0.22
(1,1480)	1:119:A:ARG:HA	1:119:A:ARG:HG2	15	0.22
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG13	15	0.22
(1,1366)	1:140:A:TYR:HH	1:43:A:LYS:HD2	15	0.22
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD11	3	0.22
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD13	7	0.22
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	8	0.22
(1,1249)	1:3:A:LEU:HD21	1:3:A:LEU:H	8	0.22
(1,1249)	1:3:A:LEU:HD22	1:3:A:LEU:H	14	0.22
(1,1222)	1:127:A:MET:HE1	1:118:A:TYR:HD1	2	0.22
(1,1183)	1:35:A:VAL:HB	1:32:A:MET:HE1	15	0.22
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	14	0.22
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE3	14	0.22
(1,1064)	1:36:A:ILE:HD12	1:36:A:ILE:HA	2	0.22
(1,1064)	1:36:A:ILE:HD12	1:36:A:ILE:HA	17	0.22
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	6	0.22
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	11	0.22
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG11	1	0.22
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG21	20	0.22
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	5	0.22
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	11	0.22
(1,752)	1:94:A:LEU:HD13	1:7:A:PHE:HD2	9	0.22
(1,678)	1:60:A:ASN:HB3	1:83:A:LEU:HD23	10	0.22
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	10	0.22
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB2	20	0.22
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB2	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB3	1	0.22
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB3	13	0.22
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	1	0.22
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	8	0.22
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	10	0.22
(1,446)	1:49:A:ALA:HB1	1:49:A:ALA:H	4	0.22
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD11	9	0.22
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD12	14	0.22
(1,378)	1:32:A:MET:HG2	1:32:A:MET:HE1	18	0.22
(1,310)	1:25:A:ALA:HB3	1:134:A:VAL:HB	9	0.22
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	6	0.22
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	15	0.22
(1,288)	1:23:A:LEU:HD23	1:33:A:ARG:HA	5	0.22
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB3	6	0.22
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB2	9	0.22
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	20	0.22
(1,17)	1:31:A:ILE:HD11	1:31:A:ILE:HA	11	0.22
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG23	13	0.22
(1,4)	1:112:A:ASP:H	1:105:A:ILE:HG23	3	0.22
(3,43)	1:55:A:ARG:H	1:53:A:PRO:O	18	0.21
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	11	0.21
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	17	0.21
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	19	0.21
(2,1678)	1:10:A:THR:HG22	1:44:A:LYS:HG2	12	0.21
(2,1674)	1:120:A:ARG:HB2	1:120:A:ARG:HG3	17	0.21
(2,1664)	1:88:A:HIS:HD2	1:86:A:THR:HG22	14	0.21
(2,1658)	1:19:A:PHE:HE1	2:1001:A:OLA:H21	20	0.21
(2,1654)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	19	0.21
(2,1653)	1:32:A:MET:HE2	2:1001:A:OLA:H121	18	0.21
(2,1651)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	7	0.21
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	3	0.21
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	4	0.21
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	7	0.21
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	13	0.21
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	2	0.21
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	9	0.21
(2,1619)	2:1001:A:OLA:H142	1:84:A:ASP:HB3	12	0.21
(2,1583)	1:41:A:VAL:HG23	2:1001:A:OLA:H22	1	0.21
(2,1520)	1:126:A:VAL:HG21	1:119:A:ARG:H	1	0.21
(2,1495)	1:13:A:LEU:H	1:42:A:THR:HG22	11	0.21
(2,1471)	1:102:A:GLU:HG3	1:93:A:ASP:H	16	0.21
(2,1411)	1:13:A:LEU:H	1:143:A:GLN:HE22	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	11	0.21
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	6	0.21
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	17	0.21
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	18	0.21
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	4	0.21
(2,1102)	1:58:A:MET:H	1:70:A:LYS:HG2	9	0.21
(2,1080)	1:102:A:GLU:H	1:92:A:PHE:HD2	11	0.21
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	6	0.21
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG11	19	0.21
(2,925)	1:65:A:LYS:HG3	1:67:A:THR:H	1	0.21
(2,880)	1:128:A:LYS:HE3	1:128:A:LYS:HB2	5	0.21
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	2	0.21
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	18	0.21
(2,875)	1:-5:A:HIS:HA	1:-5:A:HIS:HB2	20	0.21
(2,810)	1:52:A:LYS:HE2	1:50:A:SER:HB3	1	0.21
(2,803)	1:-2:A:HIS:HB2	1:1:A:LYS:HA	8	0.21
(2,803)	1:-5:A:HIS:HA	1:-2:A:HIS:HB2	15	0.21
(2,778)	1:119:A:ARG:HD3	1:99:A:THR:HA	2	0.21
(2,759)	1:32:A:MET:HE1	2:1001:A:OLA:H121	5	0.21
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD13	1	0.21
(2,743)	1:104:A:HIS:HD2	1:105:A:ILE:HG13	19	0.21
(2,728)	1:143:A:GLN:H	1:10:A:THR:HG21	10	0.21
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	6	0.21
(2,684)	1:125:A:LEU:HD11	1:140:A:TYR:HE2	10	0.21
(2,684)	1:125:A:LEU:HD11	1:140:A:TYR:HE2	19	0.21
(2,683)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	14	0.21
(2,680)	1:140:A:TYR:HE2	2:1001:A:OLA:H22	11	0.21
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	19	0.21
(2,675)	1:126:A:VAL:HA	1:139:A:TYR:HE2	9	0.21
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB3	14	0.21
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB2	15	0.21
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB2	18	0.21
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE2	3	0.21
(2,633)	1:128:A:LYS:H	1:128:A:LYS:HD2	17	0.21
(2,624)	1:119:A:ARG:HG2	1:126:A:VAL:HG12	20	0.21
(2,623)	1:128:A:LYS:HE2	1:126:A:VAL:HG11	1	0.21
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG12	5	0.21
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD11	7	0.21
(2,552)	1:105:A:ILE:H	1:103:A:THR:HG21	13	0.21
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG22	2	0.21
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	9	0.21
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,496)	1:90:A:ILE:HD13	1:69:A:HIS:HA	7	0.21
(2,495)	1:90:A:ILE:HD12	1:82:A:ALA:HA	9	0.21
(2,487)	1:90:A:ILE:HG21	1:92:A:PHE:HB2	1	0.21
(2,395)	1:85:A:SER:HA	1:65:A:LYS:HE3	10	0.21
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	11	0.21
(2,250)	1:26:A:ARG:HD2	1:131:A:TRP:HD1	15	0.21
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	13	0.21
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD2	20	0.21
(2,209)	1:23:A:LEU:HD12	1:36:A:ILE:HG22	16	0.21
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	15	0.21
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	7	0.21
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	14	0.21
(2,100)	1:8:A:LEU:HD13	1:5:A:ASP:HB3	13	0.21
(2,98)	1:8:A:LEU:HD22	1:5:A:ASP:HA	6	0.21
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	7	0.21
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	2	0.21
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD3	1	0.21
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD2	3	0.21
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD3	12	0.21
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	13	0.21
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	14	0.21
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	16	0.21
(2,53)	1:33:A:ARG:HD3	1:30:A:TRP:HA	6	0.21
(1,2839)	2:1001:A:OLA:H182	1:19:A:PHE:HE1	5	0.21
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	5	0.21
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	14	0.21
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	16	0.21
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG22	17	0.21
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	1	0.21
(1,2789)	2:1001:A:OLA:H182	1:36:A:ILE:HA	18	0.21
(1,2762)	1:36:A:ILE:H	1:35:A:VAL:HG12	18	0.21
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	5	0.21
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	6	0.21
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	5	0.21
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	9	0.21
(1,2243)	1:23:A:LEU:HD22	1:37:A:LYS:H	16	0.21
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG22	18	0.21
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG23	16	0.21
(1,1981)	1:8:A:LEU:HD23	1:47:A:ASN:H	14	0.21
(1,1972)	1:21:A:GLU:H	1:21:A:GLU:HG2	8	0.21
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	8	0.21
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1762)	1:8:A:LEU:HD13	1:47:A:ASN:HD21	2	0.21
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	12	0.21
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	18	0.21
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	18	0.21
(1,1259)	1:125:A:LEU:HA	1:125:A:LEU:HD11	14	0.21
(1,1171)	1:32:A:MET:HE3	1:33:A:ARG:H	13	0.21
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	19	0.21
(1,1168)	1:32:A:MET:HE3	1:35:A:VAL:H	10	0.21
(1,1108)	1:58:A:MET:HE3	1:43:A:LYS:HA	14	0.21
(1,1064)	1:36:A:ILE:HD12	1:36:A:ILE:HA	19	0.21
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG23	12	0.21
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	8	0.21
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG13	13	0.21
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG11	15	0.21
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG11	16	0.21
(1,923)	1:125:A:LEU:HD22	1:118:A:TYR:HB2	17	0.21
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	3	0.21
(1,843)	1:108:A:ASP:HB2	1:108:A:ASP:H	14	0.21
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	6	0.21
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG23	10	0.21
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG23	14	0.21
(1,805)	1:101:A:THR:HG22	1:102:A:GLU:H	11	0.21
(1,793)	1:100:A:LEU:HD13	1:118:A:TYR:HB3	3	0.21
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	2	0.21
(1,785)	1:100:A:LEU:HD23	1:45:A:PHE:HE2	5	0.21
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG23	11	0.21
(1,771)	1:99:A:THR:H	1:99:A:THR:HG23	6	0.21
(1,719)	1:90:A:ILE:HG22	1:104:A:HIS:HD2	7	0.21
(1,678)	1:60:A:ASN:HB3	1:83:A:LEU:HD23	15	0.21
(1,676)	1:83:A:LEU:HA	1:83:A:LEU:HD21	17	0.21
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD13	8	0.21
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD12	18	0.21
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB1	19	0.21
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	15	0.21
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	3	0.21
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	2	0.21
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD13	15	0.21
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD12	16	0.21
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD12	20	0.21
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD12	7	0.21
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	10	0.21
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	16	0.21
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	1	0.21
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB1	3	0.21
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	12	0.21
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB2	19	0.21
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB1	10	0.21
(1,17)	1:31:A:ILE:HD11	1:31:A:ILE:HA	7	0.21
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD11	18	0.21
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG23	17	0.21
(3,89)	1:117:A:GLU:H	1:128:A:LYS:O	16	0.2
(3,31)	1:12:A:LYS:H	1:142:A:LYS:O	1	0.2
(2,1671)	1:24:A:LYS:HB3	1:24:A:LYS:HG2	8	0.2
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	6	0.2
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	18	0.2
(2,1626)	2:1001:A:OLA:H22	1:19:A:PHE:HE1	14	0.2
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	8	0.2
(2,1619)	2:1001:A:OLA:H142	1:84:A:ASP:HB3	3	0.2
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	11	0.2
(2,1542)	1:23:A:LEU:HB3	1:33:A:ARG:H	9	0.2
(2,1539)	1:125:A:LEU:HA	1:120:A:ARG:H	4	0.2
(2,1480)	1:71:A:ASP:H	1:55:A:ARG:HG3	15	0.2
(2,1471)	1:102:A:GLU:HG3	1:93:A:ASP:H	10	0.2
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	6	0.2
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	7	0.2
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	12	0.2
(2,1193)	1:42:A:THR:HG22	1:61:A:LEU:H	12	0.2
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	12	0.2
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD12	17	0.2
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	16	0.2
(2,1168)	1:56:A:TYR:H	1:55:A:ARG:HD2	11	0.2
