



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:57 PM UTC

PDB ID : 6G7G / pdb_00006g7g
BMRB ID : 27439
Title : Structure of SPH (Self-Incompatibility Protein Homologue) proteins, a widespread family of small, highly stable, secreted proteins from plants
Authors : Rajasekar, K.V.; Coulthard, R.J.; Ride, J.P.; Ji, S.; Winn, P.J.; Wheeler, M.P.; Hyde, E.I.; Smith, L.J.
Deposited on : 2018-04-06

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

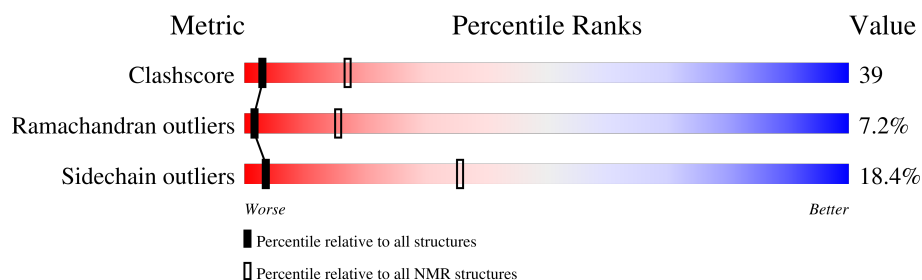
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 66%.

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	115	25% 50% 9% 17%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:48, A:56-A:76, A:85-A:115 (96)	1.95	7

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1908 atoms, of which 956 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S-protein homolog 15.

Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1908	603	956	175	166	8	

There are 3 discrepancies between the modelled and reference sequences:

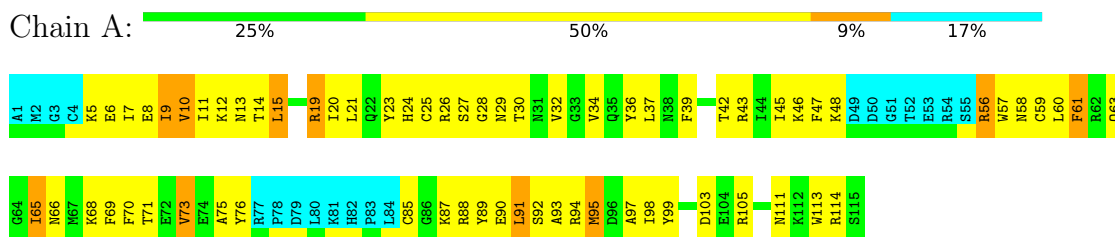
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP Q9FLY6
A	2	MET	-	expression tag	UNP Q9FLY6
A	3	GLY	-	expression tag	UNP Q9FLY6

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: S-protein homolog 15

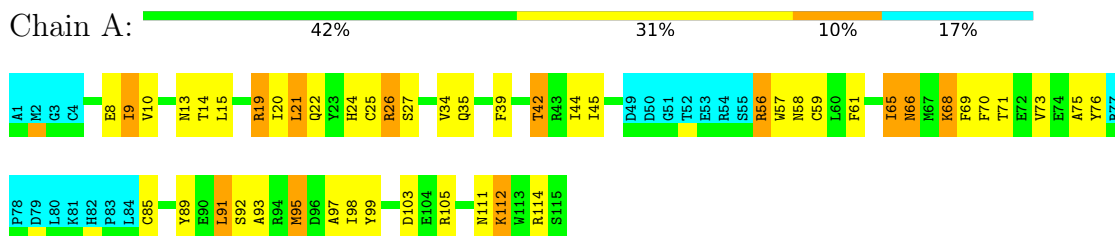


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

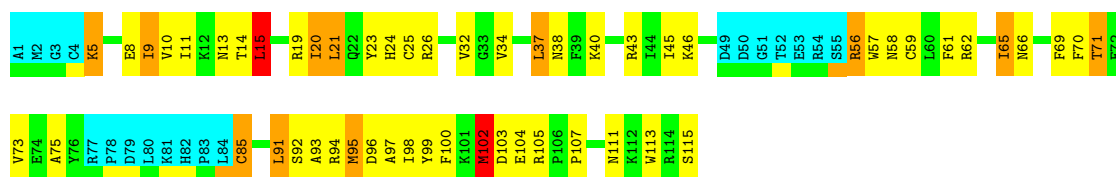
- Molecule 1: S-protein homolog 15



4.2.2 Score per residue for model 2

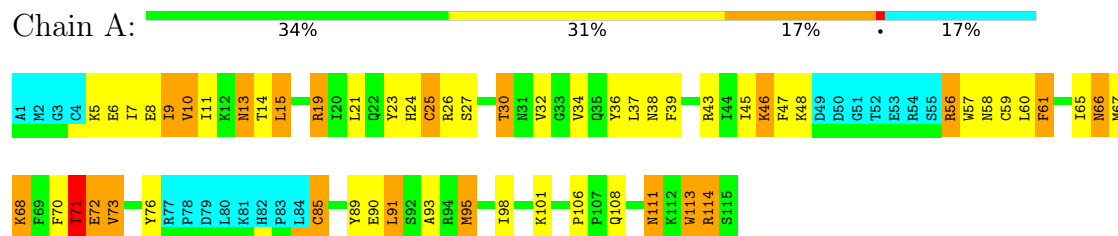
- Molecule 1: S-protein homolog 15





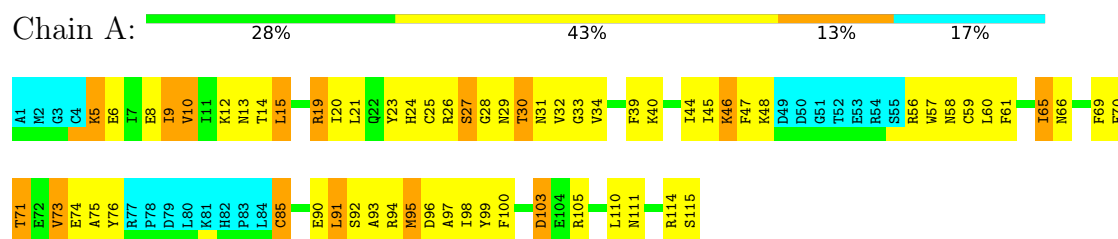
4.2.3 Score per residue for model 3

- Molecule 1: S-protein homolog 15



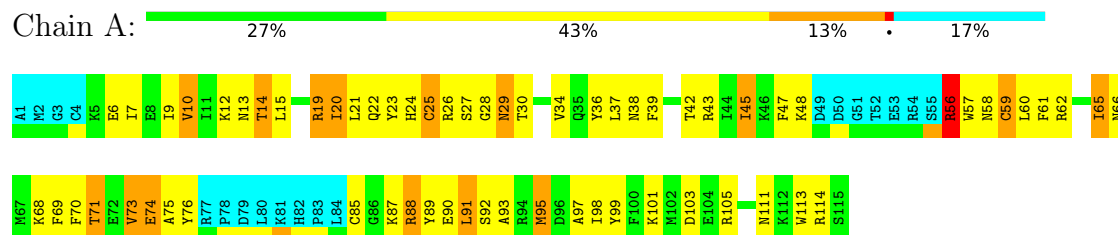
4.2.4 Score per residue for model 4

- Molecule 1: S-protein homolog 15



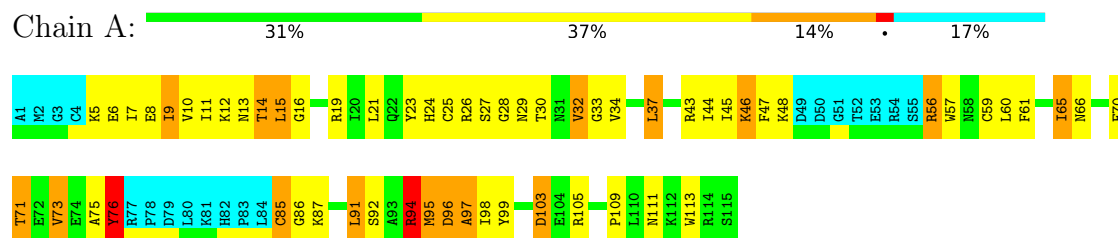
4.2.5 Score per residue for model 5

- Molecule 1: S-protein homolog 15



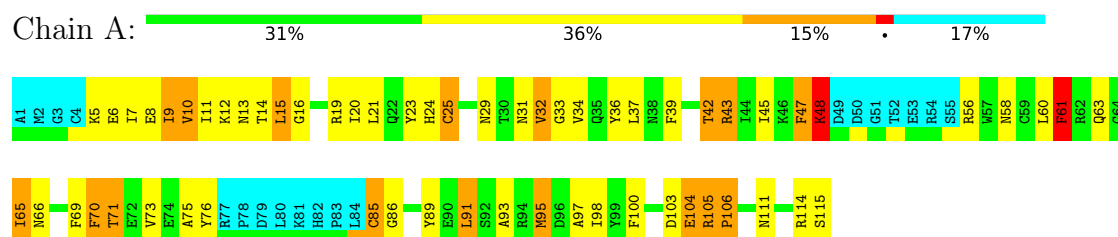
4.2.6 Score per residue for model 6

- Molecule 1: S-protein homolog 15



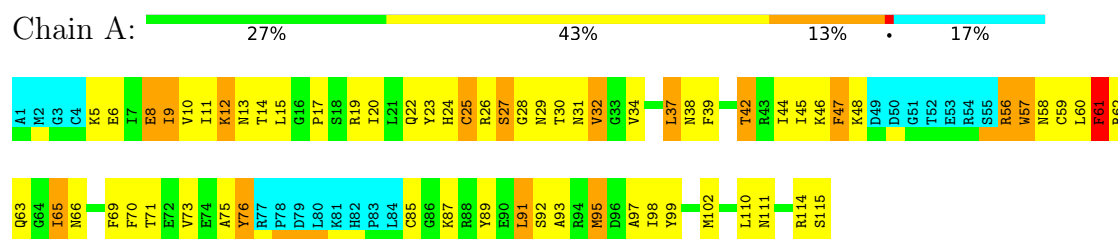
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: S-protein homolog 15



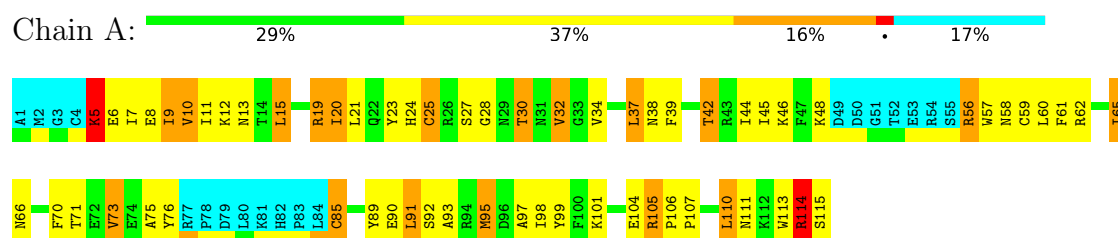
4.2.8 Score per residue for model 8

- Molecule 1: S-protein homolog 15



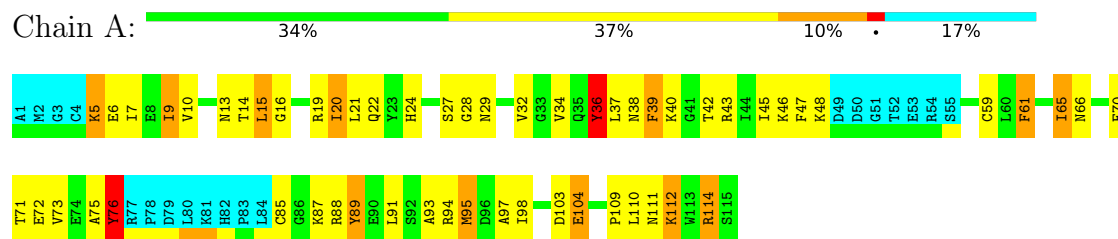
4.2.9 Score per residue for model 9

- Molecule 1: S-protein homolog 15



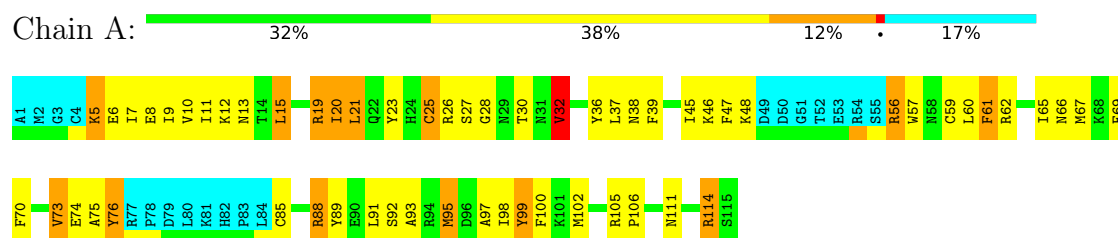
4.2.10 Score per residue for model 10

- Molecule 1: S-protein homolog 15



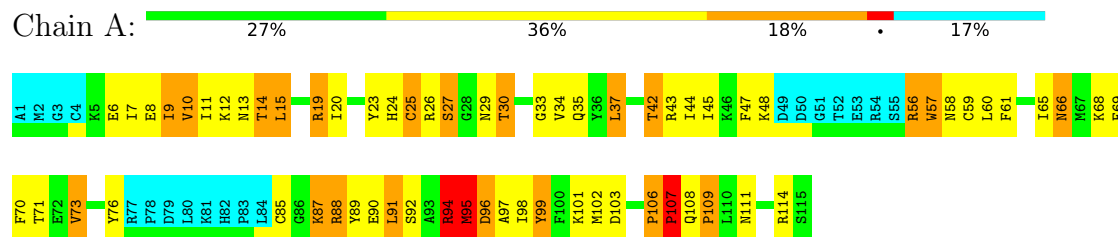
4.2.11 Score per residue for model 11

- Molecule 1: S-protein homolog 15



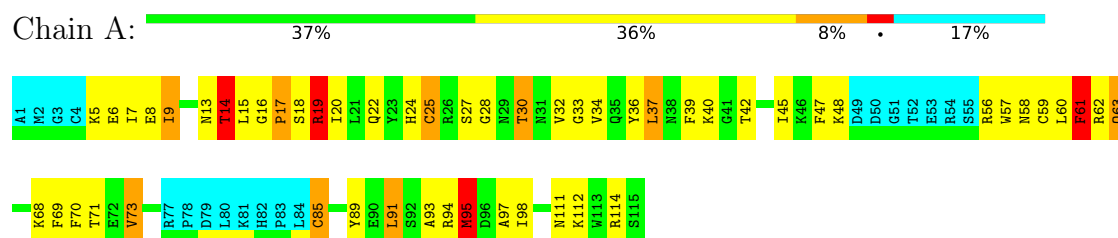
4.2.12 Score per residue for model 12

- Molecule 1: S-protein homolog 15



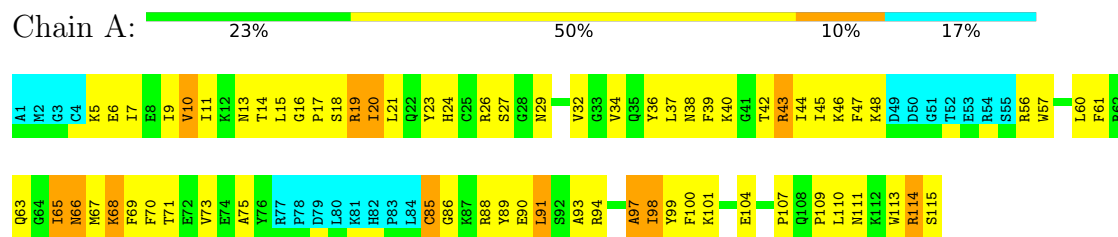
4.2.13 Score per residue for model 13

- Molecule 1: S-protein homolog 15



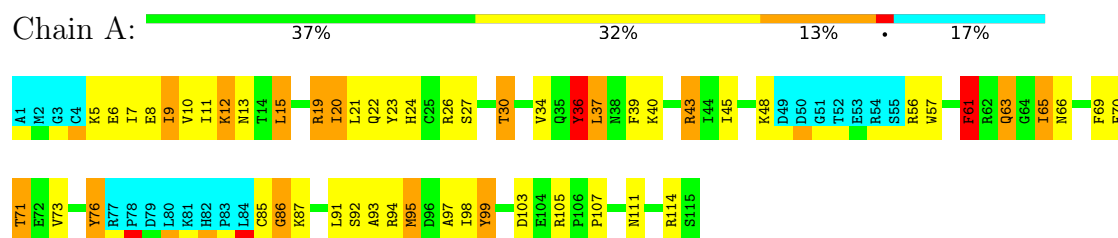
4.2.14 Score per residue for model 14

- Molecule 1: S-protein homolog 15



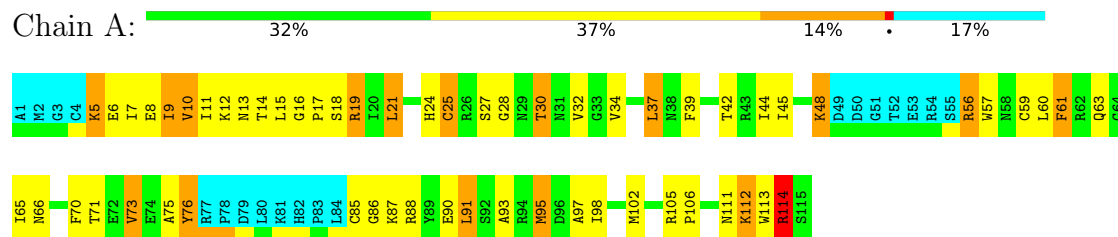
4.2.15 Score per residue for model 15

- Molecule 1: S-protein homolog 15



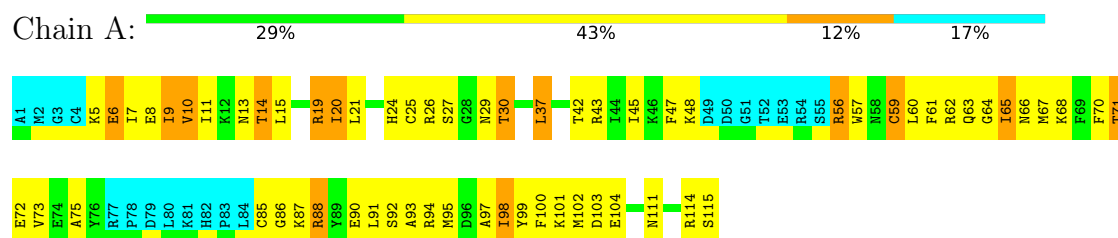
4.2.16 Score per residue for model 16

- Molecule 1: S-protein homolog 15



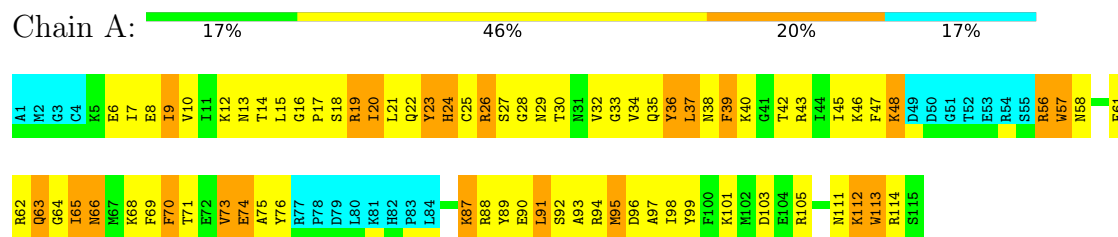
4.2.17 Score per residue for model 17

- Molecule 1: S-protein homolog 15



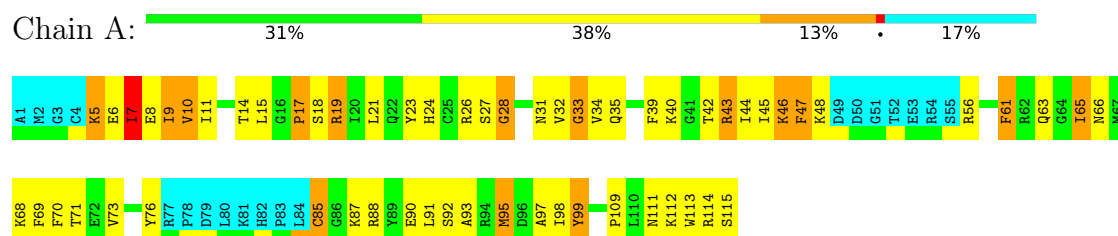
4.2.18 Score per residue for model 18

- Molecule 1: S-protein homolog 15



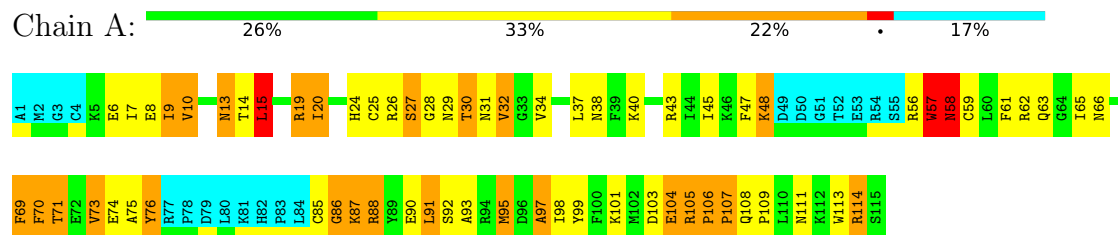
4.2.19 Score per residue for model 19

- Molecule 1: S-protein homolog 15



4.2.20 Score per residue for model 20

- Molecule 1: S-protein homolog 15



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 200 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
CNS	refinement	
ARIA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1096
Number of shifts mapped to atoms	1096
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.79±0.07	1±2/827 (0.1± 0.2%)	0.91±0.05	1±1/1107 (0.1± 0.1%)
All	All	0.79	21/16540 (0.1%)	0.91	17/22140 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.7
All	All	0	17

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	76	TYR	CE2-CZ	9.24	1.60	1.38	10	1
1	A	61	PHE	CE1-CZ	9.00	1.65	1.38	8	7
1	A	76	TYR	CE1-CZ	-8.62	1.17	1.38	10	1
1	A	57	TRP	CA-C	8.53	1.61	1.52	20	1
1	A	61	PHE	CE2-CZ	-7.68	1.15	1.38	8	4
1	A	36	TYR	CE2-CZ	6.32	1.53	1.38	10	2
1	A	36	TYR	CE1-CZ	-5.72	1.24	1.38	10	2
1	A	76	TYR	N-CA	5.28	1.52	1.45	11	1
1	A	58	ASN	N-CA	5.25	1.52	1.45	20	1
1	A	36	TYR	CA-CB	-5.11	1.44	1.53	10	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	PHE	CA-CB-CG	-6.57	107.23	113.80	18	1
1	A	67	MET	N-CA-C	-6.21	105.83	113.41	11	2
1	A	76	TYR	OH-CZ-CE2	-6.15	101.45	119.90	10	1
1	A	36	TYR	CA-CB-CG	-5.95	103.19	113.90	15	2
1	A	36	TYR	N-CA-C	5.85	118.30	109.41	15	2
1	A	56	ARG	N-CA-CB	-5.80	100.69	110.49	8	2
1	A	15	LEU	N-CA-C	-5.49	105.70	112.90	20	2
1	A	76	TYR	N-CA-C	5.35	115.60	108.38	15	1
1	A	7	ILE	N-CA-CB	5.19	119.79	111.23	19	1
1	A	107	PRO	N-CA-CB	-5.11	97.89	103.25	12	1
1	A	88	ARG	N-CA-C	5.05	115.98	108.60	17	1
1	A	56	ARG	N-CA-C	5.00	116.46	107.80	18	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	61	PHE	Sidechain	4
1	A	76	TYR	Sidechain	2
1	A	66	ASN	Peptide	2
1	A	102	MET	Peptide	1
1	A	94	ARG	Peptide	1
1	A	5	LYS	Peptide	1
1	A	14	THR	Peptide	1
1	A	36	TYR	Sidechain	1
1	A	23	TYR	Sidechain	1
1	A	39	PHE	Sidechain	1
1	A	86	GLY	Peptide	1
1	A	87	LYS	Peptide	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	808	817	816	64±17
All	All	16160	16340	16320	1281