(2,1164)	1:64:A:LYS:HG2	1:39:A:ALA:H	1	0.2
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	18	0.2
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	9	0.2
(2,1029)	1:113:A:VAL:HG13	1:104:A:HIS:H	3	0.2
(2,1018)	1:68:A:HIS:H	1:61:A:LEU:HD22	16	0.2
(2,1010)	1:114:A:GLU:H	1:113:A:VAL:HG12	9	0.2
(2,990)	1:132:A:LYS:HG3	1:132:A:LYS:H	15	0.2
(2,982)	1:26:A:ARG:HB3	1:131:A:TRP:HE1	5	0.2
(2,979)	1:132:A:LYS:HG3	1:131:A:TRP:HE1	2	0.2
(2,930)	1:134:A:VAL:H	1:25:A:ALA:HB1	6	0.2
(2,929)	1:116:A:TYR:H	1:129:A:MET:HB2	2	0.2
(2,880)	1:128:A:LYS:HE2	1:128:A:LYS:HB2	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	1	0.2
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	5	0.2
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	4	0.2
(2,810)	1:52:A:LYS:HE2	1:50:A:SER:HB3	17	0.2
(2,791)	1:131:A:TRP:HZ2	1:132:A:LYS:HE3	20	0.2
(2,785)	1:32:A:MET:HE2	2:1001:A:OLA:H131	8	0.2
(2,785)	1:32:A:MET:HE2	2:1001:A:OLA:H131	19	0.2
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	5	0.2
(2,722)	1:94:A:LEU:HD13	1:4:A:PRO:HD2	16	0.2
(2,706)	1:41:A:VAL:HG23	1:62:A:THR:HG1	20	0.2
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	3	0.2
(2,677)	1:139:A:TYR:HE2	1:121:A:ASP:HB3	12	0.2
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	5	0.2
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	8	0.2
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	13	0.2
(2,633)	1:128:A:LYS:HD3	1:128:A:LYS:H	5	0.2
(2,632)	1:128:A:LYS:HB3	1:128:A:LYS:HE2	14	0.2
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	11	0.2
(2,616)	1:125:A:LEU:HD21	1:140:A:TYR:HD2	17	0.2
(2,612)	1:125:A:LEU:HD21	1:125:A:LEU:HB3	2	0.2
(2,612)	1:125:A:LEU:HD21	1:125:A:LEU:HB3	13	0.2
(2,612)	1:125:A:LEU:HD21	1:125:A:LEU:HB3	15	0.2
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HA	12	0.2
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HB	14	0.2
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD12	16	0.2
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	8	0.2
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	9	0.2
(2,490)	1:90:A:ILE:HG13	1:90:A:ILE:HG21	12	0.2
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HB3	9	0.2
(2,447)	1:84:A:ASP:HA	2:1001:A:OLA:H112	17	0.2
(2,441)	1:141:A:LYS:H	1:141:A:LYS:HG3	13	0.2
(2,426)	1:15:A:ARG:HB3	1:13:A:LEU:HD21	5	0.2
(2,360)	1:60:A:ASN:HB3	1:67:A:THR:H	18	0.2
(2,319)	1:61:A:LEU:HD23	1:42:A:THR:HB	3	0.2
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	7	0.2
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	16	0.2
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	16	0.2
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	5	0.2
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	1	0.2
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	7	0.2
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	9	0.2
(2,158)	1:15:A:ARG:HA	1:13:A:LEU:HB3	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:12:A:LYS:HE2	1:12:A:LYS:HA	3	0.2
(2,136)	1:139:A:TYR:HA	1:140:A:TYR:HD2	14	0.2
(2,116)	1:46:A:ARG:H	1:8:A:LEU:HD23	14	0.2
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	5	0.2
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	7	0.2
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	15	0.2
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD3	19	0.2
(2,65)	1:12:A:LYS:HE2	1:12:A:LYS:HG3	3	0.2
(2,59)	1:0:A:SER:HB2	1:2:A:THR:HG22	19	0.2
(2,51)	1:48:A:ALA:HB1	1:56:A:TYR:HB3	1	0.2
(2,26)	1:4:A:PRO:HG3	1:94:A:LEU:HD23	7	0.2
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG23	16	0.2
(1,2839)	2:1001:A:OLA:H183	1:19:A:PHE:HE1	10	0.2
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	12	0.2
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG22	7	0.2
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	11	0.2
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	13	0.2
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	16	0.2
(1,2813)	1:127:A:MET:HE2	1:118:A:TYR:HH	8	0.2
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H181	12	0.2
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	16	0.2
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	20	0.2
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	7	0.2
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	13	0.2
(1,2413)	1:23:A:LEU:HD22	1:33:A:ARG:H	2	0.2
(1,2331)	1:60:A:ASN:HB3	1:67:A:THR:H	4	0.2
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	4	0.2
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	20	0.2
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG23	7	0.2
(1,1762)	1:8:A:LEU:HD12	1:47:A:ASN:HD21	18	0.2
(1,1461)	1:55:A:ARG:HG2	1:56:A:TYR:H	1	0.2
(1,1386)	1:83:A:LEU:HD12	1:84:A:ASP:H	12	0.2
(1,1297)	1:8:A:LEU:HD23	1:8:A:LEU:H	6	0.2
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	3	0.2
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB2	16	0.2
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG21	8	0.2
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	7	0.2
(1,1171)	1:32:A:MET:HE2	1:33:A:ARG:H	9	0.2
(1,1168)	1:32:A:MET:HE1	1:35:A:VAL:H	19	0.2
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	7	0.2
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	3	0.2
(1,1111)	1:58:A:MET:HE2	1:43:A:LYS:HE2	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:58:A:MET:HE2	1:45:A:PHE:HE1	18	0.2
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	5	0.2
(1,1064)	1:36:A:ILE:HD12	1:36:A:ILE:HA	15	0.2
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	18	0.2
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	15	0.2
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	5	0.2
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	18	0.2
(1,954)	1:129:A:MET:HG3	1:116:A:TYR:HD1	13	0.2
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG22	11	0.2
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG22	13	0.2
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	9	0.2
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	15	0.2
(1,843)	1:108:A:ASP:HB2	1:108:A:ASP:H	18	0.2
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD11	6	0.2
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG21	4	0.2
(1,752)	1:94:A:LEU:HD11	1:7:A:PHE:HD2	1	0.2
(1,752)	1:94:A:LEU:HD12	1:7:A:PHE:HD2	6	0.2
(1,697)	1:88:A:HIS:HE1	1:90:A:ILE:HG22	13	0.2
(1,598)	1:70:A:LYS:HA	1:70:A:LYS:HE3	16	0.2
(1,548)	1:62:A:THR:HG23	1:60:A:ASN:HB2	13	0.2
(1,449)	1:61:A:LEU:HB2	1:42:A:THR:HB	4	0.2
(1,441)	1:38:A:LEU:HD22	1:38:A:LEU:HA	3	0.2
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD13	11	0.2
(1,349)	1:28:A:TYR:HD1	1:23:A:LEU:HD12	17	0.2
(1,310)	1:25:A:ALA:HB3	1:134:A:VAL:HB	6	0.2
(1,288)	1:23:A:LEU:HD21	1:33:A:ARG:HA	12	0.2
(1,191)	1:10:A:THR:HB	1:143:A:GLN:H	5	0.2
(1,191)	1:10:A:THR:HB	1:143:A:GLN:H	16	0.2
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	19	0.2
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB1	4	0.2
(1,100)	1:48:A:ALA:HB1	1:50:A:SER:H	14	0.2
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB1	5	0.2
(1,44)	1:58:A:MET:HG2	1:118:A:TYR:HE2	5	0.2
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	19	0.2
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	10	0.19
(2,1677)	2:1001:A:OLA:H161	2:1001:A:OLA:H182	4	0.19
(2,1664)	1:102:A:GLU:HG3	1:118:A:TYR:HE2	10	0.19
(2,1659)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	9	0.19
(2,1653)	1:32:A:MET:HE1	2:1001:A:OLA:H121	5	0.19
(2,1644)	2:1001:A:OLA:H10	2:1001:A:OLA:H111	6	0.19
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	12	0.19
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	3	0.19
(2,1610)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	9	0.19
(2,1580)	2:1001:A:OLA:H32	2:1001:A:OLA:H183	19	0.19
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	3	0.19
(2,1409)	1:34:A:GLN:H	1:34:A:GLN:HE22	5	0.19
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	7	0.19
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	1	0.19
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	7	0.19
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	17	0.19
(2,1185)	1:17:A:GLU:H	1:16:A:ASP:HB3	18	0.19
(2,1168)	1:128:A:LYS:HE3	1:135:A:SER:H	2	0.19
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD12	18	0.19
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	1	0.19
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	4	0.19
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	2	0.19
(2,1075)	1:93:A:ASP:H	1:74:A:LEU:HD21	9	0.19
(2,1074)	1:95:A:LYS:HB2	1:96:A:ASP:H	15	0.19
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	10	0.19
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	15	0.19
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	11	0.19
(2,990)	1:132:A:LYS:HG3	1:132:A:LYS:H	19	0.19
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	4	0.19
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	8	0.19
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	11	0.19
(2,927)	1:38:A:LEU:H	1:37:A:LYS:HB3	15	0.19
(2,925)	1:65:A:LYS:HG3	1:67:A:THR:H	17	0.19
(2,917)	1:86:A:THR:H	1:82:A:ALA:HB2	16	0.19
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	19	0.19
(2,846)	1:88:A:HIS:HE1	1:82:A:ALA:HB3	16	0.19
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	19	0.19
(2,819)	1:36:A:ILE:HG21	2:1001:A:OLA:H82	16	0.19
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	1	0.19
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	18	0.19
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	2	0.19
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG23	19	0.19
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	3	0.19
(2,612)	1:125:A:LEU:HD22	1:125:A:LEU:HB3	8	0.19
(2,612)	1:125:A:LEU:HD22	1:125:A:LEU:HB3	12	0.19
(2,596)	1:118:A:TYR:HD1	1:125:A:LEU:HG	3	0.19
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HB	4	0.19
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HB	8	0.19
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HB	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,564)	1:88:A:HIS:HB2	1:107:A:VAL:HA	11	0.19
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	11	0.19
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	12	0.19
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	18	0.19
(2,456)	1:85:A:SER:HA	1:65:A:LYS:HB3	16	0.19
(2,374)	2:1001:A:OLA:H81	1:62:A:THR:HG23	2	0.19
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG21	14	0.19
(2,331)	1:44:A:LYS:HA	1:11:A:PHE:HB2	8	0.19
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	7	0.19
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	18	0.19
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	3	0.19
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	4	0.19
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	9	0.19
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD13	14	0.19
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	18	0.19
(2,122)	1:9:A:GLY:HA3	1:142:A:LYS:HE3	4	0.19
(2,121)	1:142:A:LYS:HE2	1:9:A:GLY:HA2	8	0.19
(2,45)	1:48:A:ALA:HA	1:46:A:ARG:HG3	13	0.19
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	9	0.19
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG22	8	0.19
(1,2839)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	14	0.19
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG23	4	0.19
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	7	0.19
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	2	0.19
(1,2815)	1:23:A:LEU:HA	2:1001:A:OLA:H183	1	0.19
(1,2813)	1:127:A:MET:HE3	1:118:A:TYR:HH	5	0.19
(1,2809)	2:1001:A:OLA:H182	1:36:A:ILE:HD13	20	0.19
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	2	0.19
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	3	0.19
(1,2789)	2:1001:A:OLA:H183	1:36:A:ILE:HA	12	0.19
(1,2759)	1:108:A:ASP:H	1:107:A:VAL:HG12	6	0.19
(1,2736)	1:47:A:ASN:HD22	1:8:A:LEU:HD22	6	0.19
(1,2694)	1:28:A:TYR:H	1:28:A:TYR:HE1	13	0.19
(1,2499)	1:66:A:ASP:HB2	1:66:A:ASP:H	2	0.19
(1,2300)	1:90:A:ILE:HD13	1:90:A:ILE:H	12	0.19
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	19	0.19
(1,2243)	1:23:A:LEU:HD23	1:37:A:LYS:H	1	0.19
(1,2029)	1:114:A:GLU:H	1:103:A:THR:HG23	6	0.19
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	11	0.19
(1,1676)	1:87:A:GLN:H	1:87:A:GLN:HE22	13	0.19
(1,1643)	1:19:A:PHE:H	1:19:A:PHE:HD1	7	0.19
(1,1480)	1:119:A:ARG:HA	1:119:A:ARG:HG2	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	20	0.19
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD11	12	0.19
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG11	4	0.19
(1,1333)	1:106:A:LYS:HA	1:106:A:LYS:HD3	12	0.19
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	7	0.19
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	10	0.19