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 39.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ARG:HA	1:A:70:PHE:CG	0.96	1.95	18	2
1:A:34:VAL:HG12	1:A:35:GLN:H	0.90	1.26	18	1
1:A:19:ARG:HB2	1:A:39:PHE:CZ	0.86	2.05	13	1
1:A:7:ILE:HD12	1:A:7:ILE:N	0.86	1.82	19	1
1:A:61:PHE:O	1:A:70:PHE:HA	0.85	1.70	13	16
1:A:13:ASN:HA	1:A:93:ALA:HB3	0.85	1.48	18	1
1:A:14:THR:HA	1:A:93:ALA:C	0.83	1.98	13	1
1:A:76:TYR:CE2	1:A:87:LYS:HB3	0.83	2.09	10	1
1:A:27:SER:O	1:A:58:ASN:HB2	0.82	1.75	4	1
1:A:27:SER:H	1:A:58:ASN:N	0.82	1.73	4	2
1:A:27:SER:N	1:A:57:TRP:HA	0.80	1.91	4	2
1:A:76:TYR:OH	1:A:88:ARG:N	0.80	2.13	10	1
1:A:98:ILE:HB	1:A:111:ASN:O	0.79	1.78	3	1
1:A:30:THR:HB	1:A:57:TRP:NE1	0.79	1.93	8	1
1:A:61:PHE:HB2	1:A:71:THR:HG22	0.79	1.55	13	12
1:A:30:THR:HB	1:A:57:TRP:CE2	0.78	2.12	8	1
1:A:29:ASN:H	1:A:57:TRP:N	0.78	1.77	20	1
1:A:8:GLU:O	1:A:9:ILE:HD13	0.76	1.80	11	1
1:A:30:THR:C	1:A:57:TRP:HB2	0.76	2.05	4	1
1:A:15:LEU:CD1	1:A:94:ARG:HB3	0.75	2.11	14	2
1:A:31:ASN:HB2	1:A:57:TRP:CD2	0.75	2.15	4	1
1:A:9:ILE:HD12	1:A:75:ALA:HB1	0.75	1.58	11	1
1:A:15:LEU:HD11	1:A:94:ARG:HB3	0.75	1.56	17	2
1:A:29:ASN:N	1:A:57:TRP:H	0.74	1.78	4	1
1:A:9:ILE:HA	1:A:88:ARG:O	0.74	1.82	17	1
1:A:90:GLU:HG3	1:A:91:LEU:N	0.74	1.95	3	1
1:A:25:CYS:HA	1:A:58:ASN:O	0.74	1.81	4	10
1:A:6:GLU:H	1:A:48:LYS:HA	0.74	1.43	19	1
1:A:10:VAL:HG13	1:A:90:GLU:HB2	0.73	1.58	14	3
1:A:7:ILE:HG21	1:A:88:ARG:CZ	0.73	2.14	19	1
1:A:32:VAL:HG22	1:A:57:TRP:CE3	0.72	2.18	8	1
1:A:14:THR:O	1:A:95:MET:HG2	0.72	1.84	17	2
1:A:6:GLU:C	1:A:7:ILE:HD12	0.72	2.07	19	1
1:A:62:ARG:HB3	1:A:70:PHE:CE1	0.72	2.19	17	1
1:A:8:GLU:HB2	1:A:76:TYR:CE2	0.72	2.20	11	1
1:A:24:HIS:CG	1:A:34:VAL:HG22	0.72	2.19	9	17
1:A:27:SER:H	1:A:57:TRP:N	0.71	1.83	8	2
1:A:29:ASN:C	1:A:57:TRP:H	0.71	1.93	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ALA:HB1	1:A:111:ASN:O	0.71	1.84	6	19
1:A:15:LEU:HG	1:A:94:ARG:O	0.71	1.85	6	2
1:A:27:SER:H	1:A:57:TRP:C	0.70	1.94	4	2
1:A:60:LEU:HG	1:A:70:PHE:CD1	0.70	2.20	17	3
1:A:27:SER:C	1:A:56:ARG:HB2	0.70	2.10	13	1
1:A:13:ASN:O	1:A:39:PHE:HA	0.70	1.86	8	9
1:A:26:ARG:HA	1:A:56:ARG:O	0.70	1.87	8	2
1:A:62:ARG:HA	1:A:70:PHE:CD2	0.70	2.20	18	1
1:A:61:PHE:O	1:A:70:PHE:HB3	0.70	1.86	11	2
1:A:13:ASN:HB2	1:A:19:ARG:CZ	0.69	2.17	1	1
1:A:21:LEU:HD12	1:A:93:ALA:HB1	0.69	1.64	17	2
1:A:25:CYS:SG	1:A:57:TRP:HB3	0.68	2.28	5	2
1:A:42:THR:HB	1:A:44:ILE:HD11	0.68	1.63	9	4
1:A:24:HIS:HA	1:A:34:VAL:HB	0.68	1.66	18	1
1:A:27:SER:O	1:A:30:THR:HB	0.68	1.88	18	1
1:A:75:ALA:O	1:A:88:ARG:HB2	0.68	1.88	17	1
1:A:30:THR:HG22	1:A:47:PHE:CD1	0.68	2.24	20	2
1:A:65:ILE:HG23	1:A:66:ASN:H	0.67	1.47	9	12
1:A:8:GLU:O	1:A:88:ARG:HB2	0.67	1.89	19	1
1:A:27:SER:O	1:A:58:ASN:HB3	0.67	1.90	20	1
1:A:100:PHE:CD2	1:A:107:PRO:HB2	0.67	2.25	14	1
1:A:62:ARG:HA	1:A:70:PHE:CB	0.67	2.18	11	2
1:A:76:TYR:OH	1:A:87:LYS:HB2	0.67	1.90	15	1
1:A:15:LEU:HD12	1:A:15:LEU:N	0.66	2.06	13	16
1:A:9:ILE:HG13	1:A:75:ALA:HB1	0.66	1.67	8	2
1:A:57:TRP:CZ3	1:A:76:TYR:HB3	0.66	2.25	12	1
1:A:70:PHE:O	1:A:114:ARG:HG3	0.66	1.91	13	1
1:A:14:THR:HA	1:A:39:PHE:CD1	0.66	2.26	4	1
1:A:73:VAL:HB	1:A:91:LEU:HD13	0.66	1.65	16	5
1:A:9:ILE:HG23	1:A:75:ALA:HB1	0.66	1.67	11	1
1:A:100:PHE:CG	1:A:107:PRO:HB2	0.66	2.26	14	1
1:A:7:ILE:HG21	1:A:76:TYR:CE2	0.66	2.26	15	1
1:A:16:GLY:HA2	1:A:39:PHE:CZ	0.66	2.26	18	1
1:A:26:ARG:HG2	1:A:32:VAL:N	0.66	2.06	18	1
1:A:5:LYS:O	1:A:85:CYS:HB3	0.66	1.91	19	1
1:A:28:GLY:N	1:A:57:TRP:HD1	0.65	1.89	18	1
1:A:93:ALA:HA	1:A:98:ILE:HD13	0.65	1.68	10	17
1:A:16:GLY:HA2	1:A:39:PHE:CE2	0.65	2.26	18	1
1:A:24:HIS:HA	1:A:34:VAL:CB	0.65	2.21	18	1
1:A:22:GLN:HA	1:A:36:TYR:CD1	0.65	2.26	10	2
1:A:76:TYR:CZ	1:A:87:LYS:HB3	0.65	2.26	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:GLU:HB3	1:A:101:LYS:CB	0.65	2.22	14	1
1:A:24:HIS:HA	1:A:34:VAL:CG2	0.65	2.21	18	1
1:A:15:LEU:HB2	1:A:19:ARG:HG2	0.65	1.68	10	14
1:A:30:THR:HB	1:A:47:PHE:CD2	0.65	2.26	6	1
1:A:92:SER:O	1:A:98:ILE:HA	0.65	1.91	12	9
1:A:45:ILE:HG23	1:A:57:TRP:CZ3	0.65	2.27	8	1
1:A:113:TRP:O	1:A:114:ARG:HG2	0.65	1.91	18	1
1:A:91:LEU:HA	1:A:99:TYR:O	0.64	1.92	8	10
1:A:26:ARG:O	1:A:57:TRP:HB2	0.64	1.92	6	1
1:A:93:ALA:HB1	1:A:113:TRP:CZ2	0.64	2.27	18	1
1:A:20:ILE:HD13	1:A:38:ASN:HA	0.64	1.68	10	3
1:A:9:ILE:HD13	1:A:87:LYS:HA	0.64	1.69	17	1
1:A:19:ARG:HB2	1:A:39:PHE:CE2	0.64	2.27	13	1
1:A:26:ARG:HA	1:A:57:TRP:HB3	0.64	1.70	20	2
1:A:30:THR:O	1:A:56:ARG:HG2	0.64	1.92	13	1
1:A:30:THR:HB	1:A:57:TRP:CZ2	0.64	2.28	9	1
1:A:70:PHE:O	1:A:71:THR:HB	0.63	1.93	3	2
1:A:31:ASN:HB2	1:A:57:TRP:CG	0.63	2.28	20	2
1:A:8:GLU:C	1:A:89:TYR:HB3	0.63	2.17	7	1
1:A:14:THR:O	1:A:95:MET:HG3	0.63	1.92	12	1
1:A:6:GLU:H	1:A:48:LYS:CA	0.63	2.04	19	1
1:A:26:ARG:HA	1:A:57:TRP:CB	0.63	2.23	20	1
1:A:15:LEU:HD11	1:A:94:ARG:CB	0.63	2.24	12	2
1:A:20:ILE:HA	1:A:37:LEU:O	0.63	1.93	20	6
1:A:19:ARG:CB	1:A:39:PHE:CZ	0.63	2.81	13	1
1:A:29:ASN:N	1:A:57:TRP:N	0.63	2.46	20	1
1:A:27:SER:CA	1:A:56:ARG:HB2	0.63	2.24	8	2
1:A:14:THR:O	1:A:94:ARG:HA	0.63	1.93	13	1
1:A:13:ASN:N	1:A:37:LEU:HD21	0.63	2.09	12	2
1:A:16:GLY:HA2	1:A:39:PHE:CE1	0.63	2.29	18	2
1:A:69:PHE:HA	1:A:114:ARG:O	0.62	1.93	5	6
1:A:25:CYS:SG	1:A:75:ALA:HB2	0.62	2.34	4	3
1:A:57:TRP:HB2	1:A:75:ALA:O	0.62	1.94	16	2
1:A:102:MET:HA	1:A:105:ARG:O	0.62	1.93	2	1
1:A:88:ARG:O	1:A:88:ARG:HD3	0.62	1.94	20	1
1:A:24:HIS:HA	1:A:33:GLY:O	0.62	1.93	4	3
1:A:27:SER:H	1:A:57:TRP:HA	0.62	1.53	4	2
1:A:27:SER:H	1:A:57:TRP:CA	0.62	2.07	20	3
1:A:94:ARG:C	1:A:96:ASP:N	0.62	2.55	6	2
1:A:26:ARG:HG3	1:A:30:THR:O	0.62	1.94	18	1
1:A:10:VAL:HG13	1:A:90:GLU:HA	0.62	1.71	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:SER:HB2	1:A:99:TYR:CD1	0.62	2.30	19	1
1:A:8:GLU:O	1:A:76:TYR:HB2	0.62	1.94	11	1
1:A:74:GLU:CB	1:A:89:TYR:HB2	0.62	2.25	11	1
1:A:6:GLU:N	1:A:48:LYS:HA	0.62	2.08	19	1
1:A:27:SER:N	1:A:58:ASN:N	0.61	2.48	4	2
1:A:19:ARG:NE	1:A:39:PHE:HB3	0.61	2.10	16	2
1:A:62:ARG:HA	1:A:69:PHE:O	0.61	1.95	2	1
1:A:15:LEU:H	1:A:19:ARG:HG2	0.61	1.54	16	4
1:A:27:SER:HB3	1:A:30:THR:O	0.61	1.94	15	3
1:A:7:ILE:N	1:A:7:ILE:CD1	0.61	2.59	19	1
1:A:45:ILE:HD11	1:A:57:TRP:CD2	0.61	2.30	5	1
1:A:9:ILE:O	1:A:44:ILE:HA	0.61	1.96	6	5
1:A:71:THR:HG21	1:A:98:ILE:HG13	0.61	1.70	18	6
1:A:29:ASN:N	1:A:56:ARG:HG2	0.61	2.10	5	1
1:A:27:SER:N	1:A:57:TRP:HD1	0.61	1.94	6	1
1:A:106:PRO:CB	1:A:107:PRO:HD2	0.61	2.26	12	1
1:A:34:VAL:CG1	1:A:35:GLN:H	0.61	2.05	18	1
1:A:27:SER:N	1:A:58:ASN:H	0.60	1.94	20	1
1:A:76:TYR:CE2	1:A:87:LYS:CB	0.60	2.84	10	1
1:A:59:CYS:SG	1:A:75:ALA:HB2	0.60	2.37	1	3
1:A:27:SER:HB3	1:A:56:ARG:O	0.60	1.96	1	1
1:A:61:PHE:HE2	1:A:93:ALA:HB2	0.60	1.56	1	2
1:A:7:ILE:HD11	1:A:85:CYS:H	0.60	1.57	11	1
1:A:27:SER:HA	1:A:56:ARG:O	0.60	1.96	15	1
1:A:10:VAL:HG13	1:A:89:TYR:O	0.60	1.97	7	1
1:A:7:ILE:HD11	1:A:85:CYS:CA	0.60	2.26	15	1
1:A:69:PHE:C	1:A:114:ARG:HA	0.60	2.22	18	1
1:A:30:THR:HB	1:A:47:PHE:CG	0.60	2.31	6	1
1:A:67:MET:O	1:A:68:LYS:HG2	0.59	1.97	3	1
1:A:73:VAL:CG1	1:A:91:LEU:HG	0.59	2.27	11	2
1:A:7:ILE:HG21	1:A:57:TRP:CH2	0.59	2.32	18	1
1:A:5:LYS:HD3	1:A:86:GLY:O	0.59	1.97	14	1
1:A:9:ILE:HG12	1:A:45:ILE:HB	0.59	1.75	11	10
1:A:23:TYR:OH	1:A:43:ARG:HD3	0.59	1.98	7	1
1:A:24:HIS:O	1:A:59:CYS:HA	0.59	1.96	6	3
1:A:43:ARG:NE	1:A:43:ARG:HA	0.59	2.13	12	2
1:A:23:TYR:OH	1:A:43:ARG:HG2	0.59	1.97	18	1
1:A:90:GLU:CG	1:A:91:LEU:N	0.59	2.66	3	1
1:A:27:SER:HB2	1:A:58:ASN:CB	0.59	2.28	8	3
1:A:5:LYS:O	1:A:48:LYS:HB3	0.59	1.98	7	1
1:A:6:GLU:HA	1:A:48:LYS:CA	0.59	2.27	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:O	1:A:36:TYR:CG	0.59	2.56	15	2
1:A:9:ILE:HD13	1:A:87:LYS:CB	0.59	2.28	17	1
1:A:14:THR:HB	1:A:39:PHE:CD1	0.58	2.33	19	3
1:A:25:CYS:HB3	1:A:32:VAL:HG21	0.58	1.74	8	1
1:A:92:SER:HB3	1:A:99:TYR:CD1	0.58	2.33	12	1
1:A:93:ALA:O	1:A:94:ARG:HG3	0.58	1.98	13	1
1:A:25:CYS:O	1:A:32:VAL:HB	0.58	1.98	16	2
1:A:70:PHE:O	1:A:114:ARG:HB2	0.58	1.99	3	2
1:A:15:LEU:HD21	1:A:94:ARG:HB2	0.58	1.75	12	1
1:A:62:ARG:HB2	1:A:70:PHE:CE1	0.58	2.33	13	3
1:A:15:LEU:HG	1:A:95:MET:CG	0.58	2.29	13	1
1:A:8:GLU:H	1:A:88:ARG:HG2	0.58	1.57	20	1
1:A:28:GLY:HA3	1:A:56:ARG:O	0.58	1.98	19	1
1:A:56:ARG:HG3	1:A:76:TYR:O	0.57	1.99	6	2
1:A:92:SER:OG	1:A:99:TYR:HB2	0.57	1.99	5	2
1:A:13:ASN:HB2	1:A:37:LEU:HD12	0.57	1.75	8	1
1:A:15:LEU:HG	1:A:95:MET:CA	0.57	2.30	2	4
1:A:70:PHE:HA	1:A:114:ARG:H	0.57	1.59	18	2
1:A:7:ILE:HG22	1:A:88:ARG:HB2	0.57	1.75	5	1
1:A:26:ARG:C	1:A:56:ARG:HG3	0.57	2.25	8	1
1:A:91:LEU:CD1	1:A:100:PHE:HA	0.57	2.29	11	1
1:A:5:LYS:CB	1:A:85:CYS:HA	0.57	2.29	4	1
1:A:23:TYR:HE1	1:A:37:LEU:HD23	0.57	1.59	18	1
1:A:15:LEU:N	1:A:15:LEU:CD1	0.57	2.68	12	18
1:A:26:ARG:HG2	1:A:32:VAL:H	0.57	1.60	18	1
1:A:71:THR:HB	1:A:112:LYS:O	0.57	2.00	18	3
1:A:89:TYR:HB3	1:A:101:LYS:O	0.56	2.01	18	3
1:A:25:CYS:HA	1:A:59:CYS:HA	0.56	1.77	20	7
1:A:7:ILE:H	1:A:48:LYS:CB	0.56	2.14	7	1
1:A:7:ILE:HD11	1:A:85:CYS:N	0.56	2.15	11	1