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	15	0.19
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG21	3	0.19
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG21	4	0.19
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE1	4	0.19
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	12	0.19
(1,1027)	1:139:A:TYR:HE2	1:126:A:VAL:HG13	15	0.19
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	8	0.19
(1,989)	1:134:A:VAL:HG11	1:22:A:TYR:HB3	9	0.19
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD11	7	0.19
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD13	19	0.19
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD22	16	0.19
(1,720)	1:103:A:THR:HB	1:90:A:ILE:HG22	13	0.19
(1,668)	1:83:A:LEU:HA	1:82:A:ALA:HB1	4	0.19
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	19	0.19
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB2	12	0.19
(1,617)	1:73:A:ALA:HB1	1:75:A:GLY:H	11	0.19
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	19	0.19
(1,466)	1:44:A:LYS:HE3	1:44:A:LYS:HB3	5	0.19
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	9	0.19
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD13	9	0.19
(1,307)	1:25:A:ALA:HB2	1:27:A:GLY:H	2	0.19
(1,307)	1:25:A:ALA:HB1	1:27:A:GLY:H	4	0.19
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB2	5	0.19
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	3	0.19
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	8	0.19
(1,100)	1:48:A:ALA:HB1	1:50:A:SER:H	9	0.19
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	18	0.19
(1,47)	1:34:A:GLN:HA	1:37:A:LYS:HE3	2	0.19
(1,17)	1:31:A:ILE:HD11	1:31:A:ILE:HA	12	0.19
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	1	0.18
(2,1678)	1:10:A:THR:HG21	1:44:A:LYS:HG2	8	0.18
(2,1671)	2:1001:A:OLA:H41	2:1001:A:OLA:H22	16	0.18
(2,1659)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	1	0.18
(2,1651)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	11	0.18
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	8	0.18
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	20	0.18
(2,1636)	1:83:A:LEU:HB3	1:62:A:THR:HG1	14	0.18
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	1	0.18
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	3	0.18
(2,1611)	1:28:A:TYR:HE2	2:1001:A:OLA:H131	19	0.18
(2,1610)	1:19:A:PHE:HZ	2:1001:A:OLA:H22	1	0.18
(2,1568)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	3	0.18
(2,1553)	1:136:A:THR:H	1:128:A:LYS:HG2	12	0.18
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	15	0.18
(2,1495)	1:13:A:LEU:H	1:42:A:THR:HG22	14	0.18
(2,1487)	1:67:A:THR:HG23	1:65:A:LYS:H	9	0.18
(2,1432)	1:30:A:TRP:HH2	1:34:A:GLN:HE22	3	0.18
(2,1332)	1:75:A:GLY:H	1:91:A:THR:HG23	18	0.18
(2,1235)	1:39:A:ALA:H	1:35:A:VAL:HG13	18	0.18
(2,1131)	1:17:A:GLU:HA	1:137:A:SER:H	18	0.18
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	19	0.18
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD22	4	0.18
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	10	0.18
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	16	0.18
(2,990)	1:132:A:LYS:HG3	1:132:A:LYS:H	20	0.18
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG11	18	0.18
(2,893)	1:64:A:LYS:HG3	2:1001:A:OLA:H10	1	0.18
(2,875)	1:-5:A:HIS:HB3	1:-5:A:HIS:HA	16	0.18
(2,844)	1:69:A:HIS:HE1	1:82:A:ALA:HB2	3	0.18
(2,839)	1:129:A:MET:HE2	1:19:A:PHE:HE1	2	0.18
(2,820)	1:41:A:VAL:HG21	1:43:A:LYS:HE2	5	0.18
(2,782)	1:127:A:MET:HE3	1:116:A:TYR:HA	11	0.18
(2,729)	1:66:A:ASP:HA	1:61:A:LEU:HB3	15	0.18
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	14	0.18
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	19	0.18
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	17	0.18
(2,683)	1:41:A:VAL:HG22	1:140:A:TYR:HE1	18	0.18
(2,676)	1:121:A:ASP:HB2	1:139:A:TYR:HE2	14	0.18
(2,676)	1:139:A:TYR:HE2	1:139:A:TYR:HB3	15	0.18
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	20	0.18
(2,674)	1:16:A:ASP:HA	1:139:A:TYR:HE1	11	0.18
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB3	13	0.18
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	10	0.18
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	12	0.18
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	16	0.18
(2,632)	1:128:A:LYS:HE3	1:128:A:LYS:HB3	15	0.18
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	17	0.18
(2,580)	1:111:A:THR:HG21	1:110:A:PRO:HG2	11	0.18
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HB	5	0.18
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HA	16	0.18
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HB	19	0.18
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HB	20	0.18
(2,564)	1:88:A:HIS:HB2	1:107:A:VAL:HA	14	0.18
(2,561)	1:106:A:LYS:HA	1:107:A:VAL:HG13	7	0.18
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG22	8	0.18
(2,531)	1:96:A:ASP:H	1:99:A:THR:HG23	14	0.18
(2,527)	1:96:A:ASP:H	1:95:A:LYS:HD3	17	0.18
(2,500)	1:90:A:ILE:HD12	1:88:A:HIS:H	16	0.18
(2,488)	1:102:A:GLU:HB3	1:90:A:ILE:HG21	10	0.18
(2,482)	1:69:A:HIS:HD2	1:90:A:ILE:HG21	9	0.18
(2,479)	1:90:A:ILE:HG22	1:78:A:PHE:H	5	0.18
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	2	0.18
(2,452)	1:84:A:ASP:HB2	1:82:A:ALA:HB1	9	0.18
(2,433)	1:85:A:SER:H	1:81:A:GLU:HG2	3	0.18
(2,420)	1:93:A:ASP:HA	1:74:A:LEU:HD12	7	0.18
(2,418)	1:106:A:LYS:HG2	1:107:A:VAL:H	2	0.18
(2,418)	1:106:A:LYS:HG2	1:107:A:VAL:H	18	0.18
(2,395)	1:85:A:SER:HA	1:65:A:LYS:HE3	14	0.18
(2,380)	2:1001:A:OLA:H10	1:64:A:LYS:HB3	7	0.18
(2,378)	1:62:A:THR:HG21	1:83:A:LEU:HD23	11	0.18
(2,373)	1:64:A:LYS:H	1:62:A:THR:HG23	18	0.18
(2,355)	1:57:A:ASP:HA	1:70:A:LYS:HG2	19	0.18
(2,344)	1:52:A:LYS:HA	1:53:A:PRO:HG3	15	0.18
(2,322)	1:43:A:LYS:HD3	1:118:A:TYR:HE1	18	0.18
(2,297)	1:37:A:LYS:HG3	1:19:A:PHE:HD2	3	0.18
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	6	0.18
(2,262)	1:30:A:TRP:HA	1:34:A:GLN:HB2	5	0.18
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	10	0.18
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	12	0.18
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	15	0.18
(2,226)	1:134:A:VAL:HG22	1:25:A:ALA:HA	12	0.18
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	7	0.18
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	17	0.18
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	18	0.18
(2,213)	1:23:A:LEU:HD22	1:19:A:PHE:HD2	16	0.18
(2,160)	1:13:A:LEU:HD21	1:41:A:VAL:H	6	0.18
(2,130)	1:11:A:PHE:HA	1:142:A:LYS:HG2	20	0.18
(2,126)	1:11:A:PHE:HA	1:10:A:THR:HG22	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:8:A:LEU:HD22	1:5:A:ASP:HA	20	0.18
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	7	0.18
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG23	17	0.18
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	9	0.18
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	13	0.18
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	8	0.18
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG23	19	0.18
(1,2836)	2:1001:A:OLA:H182	1:36:A:ILE:HD13	20	0.18
(1,2814)	2:1001:A:OLA:H182	1:19:A:PHE:HE1	13	0.18
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	8	0.18
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	5	0.18
(1,2331)	1:60:A:ASN:HB3	1:67:A:THR:H	12	0.18
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	10	0.18
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	14	0.18
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	16	0.18
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	17	0.18
(1,2106)	1:86:A:THR:HG23	1:87:A:GLN:H	19	0.18
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG23	10	0.18
(1,2029)	1:114:A:GLU:H	1:103:A:THR:HG21	9	0.18
(1,2000)	1:8:A:LEU:HD22	1:47:A:ASN:HD21	6	0.18
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	3	0.18
(1,1537)	1:21:A:GLU:H	1:21:A:GLU:HG2	5	0.18
(1,1480)	1:119:A:ARG:HA	1:119:A:ARG:HG2	4	0.18
(1,1461)	1:55:A:ARG:HG2	1:56:A:TYR:H	8	0.18
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG13	14	0.18
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD12	6	0.18
(1,1278)	1:113:A:VAL:H	1:113:A:VAL:HG12	3	0.18
(1,1249)	1:3:A:LEU:HD22	1:3:A:LEU:H	20	0.18
(1,1222)	1:127:A:MET:HE2	1:118:A:TYR:HD1	10	0.18
(1,1220)	1:118:A:TYR:HD1	1:58:A:MET:HE1	15	0.18
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG23	13	0.18
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE1	10	0.18
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	17	0.18
(1,1159)	1:28:A:TYR:HE2	1:32:A:MET:HE2	19	0.18
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG11	10	0.18
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG12	19	0.18
(1,989)	1:134:A:VAL:HG12	1:22:A:TYR:HB3	1	0.18
(1,895)	1:118:A:TYR:HD1	1:127:A:MET:HB2	14	0.18
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	2	0.18
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	11	0.18
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	20	0.18
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD13	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,792)	1:100:A:LEU:HD11	1:118:A:TYR:HD2	15	0.18
(1,723)	1:90:A:ILE:HG23	1:102:A:GLU:HG3	1	0.18
(1,622)	1:72:A:TRP:HA	1:73:A:ALA:HB3	7	0.18
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	13	0.18
(1,449)	1:61:A:LEU:HB2	1:42:A:THR:HB	2	0.18
(1,441)	1:38:A:LEU:HD23	1:38:A:LEU:HA	18	0.18
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD11	20	0.18
(1,307)	1:25:A:ALA:HB3	1:27:A:GLY:H	5	0.18
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB1	6	0.18
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB1	4	0.18
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB2	13	0.18
(1,228)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	1	0.18
(1,228)	1:13:A:LEU:HD11	1:13:A:LEU:HB3	9	0.18
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD11	9	0.18
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	2	0.18
(1,130)	1:3:A:LEU:HD12	1:7:A:PHE:HB3	4	0.18
(1,102)	1:55:A:ARG:H	1:48:A:ALA:HB2	17	0.18
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	6	0.18
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	13	0.18
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG23	16	0.18
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG21	20	0.18
(3,43)	1:55:A:ARG:H	1:53:A:PRO:O	9	0.17
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	2	0.17
(3,32)	1:12:A:LYS:N	1:142:A:LYS:O	19	0.17
(2,1679)	1:83:A:LEU:HD21	2:1001:A:OLA:H62	4	0.17
(2,1678)	1:10:A:THR:HG21	1:44:A:LYS:HG2	1	0.17
(2,1678)	1:10:A:THR:HG21	1:44:A:LYS:HG2	15	0.17
(2,1671)	1:24:A:LYS:HB3	1:24:A:LYS:HG2	1	0.17
(2,1671)	2:1001:A:OLA:H82	2:1001:A:OLA:H71	2	0.17
(2,1665)	1:22:A:TYR:HD2	1:26:A:ARG:HG2	6	0.17
(2,1659)	1:19:A:PHE:HZ	2:1001:A:OLA:H21	5	0.17
(2,1647)	1:36:A:ILE:HD13	2:1001:A:OLA:H131	1	0.17
(2,1647)	1:36:A:ILE:HD11	2:1001:A:OLA:H131	4	0.17
(2,1644)	2:1001:A:OLA:H10	2:1001:A:OLA:H111	12	0.17
(2,1634)	1:22:A:TYR:HD1	2:1001:A:OLA:H181	7	0.17
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	17	0.17
(2,1610)	1:19:A:PHE:HZ	2:1001:A:OLA:H21	5	0.17
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	8	0.17
(2,1521)	1:7:A:PHE:H	1:120:A:ARG:HB2	2	0.17
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG13	4	0.17
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG11	11	0.17
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	14	0.17
(2,1360)	1:52:A:LYS:H	1:52:A:LYS:HG3	14	0.17
(2,1339)	1:77:A:GLU:HG3	1:78:A:PHE:H	3	0.17
(2,1328)	1:36:A:ILE:H	1:34:A:GLN:HB3	5	0.17
(2,1325)	1:129:A:MET:HE1	1:130:A:SER:H	2	0.17
(2,1315)	1:105:A:ILE:HG13	1:113:A:VAL:H	2	0.17
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	11	0.17
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	9	0.17
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	16	0.17
(2,1138)	1:13:A:LEU:H	1:13:A:LEU:HD12	8	0.17
(2,1117)	1:94:A:LEU:HG	1:99:A:THR:H	11	0.17
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD21	2	0.17
(2,1102)	1:58:A:MET:H	1:70:A:LYS:HG2	17	0.17
(2,1061)	1:118:A:TYR:HD1	1:128:A:LYS:H	5	0.17
(2,1040)	1:34:A:GLN:HE21	1:35:A:VAL:HG22	2	0.17
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD13	1	0.17
(2,1006)	1:81:A:GLU:H	1:87:A:GLN:HE22	16	0.17
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	5	0.17
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	16	0.17
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	10	0.17
(2,977)	1:26:A:ARG:HG2	1:131:A:TRP:HE1	14	0.17
(2,965)	1:55:A:ARG:H	1:55:A:ARG:HG2	4	0.17
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG13	13	0.17
(2,880)	1:128:A:LYS:HE2	1:128:A:LYS:HB2	2	0.17
(2,880)	1:128:A:LYS:HE2	1:128:A:LYS:HB2	8	0.17
(2,880)	1:128:A:LYS:HE2	1:128:A:LYS:HB2	14	0.17
(2,787)	1:39:A:ALA:HB1	1:40:A:GLY:H	2	0.17