1:A:5:LYS:HB2	1:A:85:CYS:O	0.56	2.00	13	1
1:A:10:VAL:H	1:A:90:GLU:CB	0.56	2.13	3	1
1:A:19:ARG:CZ	1:A:39:PHE:HB3	0.56	2.30	19	2
1:A:28:GLY:C	1:A:30:THR:H	0.56	2.08	18	1
1:A:10:VAL:CG1	1:A:90:GLU:HB2	0.56	2.30	14	2
1:A:15:LEU:HD11	1:A:95:MET:N	0.56	2.15	18	1
1:A:15:LEU:HA	1:A:95:MET:HG2	0.56	1.76	20	14
1:A:7:ILE:HG23	1:A:87:LYS:C	0.56	2.26	18	3
1:A:56:ARG:HD2	1:A:76:TYR:O	0.56	2.01	19	2
1:A:93:ALA:HB1	1:A:113:TRP:CH2	0.56	2.36	18	1
1:A:23:TYR:HA	1:A:60:LEU:O	0.56	2.01	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ARG:NE	1:A:19:ARG:HA	0.56	2.16	4	3
1:A:6:GLU:CG	1:A:48:LYS:HB3	0.56	2.31	16	1
1:A:6:GLU:HA	1:A:48:LYS:N	0.55	2.17	7	1
1:A:101:LYS:HB2	1:A:107:PRO:HB3	0.55	1.78	12	1
1:A:9:ILE:CD1	1:A:87:LYS:HA	0.55	2.31	17	1
1:A:28:GLY:C	1:A:56:ARG:HA	0.55	2.27	4	1
1:A:6:GLU:HG2	1:A:48:LYS:HB3	0.55	1.77	14	3
1:A:9:ILE:HG22	1:A:89:TYR:HB2	0.55	1.77	1	1
1:A:15:LEU:HB2	1:A:19:ARG:CG	0.55	2.31	15	12
1:A:27:SER:H	1:A:56:ARG:C	0.55	2.09	12	2
1:A:65:ILE:CG2	1:A:68:LYS:HA	0.55	2.31	14	1
1:A:15:LEU:HD13	1:A:19:ARG:HG2	0.55	1.78	12	4
1:A:28:GLY:HA2	1:A:56:ARG:H	0.55	1.62	18	1
1:A:11:ILE:HG13	1:A:23:TYR:CD2	0.55	2.36	9	6
1:A:92:SER:HB2	1:A:99:TYR:CE1	0.55	2.36	4	1
1:A:15:LEU:HD21	1:A:113:TRP:CZ2	0.55	2.37	20	4
1:A:11:ILE:HG21	1:A:23:TYR:CD1	0.54	2.37	3	3
1:A:14:THR:HA	1:A:93:ALA:O	0.54	2.01	13	1
1:A:70:PHE:C	1:A:114:ARG:HA	0.54	2.26	14	1
1:A:15:LEU:HG	1:A:95:MET:HA	0.54	1.79	2	14
1:A:100:PHE:O	1:A:107:PRO:HA	0.54	2.02	2	1
1:A:15:LEU:N	1:A:15:LEU:HD12	0.54	2.17	12	4
1:A:13:ASN:OD1	1:A:19:ARG:HB3	0.54	2.01	15	4
1:A:7:ILE:HD11	1:A:85:CYS:HB3	0.54	1.79	6	2
1:A:76:TYR:CD2	1:A:87:LYS:HB2	0.54	2.37	6	1
1:A:20:ILE:HG23	1:A:37:LEU:O	0.54	2.02	10	2
1:A:9:ILE:HG13	1:A:45:ILE:HB	0.54	1.79	19	4
1:A:37:LEU:HD23	1:A:43:ARG:HG2	0.54	1.79	15	1
1:A:65:ILE:HG13	1:A:66:ASN:N	0.54	2.17	3	5
1:A:19:ARG:HD2	1:A:39:PHE:CD2	0.54	2.37	16	2
1:A:15:LEU:HD11	1:A:94:ARG:HB2	0.54	1.79	12	1
1:A:88:ARG:O	1:A:102:MET:HB3	0.54	2.03	16	1
1:A:9:ILE:CG1	1:A:45:ILE:HB	0.54	2.32	17	8
1:A:24:HIS:ND1	1:A:34:VAL:HG22	0.54	2.17	15	6
1:A:27:SER:N	1:A:57:TRP:CA	0.54	2.68	4	2
1:A:30:THR:HB	1:A:56:ARG:HB2	0.54	1.79	5	1
1:A:30:THR:O	1:A:57:TRP:HD1	0.54	1.86	12	1
1:A:88:ARG:HD3	1:A:89:TYR:N	0.54	2.17	12	1
1:A:7:ILE:HG21	1:A:57:TRP:HH2	0.54	1.62	18	1
1:A:14:THR:CG2	1:A:19:ARG:HB2	0.54	2.33	18	1
1:A:6:GLU:CG	1:A:48:LYS:HB2	0.54	2.33	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:H	1:A:19:ARG:HG3	0.54	1.63	5	2
1:A:60:LEU:HB3	1:A:70:PHE:CZ	0.54	2.38	14	3
1:A:8:GLU:HB2	1:A:89:TYR:CD2	0.53	2.38	7	1
1:A:15:LEU:HD13	1:A:19:ARG:CG	0.53	2.34	12	5
1:A:20:ILE:C	1:A:21:LEU:HD22	0.53	2.28	18	1
1:A:11:ILE:HD11	1:A:59:CYS:SG	0.53	2.44	11	3
1:A:21:LEU:HD23	1:A:113:TRP:CZ3	0.53	2.38	18	1
1:A:23:TYR:O	1:A:34:VAL:HB	0.53	2.03	18	1
1:A:19:ARG:O	1:A:38:ASN:HA	0.53	2.03	5	1
1:A:9:ILE:HD13	1:A:87:LYS:CA	0.53	2.34	17	1
1:A:64:GLY:O	1:A:65:ILE:HG22	0.53	2.04	18	1
1:A:29:ASN:CG	1:A:74:GLU:HB3	0.53	2.28	20	1
1:A:32:VAL:HG22	1:A:47:PHE:CE1	0.53	2.39	3	1
1:A:12:LYS:HB3	1:A:92:SER:CB	0.53	2.33	5	3
1:A:19:ARG:N	1:A:19:ARG:HE	0.53	2.01	16	1
1:A:57:TRP:CH2	1:A:76:TYR:HD2	0.53	2.21	18	1
1:A:76:TYR:C	1:A:76:TYR:CD2	0.53	2.86	9	1
1:A:101:LYS:CB	1:A:107:PRO:HB3	0.53	2.34	12	1
1:A:16:GLY:C	1:A:19:ARG:HD3	0.53	2.28	16	2
1:A:29:ASN:HB2	1:A:58:ASN:CA	0.52	2.34	20	1
1:A:94:ARG:O	1:A:96:ASP:N	0.52	2.42	18	2
1:A:22:GLN:HB3	1:A:62:ARG:O	0.52	2.03	8	2
1:A:103:ASP:OD2	1:A:105:ARG:HG2	0.52	2.04	1	1
1:A:28:GLY:N	1:A:56:ARG:HB2	0.52	2.18	8	2
1:A:69:PHE:CB	1:A:114:ARG:HB2	0.52	2.34	14	1
1:A:7:ILE:CG2	1:A:87:LYS:HB2	0.52	2.34	17	1
1:A:9:ILE:HG21	1:A:75:ALA:HB1	0.52	1.81	7	1
1:A:6:GLU:HG2	1:A:48:LYS:HB2	0.52	1.80	13	3
1:A:59:CYS:SG	1:A:75:ALA:HA	0.52	2.44	6	1
1:A:9:ILE:HD12	1:A:75:ALA:CB	0.52	2.33	11	1
1:A:65:ILE:HG13	1:A:66:ASN:H	0.52	1.64	14	3
1:A:113:TRP:C	1:A:114:ARG:HG3	0.52	2.30	16	2
1:A:12:LYS:O	1:A:92:SER:HA	0.52	2.05	12	3
1:A:8:GLU:C	1:A:9:ILE:HD13	0.52	2.30	11	1
1:A:103:ASP:C	1:A:105:ARG:H	0.52	2.12	15	6
1:A:7:ILE:CB	1:A:87:LYS:HB2	0.52	2.35	17	1
1:A:6:GLU:HA	1:A:48:LYS:CB	0.52	2.35	7	1
1:A:47:PHE:HE2	1:A:57:TRP:NE1	0.52	2.03	8	1
1:A:26:ARG:O	1:A:57:TRP:HA	0.52	2.04	11	5
1:A:105:ARG:H	1:A:106:PRO:CD	0.52	2.17	20	2
1:A:24:HIS:CA	1:A:34:VAL:HB	0.52	2.35	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:VAL:HG12	1:A:35:GLN:N	0.52	2.07	18	1