(2,731)	1:58:A:MET:HE2	1:61:A:LEU:H	1	0.17
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	4	0.17
(2,706)	1:41:A:VAL:HG22	1:62:A:THR:HG1	2	0.17
(2,698)	1:142:A:LYS:HG2	1:142:A:LYS:HE3	3	0.17
(2,698)	1:142:A:LYS:HG2	1:142:A:LYS:HE3	18	0.17
(2,697)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	5	0.17
(2,684)	1:125:A:LEU:HD12	1:140:A:TYR:HE2	15	0.17
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB3	1	0.17
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	4	0.17
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	6	0.17
(2,658)	1:25:A:ALA:HB1	1:134:A:VAL:HG21	10	0.17
(2,640)	1:34:A:GLN:HG3	1:30:A:TRP:HZ2	12	0.17
(2,628)	1:116:A:TYR:HB3	1:127:A:MET:HG3	8	0.17
(2,622)	1:127:A:MET:HA	1:126:A:VAL:HG11	2	0.17
(2,622)	1:127:A:MET:HA	1:126:A:VAL:HG11	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	9	0.17
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	10	0.17
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	18	0.17
(2,611)	1:125:A:LEU:HD22	1:7:A:PHE:HD1	9	0.17
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	12	0.17
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG23	15	0.17
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HB	7	0.17
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HB	13	0.17
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HA	18	0.17
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD13	14	0.17
(2,498)	1:90:A:ILE:HD11	1:78:A:PHE:HD2	6	0.17
(2,498)	1:90:A:ILE:HD12	1:78:A:PHE:HD2	10	0.17
(2,482)	1:69:A:HIS:HD2	1:90:A:ILE:HG23	16	0.17
(2,479)	1:90:A:ILE:HG21	1:78:A:PHE:H	8	0.17
(2,374)	1:62:A:THR:HG22	1:83:A:LEU:HG	6	0.17
(2,367)	1:61:A:LEU:H	1:61:A:LEU:HD11	15	0.17
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	11	0.17
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	16	0.17
(2,313)	1:129:A:MET:HE1	1:22:A:TYR:HD1	6	0.17
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	1	0.17
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	5	0.17
(2,247)	1:26:A:ARG:HD2	1:131:A:TRP:HE3	8	0.17
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	5	0.17
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	12	0.17
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	15	0.17
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD2	4	0.17
(2,212)	1:23:A:LEU:HD22	1:26:A:ARG:H	6	0.17
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG23	5	0.17
(2,205)	1:33:A:ARG:HD3	1:23:A:LEU:HD12	4	0.17
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	6	0.17
(2,152)	1:12:A:LYS:HA	1:12:A:LYS:HD2	10	0.17
(2,150)	1:12:A:LYS:HA	1:12:A:LYS:HG2	1	0.17
(2,150)	1:12:A:LYS:HA	1:12:A:LYS:HG2	5	0.17
(2,150)	1:12:A:LYS:HA	1:12:A:LYS:HG2	16	0.17
(2,150)	1:12:A:LYS:HA	1:12:A:LYS:HG2	20	0.17
(2,68)	1:12:A:LYS:HE3	1:12:A:LYS:HD2	8	0.17
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD3	20	0.17
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	3	0.17
(1,2838)	1:136:A:THR:HG1	1:136:A:THR:HG21	10	0.17
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	4	0.17
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	6	0.17
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	14	0.17
(1,2694)	1:28:A:TYR:H	1:28:A:TYR:HE1	14	0.17
(1,2463)	1:111:A:THR:HG23	1:113:A:VAL:H	7	0.17
(1,2413)	1:23:A:LEU:HD22	1:33:A:ARG:H	18	0.17
(1,2403)	1:98:A:ASN:HB3	1:98:A:ASN:H	8	0.17
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	6	0.17
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG21	11	0.17
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	15	0.17
(1,1925)	1:107:A:VAL:HG21	1:79:A:GLN:HE22	9	0.17
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	5	0.17
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	17	0.17
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	18	0.17
(1,1626)	1:61:A:LEU:HG	1:61:A:LEU:H	18	0.17
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	8	0.17
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	2	0.17
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	8	0.17
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	15	0.17
(1,1386)	1:83:A:LEU:HD12	1:84:A:ASP:H	19	0.17
(1,1297)	1:8:A:LEU:HD23	1:8:A:LEU:H	10	0.17
(1,1228)	1:139:A:TYR:HE2	1:126:A:VAL:HG21	7	0.17
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	1	0.17
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	2	0.17
(1,1194)	1:139:A:TYR:HE2	1:126:A:VAL:HG21	7	0.17
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	3	0.17
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	17	0.17
(1,1148)	1:37:A:LYS:H	1:36:A:ILE:HG22	11	0.17
(1,1124)	1:30:A:TRP:HZ3	1:34:A:GLN:HG2	19	0.17
(1,1103)	1:58:A:MET:HE3	1:69:A:HIS:HD2	19	0.17
(1,1037)	1:124:A:TYR:HE2	1:141:A:LYS:HD3	19	0.17
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG21	12	0.17
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	10	0.17
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD13	15	0.17
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG22	4	0.17
(1,793)	1:100:A:LEU:HD12	1:118:A:TYR:HB3	10	0.17
(1,793)	1:100:A:LEU:HD13	1:118:A:TYR:HB3	14	0.17
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD22	6	0.17
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD21	13	0.17
(1,698)	1:88:A:HIS:HA	1:88:A:HIS:HD2	10	0.17
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD11	4	0.17
(1,631)	1:4:A:PRO:HD3	1:74:A:LEU:HD13	14	0.17
(1,571)	1:65:A:LYS:HD3	1:66:A:ASP:H	4	0.17
(1,451)	1:67:A:THR:HG23	1:67:A:THR:HG1	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD13	6	0.17
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD12	18	0.17
(1,407)	1:36:A:ILE:H	1:36:A:ILE:HG22	7	0.17
(1,374)	1:32:A:MET:HG2	1:36:A:ILE:HD11	15	0.17
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	9	0.17
(1,228)	1:13:A:LEU:HD12	1:13:A:LEU:HB3	12	0.17
(1,82)	1:96:A:ASP:HB3	1:97:A:PRO:HD3	20	0.17
(1,17)	1:31:A:ILE:HD11	1:31:A:ILE:HA	10	0.17
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD11	11	0.17
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG23	1	0.17
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	3	0.17
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG23	15	0.17
(3,65)	1:88:A:HIS:H	1:80:A:ASP:O	14	0.16
(2,1679)	2:1001:A:OLA:H71	1:36:A:ILE:HG21	2	0.16
(2,1675)	1:94:A:LEU:HB3	1:94:A:LEU:HD21	7	0.16
(2,1671)	2:1001:A:OLA:H41	2:1001:A:OLA:H21	3	0.16
(2,1671)	2:1001:A:OLA:H81	2:1001:A:OLA:H62	4	0.16
(2,1643)	2:1001:A:OLA:H10	1:35:A:VAL:HG12	11	0.16
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	15	0.16
(2,1635)	2:1001:A:OLA:H81	1:62:A:THR:HG1	16	0.16
(2,1591)	2:1001:A:OLA:H131	2:1001:A:OLA:H72	5	0.16
(2,1583)	2:1001:A:OLA:H161	2:1001:A:OLA:H22	2	0.16
(2,1581)	1:36:A:ILE:HD12	2:1001:A:OLA:H82	9	0.16
(2,1553)	1:136:A:THR:H	1:128:A:LYS:HG2	14	0.16
(2,1488)	1:81:A:GLU:H	1:87:A:GLN:HE21	15	0.16
(2,1471)	1:101:A:THR:HG23	1:93:A:ASP:H	17	0.16
(2,1461)	1:136:A:THR:H	1:128:A:LYS:HB3	14	0.16
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	8	0.16
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	9	0.16
(2,1332)	1:75:A:GLY:H	1:91:A:THR:HG22	12	0.16
(2,1302)	1:28:A:TYR:H	1:131:A:TRP:HE1	7	0.16
(2,1259)	1:120:A:ARG:H	1:7:A:PHE:HD1	6	0.16
(2,1184)	1:141:A:LYS:HG3	1:143:A:GLN:HE22	1	0.16
(2,1155)	1:60:A:ASN:H	1:61:A:LEU:HD21	11	0.16
(2,1103)	1:87:A:GLN:H	1:82:A:ALA:HB3	15	0.16
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD22	6	0.16
(2,1080)	1:102:A:GLU:H	1:92:A:PHE:HD2	15	0.16
(2,1075)	1:94:A:LEU:HD22	1:93:A:ASP:H	14	0.16
(2,993)	1:38:A:LEU:HB3	1:39:A:ALA:H	13	0.16
(2,990)	1:132:A:LYS:HG3	1:132:A:LYS:H	11	0.16
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG11	15	0.16
(2,946)	1:56:A:TYR:H	1:55:A:ARG:HG3	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,946)	1:56:A:TYR:H	1:55:A:ARG:HG3	18	0.16
(2,904)	1:106:A:LYS:H	1:106:A:LYS:HE2	14	0.16
(2,894)	1:64:A:LYS:HG3	1:64:A:LYS:H	18	0.16
(2,880)	1:128:A:LYS:HE2	1:128:A:LYS:HB2	3	0.16
(2,880)	1:128:A:LYS:HE2	1:128:A:LYS:HB2	12	0.16
(2,860)	1:64:A:LYS:HB2	2:1001:A:OLA:H10	10	0.16
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	5	0.16
(2,837)	1:58:A:MET:HE1	1:60:A:ASN:HD21	6	0.16
(2,828)	1:23:A:LEU:HG	1:22:A:TYR:HB2	13	0.16
(2,802)	1:62:A:THR:HA	1:41:A:VAL:HG13	4	0.16
(2,789)	1:26:A:ARG:HD2	1:131:A:TRP:HZ3	10	0.16
(2,782)	1:127:A:MET:HE2	1:116:A:TYR:HA	2	0.16
(2,778)	1:119:A:ARG:HD3	1:99:A:THR:HA	12	0.16
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	17	0.16
(2,718)	1:0:A:SER:HA	1:1:A:LYS:HG2	9	0.16
(2,706)	1:41:A:VAL:HG23	1:62:A:THR:HG1	19	0.16
(2,698)	1:142:A:LYS:HG2	1:142:A:LYS:HE3	13	0.16
(2,687)	1:141:A:LYS:HD2	1:141:A:LYS:HA	13	0.16
(2,680)	1:140:A:TYR:HE2	1:43:A:LYS:HG2	8	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	1	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	3	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	8	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	9	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	11	0.16
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG23	14	0.16
(2,633)	1:128:A:LYS:HD3	1:128:A:LYS:H	20	0.16
(2,612)	1:125:A:LEU:HD21	1:125:A:LEU:HB3	11	0.16
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	20	0.16
(2,602)	1:124:A:TYR:HA	1:126:A:VAL:HG21	10	0.16
(2,596)	1:118:A:TYR:HD1	1:125:A:LEU:HG	14	0.16
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HA	1	0.16
(2,579)	1:111:A:THR:HG23	1:111:A:THR:HB	2	0.16
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HB	3	0.16
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HB	6	0.16
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HA	9	0.16
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HA	10	0.16
(2,545)	1:100:A:LEU:HD22	1:94:A:LEU:HD23	16	0.16
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD23	16	0.16
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	10	0.16
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	8	0.16
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	10	0.16
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,498)	1:90:A:ILE:HD12	1:78:A:PHE:HD2	5	0.16
(2,487)	1:90:A:ILE:HG22	1:92:A:PHE:HB2	14	0.16
(2,457)	1:86:A:THR:HB	1:87:A:GLN:HG2	10	0.16
(2,438)	1:88:A:HIS:H	1:82:A:ALA:HB1	13	0.16
(2,416)	1:72:A:TRP:H	1:73:A:ALA:HB3	4	0.16
(2,412)	1:73:A:ALA:HB3	1:55:A:ARG:H	7	0.16
(2,405)	1:66:A:ASP:HA	1:61:A:LEU:HB2	17	0.16
(2,402)	1:66:A:ASP:HA	1:62:A:THR:HG21	2	0.16
(2,378)	1:83:A:LEU:HD12	1:62:A:THR:HG21	1	0.16
(2,378)	1:62:A:THR:HG23	1:83:A:LEU:HD21	4	0.16
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG21	7	0.16
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG13	6	0.16
(2,327)	1:43:A:LYS:HE2	1:45:A:PHE:HE1	14	0.16
(2,326)	1:45:A:PHE:HE1	1:43:A:LYS:HE3	19	0.16
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	4	0.16
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	10	0.16
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	14	0.16
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	15	0.16
(2,263)	1:30:A:TRP:HA	1:34:A:GLN:H	17	0.16
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	4	0.16
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	3	0.16
(2,226)	1:134:A:VAL:HG23	1:25:A:ALA:HA	11	0.16
(2,225)	1:26:A:ARG:HA	1:25:A:ALA:HA	2	0.16
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	8	0.16
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG13	18	0.16
(2,150)	1:12:A:LYS:HA	1:12:A:LYS:HG2	12	0.16
(2,83)	1:11:A:PHE:HB3	1:125:A:LEU:HD13	17	0.16
(2,53)	1:33:A:ARG:HD3	1:30:A:TRP:HA	17	0.16
(2,41)	1:53:A:PRO:HG2	1:54:A:ASP:H	18	0.16
(1,2839)	2:1001:A:OLA:H182	1:19:A:PHE:HE1	15	0.16
(1,2836)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	16	0.16
(1,2809)	2:1001:A:OLA:H182	1:36:A:ILE:HD11	16	0.16
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	8	0.16
(1,2799)	1:83:A:LEU:HD23	1:62:A:THR:HG1	11	0.16
(1,2756)	1:142:A:LYS:H	1:124:A:TYR:HE2	2	0.16
(1,2694)	1:28:A:TYR:H	1:28:A:TYR:HE1	20	0.16
(1,2489)	1:13:A:LEU:HD23	1:17:A:GLU:H	7	0.16
(1,2429)	1:65:A:LYS:HA	1:66:A:ASP:H	19	0.16
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	13	0.16
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	13	0.16
(1,2209)	1:124:A:TYR:HE2	1:15:A:ARG:H	20	0.16
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	10	0.16
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	13	0.16
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG22	19	0.16
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	18	0.16
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	8	0.16
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	14	0.16
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD12	15	0.16
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD13	12	0.16