1:A:85:CYS:O	1:A:87:LYS:N	0.51	2.43	15	1
1:A:45:ILE:HG23	1:A:57:TRP:CE3	0.51	2.40	8	1
1:A:19:ARG:HD2	1:A:39:PHE:CB	0.51	2.35	16	2
1:A:27:SER:CB	1:A:47:PHE:HB2	0.51	2.36	18	1
1:A:10:VAL:HG22	1:A:90:GLU:HB3	0.51	1.82	3	1
1:A:114:ARG:HG2	1:A:115:SER:N	0.51	2.21	8	1
1:A:35:GLN:OE1	1:A:43:ARG:HD3	0.51	2.05	12	1
1:A:13:ASN:OD1	1:A:37:LEU:HB3	0.51	2.04	20	1
1:A:69:PHE:HA	1:A:115:SER:HA	0.51	1.82	2	1
1:A:58:ASN:ND2	1:A:74:GLU:HA	0.51	2.20	4	1
1:A:29:ASN:N	1:A:56:ARG:HA	0.51	2.20	12	2
1:A:76:TYR:HB3	1:A:88:ARG:HA	0.51	1.82	11	1
1:A:29:ASN:HB3	1:A:76:TYR:H	0.51	1.65	20	1
1:A:7:ILE:H	1:A:48:LYS:HB2	0.51	1.64	7	1
1:A:87:LYS:HB3	1:A:102:MET:SD	0.51	2.45	8	1
1:A:15:LEU:HD12	1:A:15:LEU:H	0.51	1.65	18	1
1:A:13:ASN:ND2	1:A:20:ILE:HA	0.51	2.21	2	1
1:A:10:VAL:N	1:A:90:GLU:CB	0.51	2.73	3	1
1:A:74:GLU:HB3	1:A:89:TYR:HB2	0.51	1.82	11	1
1:A:9:ILE:HA	1:A:88:ARG:HB3	0.51	1.82	12	1
1:A:29:ASN:OD1	1:A:74:GLU:HB3	0.51	2.06	20	1
1:A:113:TRP:H	1:A:113:TRP:CD1	0.51	2.23	18	4
1:A:13:ASN:ND2	1:A:21:LEU:HG	0.51	2.21	10	1
1:A:57:TRP:HB2	1:A:75:ALA:CB	0.51	2.36	18	1
1:A:105:ARG:N	1:A:106:PRO:CD	0.51	2.74	20	1
1:A:30:THR:HB	1:A:56:ARG:CB	0.51	2.36	5	1
1:A:56:ARG:HG2	1:A:57:TRP:N	0.51	2.20	6	2
1:A:27:SER:HB2	1:A:57:TRP:HA	0.51	1.81	17	2
1:A:10:VAL:HG13	1:A:90:GLU:CA	0.51	2.36	17	2
1:A:27:SER:HA	1:A:57:TRP:CD1	0.51	2.41	14	2
1:A:15:LEU:N	1:A:39:PHE:CZ	0.51	2.79	13	1
1:A:19:ARG:CD	1:A:39:PHE:HB3	0.51	2.35	16	1
1:A:15:LEU:HD11	1:A:95:MET:HB2	0.51	1.82	18	1
1:A:28:GLY:HA2	1:A:56:ARG:C	0.51	2.31	18	1
1:A:15:LEU:HB2	1:A:19:ARG:HG3	0.50	1.83	5	2
1:A:91:LEU:HD23	1:A:91:LEU:N	0.50	2.21	16	3
1:A:30:THR:HG21	1:A:47:PHE:HE1	0.50	1.65	11	1
1:A:8:GLU:HA	1:A:45:ILE:O	0.50	2.06	15	3
1:A:97:ALA:HB3	1:A:109:PRO:HB3	0.50	1.84	20	4
1:A:7:ILE:HB	1:A:87:LYS:HB2	0.50	1.83	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:PHE:O	1:A:114:ARG:HB3	0.50	2.05	17	1
1:A:27:SER:HB3	1:A:47:PHE:HB2	0.50	1.84	18	1
1:A:5:LYS:HA	1:A:48:LYS:HB3	0.50	1.82	19	1
1:A:46:LYS:N	1:A:46:LYS:HE3	0.50	2.21	19	1
1:A:29:ASN:C	1:A:57:TRP:HD1	0.50	2.14	4	1
1:A:16:GLY:O	1:A:19:ARG:HD3	0.50	2.06	10	3
1:A:8:GLU:O	1:A:89:TYR:HB3	0.50	2.06	7	1
1:A:89:TYR:CG	1:A:102:MET:HB2	0.50	2.41	8	1
1:A:13:ASN:CB	1:A:37:LEU:HB2	0.50	2.36	17	1
1:A:69:PHE:HA	1:A:114:ARG:C	0.50	2.32	8	2
1:A:73:VAL:HG11	1:A:91:LEU:HG	0.50	1.83	18	2
1:A:76:TYR:CE2	1:A:89:TYR:HB2	0.50	2.41	10	1
1:A:62:ARG:HG2	1:A:63:GLN:N	0.50	2.22	13	1
1:A:30:THR:OG1	1:A:75:ALA:HB1	0.50	2.06	4	1
1:A:114:ARG:CG	1:A:115:SER:N	0.50	2.75	8	1
1:A:30:THR:C	1:A:56:ARG:HG2	0.50	2.32	13	1
1:A:23:TYR:OH	1:A:43:ARG:HB3	0.50	2.07	14	1
1:A:24:HIS:CE1	1:A:26:ARG:HB3	0.50	2.42	15	1
1:A:22:GLN:O	1:A:61:PHE:HA	0.50	2.06	18	1
1:A:9:ILE:HG21	1:A:75:ALA:HA	0.50	1.83	8	2
1:A:9:ILE:HD11	1:A:57:TRP:CG	0.50	2.40	11	1
1:A:61:PHE:HB2	1:A:71:THR:HB	0.50	1.84	2	1
1:A:9:ILE:HB	1:A:45:ILE:HD12	0.50	1.82	12	3
1:A:28:GLY:HA3	1:A:56:ARG:CG	0.50	2.37	5	1
1:A:61:PHE:CE2	1:A:93:ALA:HB2	0.50	2.42	17	3
1:A:46:LYS:O	1:A:47:PHE:HD1	0.50	1.90	6	1
1:A:10:VAL:O	1:A:90:GLU:HA	0.50	2.07	17	3
1:A:28:GLY:HA2	1:A:56:ARG:HB2	0.49	1.84	20	1
1:A:13:ASN:CG	1:A:37:LEU:HB3	0.49	2.32	20	1
1:A:31:ASN:H	1:A:57:TRP:CD1	0.49	2.24	20	1
1:A:75:ALA:O	1:A:88:ARG:HD3	0.49	2.06	5	1
1:A:5:LYS:N	1:A:85:CYS:HB2	0.49	2.22	10	4
1:A:28:GLY:N	1:A:57:TRP:CD1	0.49	2.77	18	1
1:A:15:LEU:HD13	1:A:19:ARG:HG3	0.49	1.84	1	1
1:A:105:ARG:HB3	1:A:106:PRO:CD	0.49	2.37	11	1
1:A:15:LEU:HA	1:A:95:MET:CG	0.49	2.37	20	4
1:A:27:SER:HB2	1:A:47:PHE:CZ	0.49	2.42	10	1
1:A:9:ILE:CD1	1:A:87:LYS:HG3	0.49	2.37	17	1
1:A:57:TRP:CE3	1:A:76:TYR:HB2	0.49	2.42	18	1
1:A:69:PHE:HA	1:A:115:SER:N	0.49	2.22	19	1
1:A:70:PHE:H	1:A:114:ARG:HB3	0.49	1.68	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ASN:ND2	1:A:37:LEU:HB3	0.49	2.22	16	1
1:A:15:LEU:H	1:A:15:LEU:CD1	0.49	2.21	18	1
1:A:27:SER:H	1:A:58:ASN:H	0.49	1.41	20	1
1:A:93:ALA:CA	1:A:98:ILE:HD13	0.49	2.37	4	9
1:A:47:PHE:HD2	1:A:56:ARG:N	0.49	2.04	5	1
1:A:14:THR:C	1:A:94:ARG:HA	0.49	2.33	13	1
1:A:23:TYR:OH	1:A:43:ARG:CG	0.49	2.60	18	1
1:A:94:ARG:NE	1:A:96:ASP:HB3	0.49	2.23	4	1
1:A:105:ARG:HB2	1:A:106:PRO:HD2	0.49	1.83	7	1
1:A:71:THR:HB	1:A:112:LYS:C	0.49	2.33	18	1
1:A:5:LYS:HB3	1:A:47:PHE:O	0.49	2.08	19	1
1:A:103:ASP:O	1:A:104:GLU:HB2	0.48	2.08	7	3
1:A:69:PHE:HB3	1:A:115:SER:N	0.48	2.23	14	1
1:A:7:ILE:HG21	1:A:57:TRP:CZ3	0.48	2.43	16	1
1:A:13:ASN:OD1	1:A:94:ARG:HG3	0.48	2.07	17	1