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD11	15	0.16
(1,1249)	1:3:A:LEU:HD22	1:3:A:LEU:H	4	0.16
(1,1223)	1:127:A:MET:HE3	1:116:A:TYR:HD2	1	0.16
(1,1206)	1:125:A:LEU:HD13	1:118:A:TYR:HE1	5	0.16
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	4	0.16
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	6	0.16
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG21	6	0.16
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG21	14	0.16
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG23	20	0.16
(1,1168)	1:32:A:MET:HE1	1:35:A:VAL:H	12	0.16
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE2	19	0.16
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	18	0.16
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	19	0.16
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	1	0.16
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG23	4	0.16
(1,1004)	1:128:A:LYS:HA	1:136:A:THR:HG21	13	0.16
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	9	0.16
(1,989)	1:134:A:VAL:HG13	1:22:A:TYR:HB3	16	0.16
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG23	1	0.16
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG21	9	0.16
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	18	0.16
(1,787)	1:118:A:TYR:HB3	1:100:A:LEU:HD23	14	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	1	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	4	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	7	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	8	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	9	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	10	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	11	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	13	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	14	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	16	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	17	0.16
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	19	0.16
(1,548)	1:62:A:THR:HG21	1:60:A:ASN:HB2	7	0.16
(1,513)	1:48:A:ALA:HA	1:56:A:TYR:HA	12	0.16
(1,459)	1:43:A:LYS:HE3	1:118:A:TYR:HE1	14	0.16
(1,310)	1:25:A:ALA:HB1	1:134:A:VAL:HB	3	0.16
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB2	18	0.16
(1,137)	1:3:A:LEU:HD22	1:7:A:PHE:HB3	7	0.16
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD13	20	0.16
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB3	8	0.16
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	2	0.16
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	7	0.16
(1,8)	1:35:A:VAL:H	1:31:A:ILE:HG21	18	0.16
(3,89)	1:117:A:GLU:H	1:128:A:LYS:O	6	0.15
(3,67)	1:89:A:LYS:H	1:105:A:ILE:O	9	0.15
(3,65)	1:88:A:HIS:H	1:80:A:ASP:O	19	0.15
(2,1679)	2:1001:A:OLA:H61	1:36:A:ILE:HG21	20	0.15
(2,1678)	1:10:A:THR:HG22	1:44:A:LYS:HG2	2	0.15
(2,1678)	1:10:A:THR:HG23	1:44:A:LYS:HG2	10	0.15
(2,1678)	1:10:A:THR:HG21	1:44:A:LYS:HG2	13	0.15
(2,1614)	1:64:A:LYS:H	2:1001:A:OLA:H81	18	0.15
(2,1603)	1:36:A:ILE:HD13	2:1001:A:OLA:H131	5	0.15
(2,1556)	1:35:A:VAL:HG23	1:36:A:ILE:H	1	0.15
(2,1553)	1:136:A:THR:H	1:129:A:MET:HE1	3	0.15
(2,1553)	1:136:A:THR:H	1:129:A:MET:HE1	15	0.15
(2,1544)	1:134:A:VAL:HG13	1:21:A:GLU:H	7	0.15
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	10	0.15
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	9	0.15
(2,1471)	1:102:A:GLU:HG3	1:93:A:ASP:H	15	0.15
(2,1442)	1:64:A:LYS:HG3	1:64:A:LYS:H	18	0.15
(2,1396)	1:63:A:THR:HG22	1:41:A:VAL:H	1	0.15
(2,1396)	1:62:A:THR:HG21	1:41:A:VAL:H	15	0.15
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	13	0.15
(2,1315)	1:105:A:ILE:HG13	1:113:A:VAL:H	14	0.15
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	1	0.15
(2,1106)	1:42:A:THR:H	1:61:A:LEU:HD11	15	0.15
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD23	5	0.15
(2,967)	1:88:A:HIS:H	1:82:A:ALA:HB3	12	0.15
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG11	6	0.15
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	10	0.15
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	14	0.15
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG13	17	0.15
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,946)	1:56:A:TYR:H	1:55:A:ARG:HG3	6	0.15
(2,843)	1:14:A:GLU:HB3	1:139:A:TYR:HD1	2	0.15
(2,840)	1:129:A:MET:HE1	1:114:A:GLU:HG3	13	0.15
(2,839)	1:129:A:MET:HE2	1:19:A:PHE:HE1	6	0.15
(2,835)	1:20:A:ASP:HA	1:37:A:LYS:HE2	20	0.15
(2,810)	1:52:A:LYS:HE2	1:50:A:SER:HB3	19	0.15
(2,789)	1:26:A:ARG:HD2	1:131:A:TRP:HZ3	8	0.15
(2,788)	1:39:A:ALA:HB2	1:36:A:ILE:HA	19	0.15
(2,787)	1:127:A:MET:HE2	1:117:A:GLU:H	3	0.15
(2,757)	1:58:A:MET:HE2	1:43:A:LYS:HD2	2	0.15
(2,743)	1:104:A:HIS:HD2	1:102:A:GLU:HG3	7	0.15
(2,729)	1:66:A:ASP:HA	1:65:A:LYS:HB2	7	0.15
(2,716)	1:54:A:ASP:H	1:2:A:THR:HG23	2	0.15
(2,708)	1:7:A:PHE:HD2	1:94:A:LEU:HD23	9	0.15
(2,622)	1:127:A:MET:HA	1:126:A:VAL:HG13	14	0.15
(2,605)	1:14:A:GLU:HB3	1:124:A:TYR:HE2	7	0.15
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	10	0.15
(2,579)	1:111:A:THR:HG21	1:111:A:THR:HB	17	0.15
(2,570)	1:108:A:ASP:HA	1:107:A:VAL:HG22	3	0.15
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD21	9	0.15
(2,535)	1:99:A:THR:HG23	1:95:A:LYS:HB3	15	0.15
(2,534)	1:119:A:ARG:HG2	1:99:A:THR:HG21	2	0.15
(2,534)	1:99:A:THR:HG21	1:95:A:LYS:HD3	13	0.15
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	5	0.15
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	15	0.15
(2,501)	1:90:A:ILE:HD13	1:80:A:ASP:H	3	0.15
(2,495)	1:90:A:ILE:HD12	1:82:A:ALA:HA	16	0.15
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	12	0.15
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	14	0.15
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HB2	6	0.15
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD12	10	0.15
(2,418)	1:106:A:LYS:HG2	1:107:A:VAL:H	12	0.15
(2,378)	1:83:A:LEU:HD11	1:62:A:THR:HG21	8	0.15
(2,376)	1:67:A:THR:HG1	1:62:A:THR:HG21	9	0.15
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG11	18	0.15
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG22	18	0.15
(2,288)	1:36:A:ILE:HD13	1:37:A:LYS:H	7	0.15
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	9	0.15
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	14	0.15
(2,213)	1:23:A:LEU:HD23	1:19:A:PHE:HD2	9	0.15
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	1	0.15
(2,171)	1:15:A:ARG:HD2	1:16:A:ASP:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,162)	1:13:A:LEU:HD23	1:140:A:TYR:HA	19	0.15
(2,139)	1:139:A:TYR:HB2	1:124:A:TYR:HD2	8	0.15
(2,124)	1:10:A:THR:HB	1:143:A:GLN:HB3	17	0.15
(2,121)	1:142:A:LYS:HE2	1:9:A:GLY:HA2	13	0.15
(2,120)	1:8:A:LEU:HD11	1:47:A:ASN:HD21	15	0.15
(2,112)	1:7:A:PHE:H	1:8:A:LEU:HD23	10	0.15
(2,65)	1:1:A:LYS:HG2	1:1:A:LYS:HE3	6	0.15
(2,60)	1:0:A:SER:HB3	1:1:A:LYS:HB3	16	0.15
(2,33)	1:52:A:LYS:HG2	1:53:A:PRO:HD3	11	0.15
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	8	0.15
(2,23)	1:34:A:GLN:HG3	1:30:A:TRP:HZ2	14	0.15
(2,22)	1:34:A:GLN:HG2	1:30:A:TRP:HZ2	5	0.15
(2,3)	1:89:A:LYS:H	1:105:A:ILE:HG21	17	0.15
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG22	5	0.15
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG21	18	0.15
(1,2836)	2:1001:A:OLA:H183	1:36:A:ILE:HD12	2	0.15
(1,2814)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	3	0.15
(1,2809)	2:1001:A:OLA:H183	1:36:A:ILE:HD12	2	0.15
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	7	0.15
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H182	19	0.15
(1,2797)	1:116:A:TYR:HD2	1:118:A:TYR:HH	7	0.15
(1,2737)	1:86:A:THR:HG22	1:86:A:THR:H	17	0.15
(1,2413)	1:23:A:LEU:HD22	1:33:A:ARG:H	9	0.15
(1,2326)	1:74:A:LEU:HD12	1:2:A:THR:H	19	0.15
(1,2217)	1:66:A:ASP:H	1:83:A:LEU:HD22	16	0.15
(1,2213)	1:73:A:ALA:HB1	1:76:A:GLU:H	14	0.15
(1,2078)	1:76:A:GLU:H	1:91:A:THR:HG22	3	0.15
(1,2040)	1:48:A:ALA:HB2	1:50:A:SER:H	11	0.15
(1,2000)	1:8:A:LEU:HD21	1:47:A:ASN:HD21	17	0.15
(1,2000)	1:8:A:LEU:HD23	1:47:A:ASN:HD21	19	0.15
(1,1982)	1:8:A:LEU:HD11	1:47:A:ASN:HD22	6	0.15
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	19	0.15
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG22	17	0.15
(1,1680)	1:87:A:GLN:H	1:87:A:GLN:HE22	5	0.15
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	3	0.15
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	10	0.15
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	10	0.15
(1,1306)	1:125:A:LEU:H	1:125:A:LEU:HD11	10	0.15
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	4	0.15
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG22	1	0.15
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG22	15	0.15
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1168)	1:32:A:MET:HE1	1:35:A:VAL:H	7	0.15
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE3	8	0.15
(1,1104)	1:58:A:MET:HE2	1:118:A:TYR:HE1	20	0.15
(1,1064)	1:36:A:ILE:HD12	1:36:A:ILE:HA	9	0.15
(1,1037)	1:124:A:TYR:HE2	1:141:A:LYS:HD3	4	0.15
(1,1026)	1:137:A:SER:HB3	1:139:A:TYR:HE1	2	0.15
(1,1015)	1:137:A:SER:HB2	1:126:A:VAL:HG13	17	0.15
(1,989)	1:134:A:VAL:HG11	1:22:A:TYR:HB3	15	0.15
(1,968)	1:130:A:SER:HB2	1:131:A:TRP:H	15	0.15
(1,952)	1:129:A:MET:HB2	1:136:A:THR:HG22	14	0.15
(1,935)	1:121:A:ASP:HB3	1:126:A:VAL:HG11	13	0.15
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG11	2	0.15
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	1	0.15
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	12	0.15
(1,834)	1:108:A:ASP:H	1:107:A:VAL:HG12	16	0.15
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	4	0.15
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD23	9	0.15
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG22	8	0.15
(1,687)	1:86:A:THR:HG22	1:87:A:GLN:H	8	0.15
(1,636)	1:61:A:LEU:HD22	1:66:A:ASP:HB2	18	0.15
(1,620)	1:73:A:ALA:HB2	1:76:A:GLU:HB3	7	0.15
(1,616)	1:73:A:ALA:HB2	1:76:A:GLU:H	5	0.15
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	2	0.15
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	3	0.15
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	5	0.15
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	6	0.15
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	12	0.15
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	15	0.15
(1,615)	1:72:A:TRP:HZ3	1:72:A:TRP:HZ2	20	0.15
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	3	0.15
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	4	0.15
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	10	0.15
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE3	12	0.15
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	15	0.15
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD12	4	0.15
(1,375)	1:36:A:ILE:HD13	1:32:A:MET:HG3	11	0.15
(1,137)	1:3:A:LEU:HD21	1:7:A:PHE:HB3	2	0.15
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD11	6	0.15
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB1	13	0.15
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB3	1	0.15
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD12	2	0.15
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD11	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	8	0.15
(3,23)	1:114:A:GLU:H	1:104:A:HIS:O	3	0.14
(3,23)	1:114:A:GLU:H	1:104:A:HIS:O	19	0.14
(3,13)	1:48:A:ALA:H	1:55:A:ARG:O	19	0.14
(2,1679)	2:1001:A:OLA:H61	1:36:A:ILE:HG22	14	0.14
(2,1671)	1:24:A:LYS:HB3	1:24:A:LYS:HG2	14	0.14
(2,1647)	1:36:A:ILE:HD13	2:1001:A:OLA:H131	18	0.14
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	5	0.14
(2,1636)	1:64:A:LYS:HB2	1:62:A:THR:HG1	13	0.14
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H141	16	0.14
(2,1619)	1:84:A:ASP:HB3	2:1001:A:OLA:H131	20	0.14
(2,1606)	1:36:A:ILE:HD13	2:1001:A:OLA:H82	12	0.14
(2,1583)	2:1001:A:OLA:H161	2:1001:A:OLA:H21	19	0.14
(2,1556)	1:35:A:VAL:HG21	1:36:A:ILE:H	3	0.14
(2,1539)	1:120:A:ARG:H	1:121:A:ASP:HA	5	0.14
(2,1521)	1:7:A:PHE:H	1:6:A:LYS:HD3	17	0.14
(2,1489)	1:71:A:ASP:H	1:48:A:ALA:HB2	8	0.14
(2,1456)	1:95:A:LYS:HB2	1:93:A:ASP:H	16	0.14
(2,1369)	1:136:A:THR:H	1:134:A:VAL:HG11	19	0.14
(2,1332)	1:75:A:GLY:H	1:74:A:LEU:HD21	17	0.14
(2,1305)	1:116:A:TYR:H	1:127:A:MET:HG2	17	0.14
(2,1221)	1:89:A:LYS:HB3	1:78:A:PHE:H	5	0.14
(2,1221)	1:89:A:LYS:HB3	1:78:A:PHE:H	8	0.14
(2,1203)	1:112:A:ASP:H	1:106:A:LYS:HB3	12	0.14
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	16	0.14
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	20	0.14
(2,1170)	1:76:A:GLU:HA	1:73:A:ALA:H	2	0.14
(2,1169)	1:120:A:ARG:H	1:119:A:ARG:HB3	4	0.14
(2,1168)	1:128:A:LYS:HE2	1:135:A:SER:H	12	0.14
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD21	5	0.14
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD22	16	0.14
(2,1061)	1:118:A:TYR:HD1	1:128:A:LYS:H	17	0.14
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	13	0.14
(2,1031)	1:109:A:ASP:H	1:110:A:PRO:HB3	9	0.14
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD23	6	0.14
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	7	0.14
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	12	0.14
(2,930)	1:134:A:VAL:H	1:132:A:LYS:HB3	3	0.14
(2,930)	1:134:A:VAL:H	1:132:A:LYS:HB3	9	0.14
(2,916)	1:106:A:LYS:H	1:105:A:ILE:HG23	2	0.14
(2,840)	1:129:A:MET:HE2	1:114:A:GLU:HG3	14	0.14
(2,824)	1:127:A:MET:HA	1:118:A:TYR:HD2	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,792)	1:131:A:TRP:HB2	1:131:A:TRP:HZ3	3	0.14
(2,792)	1:131:A:TRP:HB2	1:131:A:TRP:HZ3	11	0.14
(2,779)	1:119:A:ARG:HA	1:119:A:ARG:HD2	18	0.14
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	13	0.14
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	17	0.14
(2,760)	1:127:A:MET:HE1	1:140:A:TYR:HH	4	0.14
(2,720)	1:14:A:GLU:H	1:124:A:TYR:HE2	9	0.14
(2,719)	1:124:A:TYR:HE2	1:141:A:LYS:HA	13	0.14
(2,697)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	12	0.14
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	14	0.14
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	7	0.14
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG23	15	0.14
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG23	17	0.14
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	20	0.14
(2,661)	1:128:A:LYS:HE2	1:135:A:SER:HB2	13	0.14
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	19	0.14
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD11	6	0.14
(2,535)	1:99:A:THR:HG21	1:95:A:LYS:HB3	20	0.14
(2,524)	1:95:A:LYS:H	1:95:A:LYS:HG3	17	0.14
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	4	0.14
(2,498)	1:90:A:ILE:HD12	1:78:A:PHE:HD2	20	0.14
(2,456)	1:85:A:SER:HA	1:81:A:GLU:HG2	4	0.14
(2,433)	1:85:A:SER:H	1:81:A:GLU:HG2	20	0.14
(2,421)	1:2:A:THR:HA	1:74:A:LEU:HD12	19	0.14
(2,413)	1:73:A:ALA:HB3	1:55:A:ARG:HD2	4	0.14
(2,385)	1:64:A:LYS:HG2	1:35:A:VAL:HG11	18	0.14
(2,350)	1:52:A:LYS:H	1:52:A:LYS:HD2	6	0.14
(2,318)	1:42:A:THR:HB	1:61:A:LEU:HB3	6	0.14
(2,301)	1:95:A:LYS:H	1:95:A:LYS:HE2	20	0.14
(2,296)	1:37:A:LYS:HA	1:36:A:ILE:HG23	7	0.14
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	7	0.14
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	10	0.14
(2,239)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	8	0.14
(2,213)	1:23:A:LEU:HD22	1:19:A:PHE:HD2	3	0.14
(2,197)	1:33:A:ARG:HD3	1:23:A:LEU:HA	17	0.14
(2,187)	1:21:A:GLU:HG3	1:134:A:VAL:HG12	13	0.14
(2,119)	1:8:A:LEU:HD13	1:46:A:ARG:H	17	0.14
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	18	0.14
(2,85)	1:125:A:LEU:HD13	1:140:A:TYR:HD2	16	0.14
(2,82)	1:125:A:LEU:HD13	1:120:A:ARG:HD3	17	0.14
(2,53)	1:33:A:ARG:HD3	1:30:A:TRP:HA	15	0.14
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2841)	1:36:A:ILE:HD11	2:1001:A:OLA:H10	2	0.14
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG23	9	0.14
(1,2836)	2:1001:A:OLA:H183	1:36:A:ILE:HD13	3	0.14
(1,2826)	1:127:A:MET:HE1	1:118:A:TYR:HH	13	0.14
(1,2809)	2:1001:A:OLA:H183	1:36:A:ILE:HD13	3	0.14
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H182	9	0.14
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H182	10	0.14
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H181	13	0.14
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	9	0.14
(1,2766)	1:111:A:THR:HG21	1:112:A:ASP:H	15	0.14
(1,2590)	1:6:A:LYS:HG2	1:7:A:PHE:H	2	0.14
(1,2429)	1:65:A:LYS:HA	1:66:A:ASP:H	13	0.14
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	12	0.14
(1,2162)	1:2:A:THR:HB	1:2:A:THR:H	11	0.14
(1,2028)	1:68:A:HIS:H	1:67:A:THR:HG23	3	0.14
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	7	0.14
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	17	0.14
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG23	9	0.14
(1,1875)	1:17:A:GLU:H	1:17:A:GLU:HG3	20	0.14
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	3	0.14
(1,1643)	1:19:A:PHE:H	1:19:A:PHE:HD1	14	0.14
(1,1483)	1:14:A:GLU:HA	1:14:A:GLU:HG2	4	0.14
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	6	0.14
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	13	0.14
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	17	0.14
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	6	0.14
(1,1367)	2:1001:A:OLA:H9	1:36:A:ILE:HD11	17	0.14
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD12	19	0.14
(1,1249)	1:3:A:LEU:HD21	1:3:A:LEU:H	7	0.14
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	17	0.14
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG22	17	0.14
(1,1183)	1:35:A:VAL:HB	1:32:A:MET:HE3	13	0.14
(1,1156)	1:127:A:MET:HG2	1:128:A:LYS:H	10	0.14
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	3	0.14
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	5	0.14
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	13	0.14
(1,1037)	1:124:A:TYR:HE2	1:141:A:LYS:HD3	8	0.14
(1,1037)	1:124:A:TYR:HE2	1:141:A:LYS:HD3	18	0.14
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	1	0.14
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	3	0.14
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	10	0.14
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1002)	1:22:A:TYR:H	1:136:A:THR:HG21	19	0.14
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	4	0.14
(1,989)	1:134:A:VAL:HG11	1:22:A:TYR:HB3	17	0.14
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG11	3	0.14
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG13	6	0.14
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	19	0.14
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG23	9	0.14
(1,772)	1:118:A:TYR:H	1:99:A:THR:HG21	8	0.14
(1,719)	1:90:A:ILE:HG23	1:104:A:HIS:HD2	8	0.14
(1,616)	1:73:A:ALA:HB3	1:76:A:GLU:H	2	0.14
(1,616)	1:73:A:ALA:HB2	1:76:A:GLU:H	18	0.14
(1,571)	1:65:A:LYS:HD3	1:66:A:ASP:H	9	0.14
(1,571)	1:65:A:LYS:HD3	1:66:A:ASP:H	17	0.14
(1,448)	1:41:A:VAL:HG21	1:140:A:TYR:HE1	10	0.14
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	7	0.14
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE1	16	0.14
(1,441)	1:38:A:LEU:HD23	1:38:A:LEU:HA	2	0.14
(1,393)	1:35:A:VAL:HB	1:35:A:VAL:H	18	0.14
(1,383)	1:23:A:LEU:HD21	1:33:A:ARG:HA	19	0.14
(1,305)	1:131:A:TRP:HE1	1:25:A:ALA:HB2	12	0.14
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	11	0.14
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	14	0.14
(1,63)	1:4:A:PRO:HG3	1:7:A:PHE:HD2	5	0.14
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD11	1	0.14
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	3	0.14
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	14	0.14
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD11	16	0.14
(1,17)	1:31:A:ILE:HD13	1:31:A:ILE:HA	9	0.14
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD11	7	0.14
(1,11)	1:32:A:MET:HG3	1:31:A:ILE:HG21	13	0.14
(3,89)	1:117:A:GLU:H	1:128:A:LYS:O	5	0.13
(3,53)	1:70:A:LYS:H	1:68:A:HIS:O	5	0.13
(3,19)	1:82:A:ALA:H	1:86:A:THR:O	1	0.13
(2,1678)	1:10:A:THR:HG22	1:44:A:LYS:HG2	20	0.13
(2,1675)	2:1001:A:OLA:H172	2:1001:A:OLA:H183	9	0.13
(2,1671)	2:1001:A:OLA:H82	2:1001:A:OLA:H71	10	0.13
(2,1671)	2:1001:A:OLA:H42	2:1001:A:OLA:H22	17	0.13
(2,1671)	2:1001:A:OLA:H122	2:1001:A:OLA:H111	20	0.13
(2,1640)	1:140:A:TYR:HH	2:1001:A:OLA:H32	4	0.13
(2,1639)	1:62:A:THR:HA	1:62:A:THR:HG1	9	0.13
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H131	17	0.13
(2,1619)	1:84:A:ASP:HB3	2:1001:A:OLA:H131	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1580)	1:129:A:MET:HE1	2:1001:A:OLA:H181	8	0.13
(2,1564)	2:1001:A:OLA:H81	1:83:A:LEU:HD11	10	0.13
(2,1461)	1:136:A:THR:H	1:128:A:LYS:HB3	16	0.13
(2,1456)	1:95:A:LYS:HB2	1:93:A:ASP:H	11	0.13
(2,1390)	1:53:A:PRO:HG2	1:54:A:ASP:H	5	0.13
(2,1267)	1:80:A:ASP:H	1:82:A:ALA:HB2	9	0.13
(2,1179)	1:100:A:LEU:H	1:94:A:LEU:HD12	10	0.13
(2,1162)	1:86:A:THR:HG22	1:85:A:SER:H	20	0.13
(2,1155)	1:60:A:ASN:H	1:83:A:LEU:HD23	20	0.13
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	2	0.13
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD21	7	0.13
(2,1074)	1:95:A:LYS:HB2	1:96:A:ASP:H	7	0.13
(2,936)	1:67:A:THR:H	1:83:A:LEU:HD13	18	0.13
(2,928)	1:90:A:ILE:H	1:89:A:LYS:HE3	1	0.13
(2,928)	1:89:A:LYS:HE2	1:90:A:ILE:H	8	0.13
(2,837)	1:58:A:MET:HE1	1:60:A:ASN:HD21	4	0.13
(2,803)	1:1:A:LYS:HA	1:-2:A:HIS:HB3	19	0.13
(2,774)	1:119:A:ARG:HA	1:119:A:ARG:HG3	16	0.13
(2,751)	1:104:A:HIS:HE1	1:83:A:LEU:HD21	10	0.13
(2,701)	1:143:A:GLN:HG3	1:11:A:PHE:HA	15	0.13
(2,694)	1:141:A:LYS:HE2	1:141:A:LYS:H	10	0.13
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	17	0.13
(2,674)	1:16:A:ASP:HA	1:139:A:TYR:HE1	19	0.13
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB2	4	0.13
(2,671)	1:137:A:SER:HB3	1:17:A:GLU:HB2	6	0.13
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	18	0.13
(2,660)	1:135:A:SER:HB3	1:128:A:LYS:HE2	17	0.13
(2,623)	1:121:A:ASP:HB2	1:126:A:VAL:HG12	12	0.13
(2,617)	1:120:A:ARG:H	1:125:A:LEU:HD23	18	0.13
(2,612)	1:125:A:LEU:HD23	1:125:A:LEU:HB3	6	0.13
(2,612)	1:125:A:LEU:HD21	1:125:A:LEU:HB3	7	0.13
(2,607)	1:124:A:TYR:HE2	1:141:A:LYS:HG3	15	0.13
(2,597)	1:118:A:TYR:HD1	1:127:A:MET:HG3	18	0.13
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	3	0.13
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	6	0.13
(2,501)	1:90:A:ILE:HD13	1:80:A:ASP:H	19	0.13
(2,457)	1:86:A:THR:HB	1:87:A:GLN:HG2	12	0.13
(2,446)	1:83:A:LEU:HD11	1:60:A:ASN:HD21	12	0.13
(2,433)	1:85:A:SER:H	1:81:A:GLU:HG2	18	0.13
(2,413)	1:73:A:ALA:HB3	1:54:A:ASP:HB3	16	0.13
(2,405)	1:66:A:ASP:HA	1:61:A:LEU:HB2	13	0.13
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG12	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG11	17	0.13
(2,299)	1:37:A:LYS:HG3	1:36:A:ILE:HG22	16	0.13
(2,282)	1:19:A:PHE:HD2	1:36:A:ILE:HG23	7	0.13
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	2	0.13
(2,239)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	6	0.13
(2,231)	1:25:A:ALA:HB2	1:134:A:VAL:HG22	4	0.13
(2,231)	1:25:A:ALA:HB1	1:134:A:VAL:HG23	5	0.13
(2,226)	1:134:A:VAL:HG23	1:25:A:ALA:HA	5	0.13
(2,212)	1:23:A:LEU:HD22	1:26:A:ARG:H	5	0.13
(2,212)	1:23:A:LEU:HD23	1:26:A:ARG:H	15	0.13
(2,203)	1:23:A:LEU:HD13	1:19:A:PHE:HE2	8	0.13
(2,178)	1:134:A:VAL:HG11	1:18:A:ASN:HB2	19	0.13
(2,169)	1:15:A:ARG:HD2	1:139:A:TYR:HD1	18	0.13
(2,155)	1:12:A:LYS:HE2	1:12:A:LYS:HA	5	0.13
(2,130)	1:11:A:PHE:HA	1:142:A:LYS:HG2	3	0.13
(2,121)	1:9:A:GLY:HA2	1:142:A:LYS:HE3	2	0.13
(2,73)	1:8:A:LEU:HD13	1:3:A:LEU:HD12	1	0.13
(2,66)	1:12:A:LYS:HG3	1:141:A:LYS:HG3	4	0.13
(2,52)	1:49:A:ALA:HB1	1:50:A:SER:HB3	18	0.13
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	6	0.13
(2,4)	1:33:A:ARG:H	1:31:A:ILE:HG21	19	0.13
(1,2839)	2:1001:A:OLA:H181	1:19:A:PHE:HE1	7	0.13
(1,2837)	2:1001:A:OLA:H9	1:36:A:ILE:HG23	12	0.13
(1,2826)	1:127:A:MET:HE1	1:118:A:TYR:HH	10	0.13
(1,2548)	1:112:A:ASP:H	1:106:A:LYS:HD2	17	0.13
(1,2548)	1:112:A:ASP:H	1:106:A:LYS:HD2	19	0.13
(1,2497)	1:78:A:PHE:H	1:77:A:GLU:HG2	14	0.13
(1,2429)	1:65:A:LYS:HA	1:66:A:ASP:H	18	0.13
(1,2413)	1:23:A:LEU:HD22	1:33:A:ARG:H	20	0.13
(1,2331)	1:60:A:ASN:HB3	1:67:A:THR:H	9	0.13
(1,2293)	1:124:A:TYR:HE1	1:124:A:TYR:H	11	0.13
(1,2000)	1:8:A:LEU:HD23	1:47:A:ASN:HD21	18	0.13
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	5	0.13
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	16	0.13
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG22	11	0.13
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	1	0.13
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	2	0.13
(1,1643)	1:19:A:PHE:H	1:19:A:PHE:HD1	17	0.13
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	9	0.13
(1,1536)	1:14:A:GLU:H	1:14:A:GLU:HG2	3	0.13
(1,1456)	1:103:A:THR:HG21	1:104:A:HIS:H	13	0.13
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	10	0.13
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD12	19	0.13
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	5	0.13
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	7	0.13
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	11	0.13
(1,1386)	1:83:A:LEU:HD13	1:84:A:ASP:H	10	0.13
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	7	0.13
(1,1373)	1:127:A:MET:H	1:126:A:VAL:HG13	7	0.13
(1,1362)	1:3:A:LEU:HA	1:74:A:LEU:HD11	10	0.13
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	11	0.13
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	16	0.13
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	18	0.13
(1,1249)	1:3:A:LEU:HD22	1:3:A:LEU:H	18	0.13
(1,1249)	1:3:A:LEU:HD21	1:3:A:LEU:H	19	0.13
(1,1240)	1:125:A:LEU:HD22	1:120:A:ARG:HD2	20	0.13
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG21	8	0.13
(1,1228)	1:139:A:TYR:HE2	1:126:A:VAL:HG21	3	0.13
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	7	0.13