1:A:28:GLY:O	1:A:56:ARG:HA	0.48	2.08	4	1
1:A:57:TRP:N	1:A:57:TRP:CD1	0.48	2.81	8	1
1:A:103:ASP:O	1:A:104:GLU:HB3	0.48	2.08	17	1
1:A:15:LEU:HD11	1:A:95:MET:CB	0.48	2.38	18	1
1:A:61:PHE:CE2	1:A:98:ILE:HD12	0.48	2.43	12	3
1:A:47:PHE:CD2	1:A:56:ARG:N	0.48	2.81	5	1
1:A:14:THR:C	1:A:15:LEU:HD12	0.48	2.33	12	1
1:A:7:ILE:HD11	1:A:47:PHE:CB	0.48	2.39	19	1
1:A:15:LEU:HB2	1:A:19:ARG:HB2	0.48	1.84	1	1
1:A:20:ILE:O	1:A:63:GLN:HG2	0.48	2.09	8	1
1:A:22:GLN:HA	1:A:35:GLN:O	0.48	2.09	1	1
1:A:15:LEU:CB	1:A:19:ARG:HG2	0.48	2.37	4	8
1:A:6:GLU:HA	1:A:48:LYS:HB3	0.48	1.86	7	1
1:A:6:GLU:HG2	1:A:48:LYS:CB	0.48	2.39	10	3
1:A:30:THR:N	1:A:57:TRP:O	0.48	2.46	20	1
1:A:91:LEU:N	1:A:91:LEU:HD22	0.48	2.23	4	6
1:A:32:VAL:HG22	1:A:47:PHE:CZ	0.48	2.44	3	1
1:A:15:LEU:CG	1:A:94:ARG:HB3	0.48	2.38	6	1
1:A:76:TYR:O	1:A:89:TYR:C	0.48	2.56	11	1
1:A:30:THR:H	1:A:56:ARG:CG	0.48	2.22	13	1
1:A:27:SER:HA	1:A:57:TRP:HB3	0.48	1.85	18	1
1:A:26:ARG:HB2	1:A:57:TRP:CD1	0.48	2.44	6	1
1:A:56:ARG:HB2	1:A:76:TYR:CD1	0.48	2.44	7	1
1:A:91:LEU:HD22	1:A:100:PHE:CE2	0.48	2.44	7	1
1:A:70:PHE:O	1:A:114:ARG:HA	0.48	2.07	9	1
1:A:88:ARG:HA	1:A:88:ARG:HE	0.48	1.69	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HG22	1:A:37:LEU:HD13	0.48	1.85	8	1
1:A:90:GLU:HB3	1:A:101:LYS:HB2	0.48	1.86	14	1
1:A:13:ASN:HB2	1:A:19:ARG:NE	0.47	2.23	1	1
1:A:45:ILE:HG22	1:A:46:LYS:N	0.47	2.24	14	5
1:A:7:ILE:HG22	1:A:76:TYR:CE1	0.47	2.44	6	1
1:A:19:ARG:NE	1:A:19:ARG:N	0.47	2.62	18	3
1:A:28:GLY:HA2	1:A:56:ARG:N	0.47	2.24	18	1
1:A:42:THR:HB	1:A:44:ILE:CD1	0.47	2.39	1	2
1:A:71:THR:HB	1:A:113:TRP:HA	0.47	1.85	6	1
1:A:14:THR:CB	1:A:19:ARG:HB2	0.47	2.39	18	1
1:A:7:ILE:HB	1:A:88:ARG:HG2	0.47	1.84	19	1
1:A:113:TRP:O	1:A:113:TRP:HE3	0.47	1.91	3	1
1:A:94:ARG:C	1:A:96:ASP:H	0.47	2.16	12	2
1:A:26:ARG:O	1:A:26:ARG:HD3	0.47	2.09	17	1
1:A:14:THR:HB	1:A:19:ARG:HB2	0.47	1.85	18	1
1:A:76:TYR:HB3	1:A:88:ARG:HH11	0.47	1.69	19	1
1:A:56:ARG:C	1:A:57:TRP:CG	0.47	2.92	20	2
1:A:18:SER:C	1:A:19:ARG:HG3	0.47	2.34	18	1
1:A:6:GLU:HB2	1:A:48:LYS:HB3	0.47	1.86	12	1
1:A:7:ILE:HD11	1:A:85:CYS:C	0.47	2.34	15	1
1:A:5:LYS:N	1:A:85:CYS:HB3	0.47	2.24	16	1
1:A:87:LYS:O	1:A:88:ARG:HG2	0.47	2.10	19	1
1:A:94:ARG:HG2	1:A:97:ALA:O	0.47	2.09	4	1
1:A:102:MET:O	1:A:102:MET:HG3	0.47	2.09	11	1
1:A:108:GLN:HB3	1:A:109:PRO:HD2	0.47	1.85	12	1
1:A:27:SER:HB2	1:A:47:PHE:CE1	0.47	2.45	14	1
1:A:60:LEU:HB3	1:A:70:PHE:CE1	0.47	2.45	14	1
1:A:19:ARG:HD2	1:A:39:PHE:HB3	0.47	1.86	16	1
1:A:7:ILE:HG22	1:A:87:LYS:HB2	0.47	1.86	17	1
1:A:23:TYR:CZ	1:A:34:VAL:HG11	0.47	2.44	18	1
1:A:28:GLY:CA	1:A:57:TRP:HD1	0.47	2.23	18	1
1:A:7:ILE:HG22	1:A:87:LYS:O	0.47	2.10	19	1
1:A:24:HIS:CE1	1:A:26:ARG:HB2	0.47	2.45	19	1
1:A:76:TYR:CD1	1:A:87:LYS:HD2	0.47	2.45	20	1
1:A:27:SER:HB2	1:A:58:ASN:N	0.47	2.24	9	1
1:A:30:THR:O	1:A:57:TRP:CD1	0.47	2.68	12	1
1:A:9:ILE:HA	1:A:88:ARG:CB	0.47	2.40	19	1
1:A:31:ASN:HB3	1:A:47:PHE:CZ	0.47	2.44	4	1
1:A:29:ASN:H	1:A:56:ARG:HG2	0.47	1.69	5	1
1:A:26:ARG:HA	1:A:57:TRP:HA	0.47	1.87	8	1
1:A:90:GLU:H	1:A:102:MET:HB2	0.47	1.70	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:CYS:SG	1:A:86:GLY:N	0.47	2.88	17	2
1:A:10:VAL:H	1:A:90:GLU:HB2	0.47	1.70	3	1
1:A:13:ASN:OD1	1:A:21:LEU:HB2	0.47	2.10	4	1
1:A:27:SER:HA	1:A:56:ARG:HB2	0.47	1.85	8	1
1:A:37:LEU:HD13	1:A:38:ASN:O	0.46	2.09	2	2
1:A:73:VAL:HG13	1:A:100:PHE:CZ	0.46	2.46	4	1
1:A:13:ASN:ND2	1:A:21:LEU:HD23	0.46	2.25	6	1
1:A:7:ILE:CG2	1:A:88:ARG:HB2	0.46	2.39	5	2
1:A:8:GLU:O	1:A:88:ARG:HB3	0.46	2.09	18	1
1:A:19:ARG:HA	1:A:19:ARG:HE	0.46	1.69	5	2
1:A:21:LEU:HD21	1:A:69:PHE:HB3	0.46	1.85	5	1
1:A:62:ARG:HA	1:A:70:PHE:CD1	0.46	2.45	11	1
1:A:16:GLY:N	1:A:39:PHE:CZ	0.46	2.71	13	1
1:A:12:LYS:O	1:A:93:ALA:N	0.46	2.47	18	1
1:A:15:LEU:HD21	1:A:113:TRP:CE2	0.46	2.45	2	1
1:A:37:LEU:HG	1:A:38:ASN:N	0.46	2.25	3	1
1:A:89:TYR:HB3	1:A:101:LYS:HA	0.46	1.87	12	1
1:A:63:GLN:O	1:A:69:PHE:HB2	0.46	2.11	20	1
1:A:17:PRO:HA	1:A:39:PHE:CD2	0.46	2.45	8	1
1:A:19:ARG:C	1:A:20:ILE:HG12	0.46	2.35	14	2
1:A:99:TYR:CD2	1:A:107:PRO:HB2	0.46	2.46	15	1
1:A:13:ASN:HD21	1:A:37:LEU:HB3	0.46	1.71	16	1
1:A:8:GLU:HB3	1:A:46:LYS:HB3	0.46	1.87	8	1
1:A:15:LEU:N	1:A:39:PHE:CE1	0.46	2.83	13	1
1:A:21:LEU:HB2	1:A:36:TYR:CE2	0.46	2.46	15	1
1:A:57:TRP:HB2	1:A:75:ALA:HB3	0.46	1.86	18	1
1:A:37:LEU:HD13	1:A:43:ARG:HG2	0.46	1.87	3	1
1:A:48:LYS:HD3	1:A:48:LYS:C	0.46	2.35	16	1
1:A:15:LEU:CD1	1:A:95:MET:N	0.46	2.79	18	1