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG22	16	0.13
(1,1194)	1:139:A:TYR:HE2	1:126:A:VAL:HG21	3	0.13
(1,1186)	1:127:A:MET:HE1	1:125:A:LEU:HD11	14	0.13
(1,1168)	1:32:A:MET:HE1	1:35:A:VAL:H	17	0.13
(1,1148)	1:37:A:LYS:H	1:36:A:ILE:HG21	10	0.13
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE1	6	0.13
(1,1106)	1:58:A:MET:HE2	1:45:A:PHE:HE1	1	0.13
(1,1106)	1:58:A:MET:HE3	1:45:A:PHE:HE1	7	0.13
(1,1102)	1:58:A:MET:HE2	1:60:A:ASN:H	19	0.13
(1,1064)	1:36:A:ILE:HD13	1:36:A:ILE:HA	20	0.13
(1,1057)	1:143:A:GLN:HB3	1:10:A:THR:HG22	8	0.13
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	6	0.13
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	20	0.13
(1,993)	1:135:A:SER:H	1:135:A:SER:HB2	16	0.13
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	1	0.13
(1,968)	1:130:A:SER:HB2	1:131:A:TRP:H	3	0.13
(1,931)	1:119:A:ARG:H	1:126:A:VAL:HG13	5	0.13
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	4	0.13
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	14	0.13
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	19	0.13
(1,839)	1:108:A:ASP:HA	1:108:A:ASP:HB3	2	0.13
(1,839)	1:108:A:ASP:HA	1:108:A:ASP:HB3	3	0.13
(1,839)	1:108:A:ASP:HA	1:108:A:ASP:HB3	8	0.13
(1,839)	1:108:A:ASP:HA	1:108:A:ASP:HB3	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,839)	1:108:A:ASP:HA	1:108:A:ASP:HB3	13	0.13
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG11	3	0.13
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	18	0.13
(1,790)	1:100:A:LEU:H	1:100:A:LEU:HD22	1	0.13
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG22	16	0.13
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG12	5	0.13
(1,620)	1:73:A:ALA:HB3	1:76:A:GLU:HB3	9	0.13
(1,597)	1:70:A:LYS:HD2	1:70:A:LYS:HE3	2	0.13
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	5	0.13
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	11	0.13
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE1	18	0.13
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	20	0.13
(1,431)	1:19:A:PHE:HD2	1:37:A:LYS:HG2	20	0.13
(1,425)	1:37:A:LYS:HA	1:19:A:PHE:HE2	12	0.13
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB3	5	0.13
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	2	0.13
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	9	0.13
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	16	0.13
(1,110)	1:71:A:ASP:HB3	1:48:A:ALA:HB3	9	0.13
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB1	3	0.13
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	9	0.13
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	10	0.13
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	19	0.13
(1,81)	1:97:A:PRO:HD2	1:96:A:ASP:HB3	7	0.13
(1,81)	1:97:A:PRO:HD2	1:96:A:ASP:HB3	20	0.13
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD13	4	0.13
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD11	8	0.13
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	13	0.13
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	17	0.13
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	20	0.13
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	14	0.13
(3,89)	1:117:A:GLU:H	1:128:A:LYS:O	18	0.12
(3,43)	1:55:A:ARG:H	1:53:A:PRO:O	12	0.12
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	4	0.12
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	7	0.12
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	16	0.12
(2,1671)	2:1001:A:OLA:H82	2:1001:A:OLA:H61	11	0.12
(2,1651)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	18	0.12
(2,1622)	1:84:A:ASP:HB2	2:1001:A:OLA:H142	5	0.12
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	10	0.12
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	13	0.12
(2,1620)	1:19:A:PHE:HZ	2:1001:A:OLA:H161	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1617)	1:36:A:ILE:HA	2:1001:A:OLA:H71	13	0.12
(2,1496)	1:70:A:LYS:HD2	1:70:A:LYS:H	8	0.12
(2,1487)	1:65:A:LYS:H	1:35:A:VAL:HG13	15	0.12
(2,1419)	1:42:A:THR:HG22	1:43:A:LYS:H	19	0.12
(2,1351)	1:80:A:ASP:H	1:89:A:LYS:HB2	5	0.12
(2,1332)	1:75:A:GLY:H	1:91:A:THR:HG23	14	0.12
(2,1315)	1:105:A:ILE:HG13	1:113:A:VAL:H	5	0.12
(2,1305)	1:116:A:TYR:H	1:127:A:MET:HG2	14	0.12
(2,1259)	1:120:A:ARG:H	1:7:A:PHE:HD1	14	0.12
(2,1222)	1:118:A:TYR:HD1	1:119:A:ARG:H	14	0.12
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	4	0.12
(2,1193)	1:42:A:THR:HG21	1:61:A:LEU:H	20	0.12
(2,1153)	1:88:A:HIS:HB2	1:80:A:ASP:H	5	0.12
(2,1128)	1:34:A:GLN:HE22	1:31:A:ILE:HA	13	0.12
(2,1098)	1:132:A:LYS:HD2	1:131:A:TRP:HE1	14	0.12
(2,1094)	1:65:A:LYS:HG3	1:66:A:ASP:H	10	0.12
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	17	0.12
(2,1079)	1:89:A:LYS:H	1:77:A:GLU:HG3	20	0.12
(2,1017)	1:8:A:LEU:HD12	1:9:A:GLY:H	9	0.12
(2,904)	1:106:A:LYS:H	1:106:A:LYS:HE2	11	0.12
(2,894)	1:64:A:LYS:HG3	1:64:A:LYS:H	2	0.12
(2,830)	2:1001:A:OLA:H82	1:36:A:ILE:HA	11	0.12
(2,749)	1:19:A:PHE:HZ	1:36:A:ILE:HD11	16	0.12
(2,732)	1:58:A:MET:HE3	1:67:A:THR:HG1	8	0.12
(2,706)	1:41:A:VAL:HG21	1:62:A:THR:HG1	11	0.12
(2,701)	1:143:A:GLN:HG3	1:11:A:PHE:HA	5	0.12
(2,688)	1:141:A:LYS:HD3	1:141:A:LYS:HA	16	0.12
(2,675)	1:139:A:TYR:HE1	1:17:A:GLU:HA	13	0.12
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE1	9	0.12
(2,669)	1:137:A:SER:HB3	1:139:A:TYR:HE2	20	0.12
(2,668)	1:129:A:MET:HE1	1:136:A:THR:HG22	2	0.12
(2,623)	1:128:A:LYS:HE3	1:126:A:VAL:HG13	6	0.12
(2,622)	1:127:A:MET:HA	1:126:A:VAL:HG13	7	0.12
(2,615)	1:125:A:LEU:HD21	1:120:A:ARG:HA	11	0.12
(2,611)	1:125:A:LEU:HD22	1:118:A:TYR:HD1	7	0.12
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	18	0.12
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG21	14	0.12
(2,579)	1:111:A:THR:HG22	1:111:A:THR:HA	15	0.12
(2,571)	1:140:A:TYR:HB2	1:127:A:MET:HB2	2	0.12
(2,541)	1:100:A:LEU:HD21	1:118:A:TYR:HB2	7	0.12
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	11	0.12
(2,495)	1:90:A:ILE:HD11	1:82:A:ALA:HA	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,488)	1:102:A:GLU:HB3	1:90:A:ILE:HG22	4	0.12
(2,488)	1:102:A:GLU:HB3	1:90:A:ILE:HG22	18	0.12
(2,482)	1:90:A:ILE:HG21	1:78:A:PHE:HD1	6	0.12
(2,402)	1:66:A:ASP:HA	1:62:A:THR:HG22	17	0.12
(2,402)	1:66:A:ASP:HA	1:62:A:THR:HG21	18	0.12
(2,400)	1:83:A:LEU:HD12	1:65:A:LYS:HG2	6	0.12
(2,367)	1:83:A:LEU:H	1:83:A:LEU:HD13	16	0.12
(2,349)	1:52:A:LYS:H	1:52:A:LYS:HG3	14	0.12
(2,330)	1:127:A:MET:HG3	1:43:A:LYS:HE3	9	0.12
(2,313)	1:129:A:MET:HE1	1:22:A:TYR:HD1	3	0.12
(2,313)	1:129:A:MET:HE2	1:22:A:TYR:HD1	12	0.12
(2,310)	1:38:A:LEU:HD21	1:38:A:LEU:HG	1	0.12
(2,310)	1:38:A:LEU:HD22	1:38:A:LEU:HG	2	0.12
(2,310)	1:38:A:LEU:HD23	1:38:A:LEU:HG	14	0.12
(2,310)	1:38:A:LEU:HD23	1:38:A:LEU:HG	15	0.12
(2,310)	1:38:A:LEU:HD22	1:38:A:LEU:HG	18	0.12
(2,301)	1:37:A:LYS:H	1:37:A:LYS:HE3	6	0.12
(2,301)	1:37:A:LYS:H	1:37:A:LYS:HE3	17	0.12
(2,286)	2:1001:A:OLA:H41	1:36:A:ILE:HG23	19	0.12
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	12	0.12
(2,250)	1:26:A:ARG:HD2	1:131:A:TRP:HD1	5	0.12
(2,244)	1:131:A:TRP:HD1	1:26:A:ARG:HG2	14	0.12
(2,231)	1:25:A:ALA:HB2	1:134:A:VAL:HG23	7	0.12
(2,213)	1:23:A:LEU:HD22	1:19:A:PHE:HD2	19	0.12
(2,209)	1:23:A:LEU:HD13	1:36:A:ILE:HG22	18	0.12
(2,176)	1:17:A:GLU:HG3	1:17:A:GLU:HA	6	0.12
(2,130)	1:11:A:PHE:HA	1:142:A:LYS:HG2	7	0.12
(2,98)	1:8:A:LEU:HD22	1:5:A:ASP:HA	10	0.12
(2,85)	1:125:A:LEU:HD11	1:140:A:TYR:HD2	19	0.12
(2,68)	1:12:A:LYS:HE2	1:12:A:LYS:HD3	2	0.12
(2,56)	1:63:A:THR:HG22	1:40:A:GLY:HA2	7	0.12
(2,29)	1:4:A:PRO:HD3	1:94:A:LEU:HD11	1	0.12
(2,26)	1:94:A:LEU:HD13	1:4:A:PRO:HG3	19	0.12
(1,2825)	2:1001:A:OLA:H9	1:36:A:ILE:HD12	13	0.12
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	6	0.12
(1,2766)	1:111:A:THR:HG23	1:112:A:ASP:H	6	0.12
(1,2737)	1:86:A:THR:HG21	1:86:A:THR:H	8	0.12
(1,2413)	1:23:A:LEU:HD22	1:33:A:ARG:H	11	0.12
(1,2300)	1:90:A:ILE:HD11	1:90:A:ILE:H	9	0.12
(1,2132)	1:69:A:HIS:H	1:68:A:HIS:HD2	19	0.12
(1,2059)	1:143:A:GLN:H	1:142:A:LYS:HG2	20	0.12
(1,2041)	1:52:A:LYS:H	1:48:A:ALA:HB3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG22	18	0.12
(1,1643)	1:19:A:PHE:H	1:19:A:PHE:HD1	5	0.12
(1,1603)	1:86:A:THR:HG23	1:86:A:THR:H	14	0.12
(1,1603)	1:86:A:THR:HG21	1:86:A:THR:H	18	0.12
(1,1456)	1:103:A:THR:HG22	1:104:A:HIS:H	18	0.12
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	7	0.12
(1,1421)	1:3:A:LEU:HA	1:74:A:LEU:HD11	10	0.12
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD12	18	0.12
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	8	0.12
(1,1249)	1:3:A:LEU:HD22	1:3:A:LEU:H	5	0.12
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	16	0.12
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	11	0.12
(1,1195)	1:31:A:ILE:HA	1:31:A:ILE:HG23	19	0.12
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE1	10	0.12
(1,1167)	1:28:A:TYR:HD2	1:32:A:MET:HE3	20	0.12
(1,1134)	1:102:A:GLU:HG2	1:104:A:HIS:HD2	19	0.12
(1,1109)	1:60:A:ASN:HA	1:58:A:MET:HE2	13	0.12
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	4	0.12
(1,1037)	1:124:A:TYR:HE2	1:141:A:LYS:HD3	20	0.12
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	10	0.12
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	11	0.12
(1,995)	1:136:A:THR:H	1:135:A:SER:HB2	19	0.12
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	2	0.12
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	15	0.12
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	2	0.12
(1,954)	1:129:A:MET:HG3	1:116:A:TYR:HD1	14	0.12
(1,932)	1:137:A:SER:HA	1:126:A:VAL:HG11	10	0.12
(1,888)	1:118:A:TYR:HB3	1:100:A:LEU:HB2	2	0.12
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	13	0.12
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG11	4	0.12
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	14	0.12
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD12	5	0.12
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD13	20	0.12
(1,815)	1:105:A:ILE:H	1:105:A:ILE:HG21	11	0.12
(1,675)	1:101:A:THR:H	1:94:A:LEU:HD23	4	0.12
(1,633)	1:74:A:LEU:H	1:74:A:LEU:HD23	15	0.12
(1,628)	1:74:A:LEU:HD13	1:74:A:LEU:H	15	0.12
(1,621)	1:76:A:GLU:HG3	1:73:A:ALA:HB2	17	0.12
(1,593)	1:70:A:LYS:HG2	1:70:A:LYS:HE3	18	0.12
(1,569)	1:65:A:LYS:HA	1:65:A:LYS:HD2	7	0.12
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD13	11	0.12
(1,398)	1:35:A:VAL:HA	1:35:A:VAL:HG12	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,398)	1:35:A:VAL:HA	1:35:A:VAL:HG12	20	0.12
(1,369)	1:32:A:MET:H	1:32:A:MET:HG3	14	0.12
(1,304)	1:22:A:TYR:H	1:25:A:ALA:HB2	6	0.12
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	15	0.12
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	17	0.12
(1,203)	1:125:A:LEU:H	1:124:A:TYR:HD2	9	0.12
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	1	0.12
(1,120)	1:1:A:LYS:HG3	1:1:A:LYS:HA	9	0.12
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB2	20	0.12
(1,101)	1:49:A:ALA:H	1:48:A:ALA:HB2	1	0.12
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	3	0.12
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	5	0.12
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	8	0.12
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	13	0.12
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	17	0.12
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	18	0.12
(1,81)	1:97:A:PRO:HD2	1:96:A:ASP:HB3	15	0.12
(1,26)	1:30:A:TRP:HH2	1:31:A:ILE:HG12	19	0.12
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	6	0.12
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD11	15	0.12
(1,19)	1:31:A:ILE:HG12	1:31:A:ILE:HD12	19	0.12
(1,15)	1:30:A:TRP:HZ3	1:31:A:ILE:HD13	9	0.12
(1,5)	1:31:A:ILE:H	1:31:A:ILE:HG22	4	0.12
(3,67)	1:89:A:LYS:H	1:105:A:ILE:O	7	0.11
(3,67)	1:89:A:LYS:H	1:105:A:ILE:O	12	0.11
(3,33)	1:23:A:LEU:H	1:20:A:ASP:O	3	0.11
(3,33)	1:23:A:LEU:H	1:20:A:ASP:O	18	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	2	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	6	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	11	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	12	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	13	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	14	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	15	0.11
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	19	0.11
(2,1679)	2:1001:A:OLA:H71	1:36:A:ILE:HG23	10	0.11
(2,1679)	2:1001:A:OLA:H41	2:1001:A:OLA:H182	16	0.11
(2,1674)	1:129:A:MET:HE2	2:1001:A:OLA:H181	20	0.11
(2,1665)	1:22:A:TYR:HD1	2:1001:A:OLA:H182	9	0.11
(2,1652)	2:1001:A:OLA:H142	1:32:A:MET:HE1	13	0.11
(2,1644)	2:1001:A:OLA:H10	2:1001:A:OLA:H111	7	0.11
(2,1642)	1:43:A:LYS:HD3	1:118:A:TYR:HH	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1634)	1:22:A:TYR:HD1	2:1001:A:OLA:H183	6	0.11
(2,1602)	1:32:A:MET:HE1	2:1001:A:OLA:H111	13	0.11
(2,1599)	1:94:A:LEU:HD11	1:100:A:LEU:HB3	3	0.11
(2,1596)	2:1001:A:OLA:H31	2:1001:A:OLA:H182	12	0.11
(2,1577)	2:1001:A:OLA:H72	1:36:A:ILE:HG22	4	0.11
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	6	0.11
(2,1534)	1:28:A:TYR:H	1:33:A:ARG:HD2	10	0.11
(2,1478)	1:45:A:PHE:HD1	1:11:A:PHE:H	10	0.11
(2,1471)	1:101:A:THR:HG23	1:93:A:ASP:H	18	0.11
(2,1471)	1:101:A:THR:HG23	1:93:A:ASP:H	19	0.11
(2,1442)	1:64:A:LYS:HG3	1:64:A:LYS:H	2	0.11
(2,1401)	1:115:A:THR:H	1:113:A:VAL:HG12	20	0.11
(2,1387)	1:131:A:TRP:HE1	1:26:A:ARG:HD2	10	0.11
(2,1349)	1:25:A:ALA:H	1:24:A:LYS:HG2	12	0.11
(2,1325)	1:129:A:MET:HE1	1:130:A:SER:H	3	0.11
(2,1232)	1:85:A:SER:H	1:81:A:GLU:HB3	8	0.11
(2,1206)	1:65:A:LYS:H	1:64:A:LYS:HB3	19	0.11
(2,1203)	1:112:A:ASP:H	1:106:A:LYS:HB3	5	0.11
(2,1197)	1:33:A:ARG:HG2	1:34:A:GLN:H	12	0.11
(2,1162)	1:67:A:THR:HG23	1:85:A:SER:H	16	0.11
(2,1157)	1:26:A:ARG:HD2	1:26:A:ARG:H	13	0.11
(2,1157)	1:26:A:ARG:HD3	1:26:A:ARG:H	20	0.11
(2,1099)	1:61:A:LEU:H	1:61:A:LEU:HD21	9	0.11
(2,1074)	1:95:A:LYS:HB2	1:96:A:ASP:H	1	0.11
(2,1074)	1:95:A:LYS:HB2	1:96:A:ASP:H	5	0.11
(2,1074)	1:95:A:LYS:HB2	1:96:A:ASP:H	10	0.11
(2,1074)	1:95:A:LYS:HB2	1:96:A:ASP:H	18	0.11
(2,1070)	1:17:A:GLU:H	1:139:A:TYR:HE1	15	0.11
(2,1053)	1:42:A:THR:H	1:63:A:THR:H	3	0.11
(2,1048)	1:143:A:GLN:H	1:12:A:LYS:HB2	13	0.11
(2,1040)	1:34:A:GLN:HE21	1:35:A:VAL:HG23	14	0.11
(2,1001)	1:59:A:GLU:H	1:58:A:MET:HG3	11	0.11
(2,961)	1:135:A:SER:H	1:134:A:VAL:HG12	1	0.11
(2,845)	1:88:A:HIS:HD2	1:107:A:VAL:H	8	0.11
(2,837)	1:58:A:MET:HE2	1:60:A:ASN:HD21	16	0.11
(2,808)	1:78:A:PHE:H	1:77:A:GLU:HG2	18	0.11
(2,752)	1:69:A:HIS:HE1	1:67:A:THR:HG21	3	0.11
(2,743)	1:104:A:HIS:HD2	1:102:A:GLU:HG3	16	0.11
(2,731)	1:58:A:MET:HE3	1:61:A:LEU:H	20	0.11
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG21	5	0.11
(2,666)	1:136:A:THR:HA	1:136:A:THR:HG22	13	0.11
(2,661)	1:128:A:LYS:HE2	1:135:A:SER:HB2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,630)	1:128:A:LYS:HB2	1:129:A:MET:H	15	0.11
(2,591)	1:118:A:TYR:HA	1:119:A:ARG:HB2	9	0.11
(2,583)	1:102:A:GLU:H	1:115:A:THR:HG22	13	0.11
(2,564)	1:88:A:HIS:HB2	1:107:A:VAL:HA	7	0.11
(2,557)	1:110:A:PRO:HB2	1:105:A:ILE:HD11	2	0.11
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD22	13	0.11
(2,531)	1:95:A:LYS:H	1:99:A:THR:HG23	12	0.11
(2,526)	1:95:A:LYS:HG2	1:99:A:THR:HB	16	0.11
(2,513)	1:95:A:LYS:H	1:94:A:LEU:HB2	5	0.11
(2,511)	1:92:A:PHE:HB3	1:100:A:LEU:HD13	5	0.11
(2,510)	1:92:A:PHE:HB3	1:74:A:LEU:HD23	12	0.11
(2,504)	1:77:A:GLU:HA	1:91:A:THR:HB	17	0.11
(2,501)	1:90:A:ILE:HD12	1:80:A:ASP:H	8	0.11
(2,500)	1:90:A:ILE:HD11	1:88:A:HIS:H	18	0.11
(2,460)	1:41:A:VAL:HG21	1:62:A:THR:HA	6	0.11
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	4	0.11
(2,459)	1:87:A:GLN:HB2	1:86:A:THR:HB	11	0.11
(2,421)	1:74:A:LEU:HA	1:74:A:LEU:HD12	4	0.11
(2,416)	1:77:A:GLU:H	1:73:A:ALA:HB2	7	0.11
(2,384)	1:64:A:LYS:HG2	1:65:A:LYS:H	20	0.11
(2,369)	1:62:A:THR:HA	1:41:A:VAL:HG13	19	0.11
(2,311)	1:67:A:THR:HG1	1:83:A:LEU:HD23	14	0.11
(2,310)	1:38:A:LEU:HD23	1:38:A:LEU:HG	5	0.11
(2,310)	1:38:A:LEU:HD22	1:38:A:LEU:HG	6	0.11
(2,310)	1:38:A:LEU:HD23	1:38:A:LEU:HG	8	0.11
(2,310)	1:38:A:LEU:HD22	1:38:A:LEU:HG	11	0.11
(2,310)	1:38:A:LEU:HD23	1:38:A:LEU:HG	16	0.11
(2,310)	1:38:A:LEU:HD21	1:38:A:LEU:HG	17	0.11
(2,310)	1:38:A:LEU:HD23	1:38:A:LEU:HG	19	0.11
(2,286)	2:1001:A:OLA:H71	1:36:A:ILE:HG21	1	0.11
(2,259)	1:28:A:TYR:HE2	1:32:A:MET:HG3	11	0.11
(2,253)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	15	0.11
(2,239)	1:26:A:ARG:HD2	1:26:A:ARG:HB2	11	0.11
(2,183)	1:21:A:GLU:HA	1:24:A:LYS:HE3	10	0.11
(2,177)	1:139:A:TYR:HE1	1:17:A:GLU:HG2	14	0.11
(2,155)	1:12:A:LYS:HA	1:12:A:LYS:HE3	12	0.11
(2,154)	1:13:A:LEU:H	1:12:A:LYS:HE3	18	0.11
(2,130)	1:11:A:PHE:HA	1:142:A:LYS:HG2	2	0.11
(2,122)	1:9:A:GLY:HA3	1:142:A:LYS:HE2	13	0.11
(2,120)	1:8:A:LEU:HD13	1:47:A:ASN:HD21	8	0.11
(2,98)	1:8:A:LEU:HD22	1:5:A:ASP:HA	8	0.11
(2,98)	1:8:A:LEU:HD21	1:5:A:ASP:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,97)	1:8:A:LEU:HB3	1:5:A:ASP:HA	1	0.11
(2,76)	1:3:A:LEU:HD12	1:45:A:PHE:HB2	8	0.11
(2,76)	1:3:A:LEU:HD12	1:45:A:PHE:HB2	12	0.11
(2,62)	1:0:A:SER:HB2	1:2:A:THR:H	10	0.11
(2,53)	1:33:A:ARG:HD3	1:30:A:TRP:HA	4	0.11
(2,52)	1:30:A:TRP:HA	1:33:A:ARG:HG2	5	0.11
(2,32)	1:97:A:PRO:HA	1:94:A:LEU:HG	19	0.11
(1,2814)	2:1001:A:OLA:H183	1:19:A:PHE:HE1	9	0.11
(1,2808)	1:28:A:TYR:HE1	2:1001:A:OLA:H183	18	0.11
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	13	0.11
(1,2737)	1:86:A:THR:HG21	1:86:A:THR:H	11	0.11
(1,2489)	1:13:A:LEU:HD21	1:17:A:GLU:H	14	0.11
(1,2403)	1:98:A:ASN:HB3	1:98:A:ASN:H	2	0.11
(1,2370)	1:2:A:THR:H	1:1:A:LYS:HB2	16	0.11
(1,2331)	1:60:A:ASN:HB3	1:67:A:THR:H	15	0.11
(1,1931)	1:10:A:THR:H	1:10:A:THR:HG23	6	0.11
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	15	0.11
(1,1688)	1:143:A:GLN:HA	1:143:A:GLN:HE22	10	0.11
(1,1688)	1:143:A:GLN:HA	1:143:A:GLN:HE22	16	0.11
(1,1538)	1:16:A:ASP:H	1:15:A:ARG:HB2	9	0.11
(1,1483)	1:14:A:GLU:HA	1:14:A:GLU:HG2	18	0.11
(1,1456)	1:103:A:THR:HG21	1:104:A:HIS:H	16	0.11
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	16	0.11
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	19	0.11
(1,1436)	1:2:A:THR:HB	1:3:A:LEU:H	20	0.11
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	11	0.11
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	1	0.11
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	9	0.11
(1,1389)	1:65:A:LYS:HA	1:66:A:ASP:H	17	0.11
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	4	0.11
(1,1385)	1:3:A:LEU:H	1:3:A:LEU:HD13	19	0.11
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	2	0.11
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	5	0.11
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	6	0.11
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	12	0.11
(1,1234)	1:101:A:THR:HA	1:115:A:THR:HG23	11	0.11
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	1	0.11
(1,1224)	1:38:A:LEU:H	1:39:A:ALA:HB3	15	0.11
(1,1200)	1:25:A:ALA:H	1:24:A:LYS:HG2	16	0.11
(1,1183)	1:35:A:VAL:HB	1:32:A:MET:HE2	5	0.11
(1,1099)	1:58:A:MET:HE3	1:60:A:ASN:HD22	1	0.11
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1049)	1:12:A:LYS:H	1:143:A:GLN:HG3	20	0.11
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	12	0.11
(1,1036)	1:124:A:TYR:HE2	1:141:A:LYS:HD2	16	0.11
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	1	0.11
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	3	0.11
(1,993)	1:135:A:SER:H	1:135:A:SER:HB2	2	0.11
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	4	0.11
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	8	0.11
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	10	0.11
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	14	0.11
(1,968)	1:130:A:SER:HB2	1:131:A:TRP:H	10	0.11
(1,954)	1:129:A:MET:HG3	1:116:A:TYR:HD1	19	0.11
(1,952)	1:129:A:MET:HB2	1:136:A:THR:HG23	8	0.11
(1,879)	1:101:A:THR:HB	1:115:A:THR:HG21	10	0.11
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	6	0.11
(1,851)	1:109:A:ASP:H	1:110:A:PRO:HD2	8	0.11
(1,839)	1:108:A:ASP:HA	1:108:A:ASP:HB3	5	0.11
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG13	11	0.11
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	12	0.11
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	13	0.11
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	15	0.11
(1,821)	1:110:A:PRO:HA	1:105:A:ILE:HD12	12	0.11
(1,793)	1:100:A:LEU:HD11	1:118:A:TYR:HB3	8	0.11
(1,773)	1:100:A:LEU:H	1:99:A:THR:HG23	12	0.11
(1,634)	1:106:A:LYS:HA	1:107:A:VAL:HG13	7	0.11
(1,629)	1:74:A:LEU:HD12	1:75:A:GLY:H	13	0.11
(1,597)	1:70:A:LYS:HD2	1:70:A:LYS:HE3	20	0.11
(1,444)	1:19:A:PHE:HZ	1:129:A:MET:HE2	6	0.11
(1,441)	1:38:A:LEU:HD21	1:38:A:LEU:HA	6	0.11
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD13	2	0.11
(1,416)	1:36:A:ILE:H	1:36:A:ILE:HD12	6	0.11
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD12	3	0.11
(1,414)	1:32:A:MET:H	1:36:A:ILE:HD11	13	0.11
(1,399)	1:35:A:VAL:H	1:35:A:VAL:HG12	18	0.11
(1,369)	1:32:A:MET:H	1:32:A:MET:HG3	16	0.11
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	13	0.11
(1,191)	1:10:A:THR:HB	1:143:A:GLN:H	4	0.11
(1,188)	1:8:A:LEU:HD11	1:56:A:TYR:HD2	16	0.11
(1,132)	1:72:A:TRP:HZ3	1:3:A:LEU:HD11	16	0.11
(1,128)	1:100:A:LEU:HD23	1:3:A:LEU:HD13	6	0.11
(1,103)	1:55:A:ARG:HA	1:48:A:ALA:HB2	16	0.11
(1,98)	1:71:A:ASP:H	1:48:A:ALA:HB2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:51:A:GLY:H	1:48:A:ALA:HB1	20	0.11
(1,84)	1:97:A:PRO:HD3	1:96:A:ASP:HB2	16	0.11
(1,82)	1:96:A:ASP:HB3	1:97:A:PRO:HD3	12	0.11
(1,81)	1:97:A:PRO:HD2	1:96:A:ASP:HB3	12	0.11
(3,67)	1:89:A:LYS:H	1:105:A:ILE:O	4	0.1
(3,33)	1:23:A:LEU:H	1:20:A:ASP:O	5	0.1
(3,33)	1:23:A:LEU:H	1:20:A:ASP:O	13	0.1
(3,5)	1:22:A:TYR:H	1:18:A:ASN:O	10	0.1
(2,1679)	2:1001:A:OLA:H62	1:36:A:ILE:HG22	17	0.1
(2,1669)	1:83:A:LEU:HG	1:83:A:LEU:HD11	20	0.1
(2,1638)	1:65:A:LYS:HA	1:62:A:THR:HG1	7	0.1
(2,1636)	1:83:A:LEU:HB3	1:62:A:THR:HG1	20	0.1
(2,1623)	2:1001:A:OLA:H82	1:36:A:ILE:HA	7	0.1
(2,1577)	1:83:A:LEU:HD13	2:1001:A:OLA:H72	9	0.1
(2,1568)	2:1001:A:OLA:H22	2:1001:A:OLA:H181	7	0.1
(2,1491)	1:142:A:LYS:H	1:141:A:LYS:HD3	18	0.1
(2,1419)	1:42:A:THR:HG23	1:43:A:LYS:H	8	0.1
(2,1325)	1:129:A:MET:HE1	1:130:A:SER:H	6	0.1
(2,1175)	1:64:A:LYS:H	1:83:A:LEU:HD13	13	0.1
(2,1168)	1:56:A:TYR:H	1:55:A:ARG:HD2	16	0.1
(2,1031)	1:109:A:ASP:H	1:110:A:PRO:HB3	5	0.1
(2,1018)	1:68:A:HIS:H	1:83:A:LEU:HD22	18	0.1
(2,789)	1:26:A:ARG:HD2	1:131:A:TRP:HZ3	14	0.1
(2,778)	1:119:A:ARG:HA	1:119:A:ARG:HD3	1	0.1
(2,743)	1:104:A:HIS:HD2	1:102:A:GLU:HG3	8	0.1
(2,682)	1:127:A:MET:HE2	1:140:A:TYR:HE2	13	0.1
(2,635)	1:130:A:SER:HB3	1:128:A:LYS:HD2	15	0.1
(2,569)	1:114:A:GLU:H	1:113:A:VAL:HG23	20	0.1
(2,540)	1:3:A:LEU:HA	1:100:A:LEU:HD23	6	0.1
(2,524)	1:95:A:LYS:H	1:95:A:LYS:HG3	20	0.1
(2,517)	1:95:A:LYS:H	1:94:A:LEU:HD21	6	0.1
(2,448)	1:84:A:ASP:HA	2:1001:A:OLA:H121	2	0.1
(2,447)	1:84:A:ASP:HA	2:1001:A:OLA:H112	20	0.1
(2,418)	1:106:A:LYS:HG2	1:107:A:VAL:H	10	0.1
(2,412)	1:73:A:ALA:HB2	1:55:A:ARG:H	19	0.1
(2,313)	1:129:A:MET:HE3	1:22:A:TYR:HD1	18	0.1
(2,310)	1:38:A:LEU:HD21	1:38:A:LEU:HG	4	0.1
(2,310)	1:38:A:LEU:HD21	1:38:A:LEU:HG	9	0.1
(2,310)	1:38:A:LEU:HB3	1:38:A:LEU:HD22	13	0.1
(2,301)	1:37:A:LYS:H	1:37:A:LYS:HE3	11	0.1
(2,297)	1:37:A:LYS:HG3	1:19:A:PHE:HD2	20	0.1
(2,236)	1:27:A:GLY:HA2	1:26:A:ARG:HA	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,226)	1:134:A:VAL:HG22	1:25:A:ALA:HA	8	0.1
(2,219)	1:23:A:LEU:HD22	1:36:A:ILE:HB	8	0.1
(2,203)	1:23:A:LEU:HD12	1:19:A:PHE:HE2	12	0.1
(2,162)	1:13:A:LEU:HD21	1:140:A:TYR:HA	15	0.1
(1,2820)	1:36:A:ILE:HD13	1:36:A:ILE:HB	7	0.1
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	8	0.1
(1,2794)	1:89:A:LYS:HB3	1:107:A:VAL:HA	10	0.1
(1,1949)	1:54:A:ASP:H	1:55:A:ARG:H	2	0.1
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	8	0.1
(1,1785)	1:67:A:THR:H	1:66:A:ASP:HB3	11	0.1
(1,1643)	1:19:A:PHE:H	1:19:A:PHE:HD1	9	0.1
(1,1549)	1:44:A:LYS:HD2	1:44:A:LYS:H	18	0.1
(1,1461)	1:55:A:ARG:HG2	1:56:A:TYR:H	6	0.1
(1,1435)	1:59:A:GLU:H	1:58:A:MET:HG3	10	0.1
(1,1428)	1:4:A:PRO:HD3	1:3:A:LEU:HD13	17	0.1
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	1	0.1
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	15	0.1
(1,1287)	1:113:A:VAL:HB	1:113:A:VAL:H	19	0.1
(1,1171)	1:32:A:MET:HE1	1:33:A:ARG:H	8	0.1
(1,1168)	1:32:A:MET:HE3	1:35:A:VAL:H	14	0.1
(1,1148)	1:37:A:LYS:H	1:36:A:ILE:HG23	4	0.1
(1,1093)	1:39:A:ALA:HB2	1:62:A:THR:HA	13	0.1
(1,1080)	1:56:A:TYR:HD1	1:2:A:THR:HG22	1	0.1
(1,994)	1:135:A:SER:HB3	1:136:A:THR:H	17	0.1
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	3	0.1
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	9	0.1
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	11	0.1
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	18	0.1
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	19	0.1
(1,977)	1:131:A:TRP:HA	1:132:A:LYS:HA	20	0.1
(1,858)	1:109:A:ASP:HA	1:110:A:PRO:HG3	7	0.1
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	17	0.1
(1,837)	1:107:A:VAL:HB	1:107:A:VAL:HG12	20	0.1
(1,755)	1:94:A:LEU:HD11	1:4:A:PRO:HG3	15	0.1
(1,687)	1:86:A:THR:HG21	1:87:A:GLN:H	14	0.1
(1,411)	1:23:A:LEU:HD11	1:36:A:ILE:HG21	3	0.1
(1,369)	1:32:A:MET:H	1:32:A:MET:HG3	12	0.1
(1,310)	1:25:A:ALA:HB1	1:134:A:VAL:HB	12	0.1
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	14	0.1
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	18	0.1
(1,253)	1:21:A:GLU:HG3	1:21:A:GLU:HA	20	0.1
(1,137)	1:3:A:LEU:HD23	1:7:A:PHE:HB3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:7:A:PHE:H	1:3:A:LEU:HD12	5	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found