1:A:15:LEU:CD1	1:A:95:MET:H	0.46	2.24	18	1
1:A:70:PHE:CZ	1:A:114:ARG:HB3	0.46	2.46	18	1
1:A:98:ILE:HG12	1:A:113:TRP:CD1	0.46	2.46	3	1
1:A:94:ARG:HB2	1:A:113:TRP:HE1	0.46	1.71	6	1
1:A:66:ASN:O	1:A:70:PHE:HB2	0.46	2.11	10	1
1:A:65:ILE:HG23	1:A:65:ILE:O	0.46	2.10	11	1
1:A:21:LEU:O	1:A:36:TYR:HA	0.46	2.11	11	3
1:A:89:TYR:CB	1:A:101:LYS:HA	0.46	2.41	12	1
1:A:9:ILE:HA	1:A:88:ARG:HB2	0.46	1.87	19	1
1:A:6:GLU:HB3	1:A:48:LYS:CB	0.46	2.41	20	1
1:A:73:VAL:CG1	1:A:91:LEU:HD22	0.45	2.40	3	1
1:A:57:TRP:O	1:A:75:ALA:HB3	0.45	2.11	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:VAL:HA	1:A:43:ARG:O	0.45	2.11	7	1
1:A:15:LEU:HD22	1:A:19:ARG:HD2	0.45	1.87	8	1
1:A:21:LEU:O	1:A:36:TYR:CD2	0.45	2.70	10	1
1:A:30:THR:HG21	1:A:47:PHE:CE1	0.45	2.46	11	2
1:A:10:VAL:O	1:A:90:GLU:CG	0.45	2.64	3	1
1:A:47:PHE:CE2	1:A:57:TRP:NE1	0.45	2.84	8	1
1:A:105:ARG:HB3	1:A:106:PRO:HD2	0.45	1.87	11	2
1:A:32:VAL:CG2	1:A:45:ILE:HG12	0.45	2.42	4	1
1:A:30:THR:N	1:A:56:ARG:N	0.45	2.65	12	1
1:A:9:ILE:HG22	1:A:76:TYR:O	0.45	2.11	16	1
1:A:14:THR:HG23	1:A:14:THR:O	0.45	2.12	3	4
1:A:19:ARG:O	1:A:21:LEU:HD13	0.45	2.10	2	1
1:A:73:VAL:HG11	1:A:91:LEU:HB3	0.45	1.88	20	2
1:A:31:ASN:N	1:A:57:TRP:CD1	0.45	2.84	20	1
1:A:70:PHE:H	1:A:114:ARG:HB2	0.45	1.71	3	3
1:A:30:THR:H	1:A:56:ARG:HA	0.45	1.71	8	1
1:A:112:LYS:N	1:A:112:LYS:HD3	0.45	2.27	10	1
1:A:9:ILE:HG23	1:A:88:ARG:N	0.45	2.27	17	1
1:A:11:ILE:HG22	1:A:37:LEU:HG	0.45	1.88	17	1
1:A:23:TYR:CE1	1:A:37:LEU:HD23	0.45	2.44	18	1
1:A:10:VAL:O	1:A:90:GLU:HB3	0.45	2.11	3	1
1:A:12:LYS:HB3	1:A:92:SER:HB3	0.45	1.88	9	4
1:A:30:THR:HG22	1:A:47:PHE:CG	0.45	2.46	20	1
1:A:57:TRP:CH2	1:A:76:TYR:CD2	0.45	3.04	18	1
1:A:5:LYS:HB3	1:A:85:CYS:HA	0.45	1.87	4	1
1:A:11:ILE:HG13	1:A:23:TYR:CG	0.45	2.47	12	3
1:A:6:GLU:O	1:A:8:GLU:HG2	0.45	2.11	8	1
1:A:7:ILE:C	1:A:7:ILE:HD13	0.45	2.37	19	1
1:A:28:GLY:H	1:A:56:ARG:HA	0.45	1.72	6	1
1:A:12:LYS:HG3	1:A:42:THR:HG23	0.45	1.87	9	1
1:A:65:ILE:HG23	1:A:66:ASN:N	0.45	2.27	19	2
1:A:76:TYR:C	1:A:76:TYR:HD2	0.45	2.18	9	1
1:A:21:LEU:O	1:A:36:TYR:CB	0.45	2.66	10	2
1:A:8:GLU:C	1:A:88:ARG:HB2	0.45	2.37	19	1
1:A:105:ARG:H	1:A:106:PRO:HD2	0.45	1.70	20	1
1:A:6:GLU:HA	1:A:48:LYS:HA	0.44	1.87	17	3
1:A:7:ILE:CG1	1:A:86:GLY:H	0.44	2.25	7	2
1:A:86:GLY:O	1:A:87:LYS:HG3	0.44	2.12	6	1
1:A:36:TYR:CD2	1:A:37:LEU:O	0.44	2.70	15	1
1:A:70:PHE:HA	1:A:114:ARG:N	0.44	2.27	18	1
1:A:30:THR:HB	1:A:45:ILE:HG21	0.44	1.88	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:PHE:CE2	1:A:98:ILE:CD1	0.44	3.00	9	2
1:A:13:ASN:CA	1:A:37:LEU:HD11	0.44	2.43	13	1
1:A:19:ARG:NH2	1:A:21:LEU:H	0.44	2.10	1	1
1:A:27:SER:OG	1:A:58:ASN:HB3	0.44	2.11	5	1
1:A:106:PRO:CB	1:A:107:PRO:CD	0.44	2.95	12	2
1:A:29:ASN:HB2	1:A:58:ASN:HA	0.44	1.88	20	1
1:A:26:ARG:O	1:A:27:SER:HB2	0.44	2.12	1	1
1:A:25:CYS:SG	1:A:59:CYS:N	0.44	2.90	8	4
1:A:98:ILE:HB	1:A:111:ASN:HB2	0.44	1.88	12	1
1:A:22:GLN:HG2	1:A:34:VAL:HG12	0.44	1.90	1	1
1:A:12:LYS:HG2	1:A:42:THR:CG2	0.44	2.42	8	2
1:A:15:LEU:N	1:A:19:ARG:HG3	0.44	2.28	8	1
1:A:12:LYS:HG3	1:A:42:THR:CG2	0.44	2.42	9	1
1:A:70:PHE:H	1:A:114:ARG:HA	0.44	1.73	11	1
1:A:22:GLN:HA	1:A:36:TYR:HA	0.44	1.89	18	2
1:A:87:LYS:C	1:A:87:LYS:HD2	0.44	2.38	18	1
1:A:90:GLU:HG3	1:A:91:LEU:HG	0.44	1.89	3	1
1:A:73:VAL:HG13	1:A:111:ASN:HD22	0.44	1.72	5	1
1:A:7:ILE:HG23	1:A:87:LYS:O	0.44	2.13	10	1
1:A:96:ASP:O	1:A:109:PRO:HB3	0.44	2.12	12	1
1:A:7:ILE:HG21	1:A:76:TYR:CG	0.44	2.48	20	1
1:A:36:TYR:CD1	1:A:36:TYR:N	0.44	2.86	18	2
1:A:74:GLU:O	1:A:91:LEU:HD23	0.44	2.13	11	1
1:A:13:ASN:CA	1:A:93:ALA:HB3	0.44	2.34	18	1
1:A:6:GLU:HB3	1:A:48:LYS:HB2	0.44	1.90	20	1
1:A:76:TYR:CE2	1:A:87:LYS:HB2	0.44	2.48	6	1
1:A:91:LEU:HD11	1:A:100:PHE:CD2	0.44	2.48	11	1
1:A:60:LEU:HG	1:A:70:PHE:CE1	0.44	2.48	13	1
1:A:63:GLN:HB3	1:A:115:SER:CB	0.44	2.42	17	1
1:A:70:PHE:CE2	1:A:114:ARG:HB3	0.44	2.48	18	1
1:A:6:GLU:OE1	1:A:48:LYS:HE3	0.43	2.13	3	1
1:A:26:ARG:O	1:A:26:ARG:HG3	0.43	2.12	5	1
1:A:36:TYR:C	1:A:37:LEU:HD22	0.43	2.38	7	1
1:A:108:GLN:HB3	1:A:109:PRO:CD	0.43	2.43	12	1
1:A:48:LYS:NZ	1:A:48:LYS:HB2	0.43	2.28	16	1
1:A:106:PRO:HG2	1:A:108:GLN:NE2	0.43	2.28	3	1
1:A:76:TYR:O	1:A:89:TYR:N	0.43	2.51	11	1
1:A:15:LEU:H	1:A:39:PHE:HZ	0.43	1.51	13	1
1:A:108:GLN:HB2	1:A:109:PRO:HD2	0.43	1.89	20	1
1:A:25:CYS:HB3	1:A:45:ILE:CD1	0.43	2.44	2	1
1:A:19:ARG:HB2	1:A:39:PHE:HB2	0.43	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:LEU:O	1:A:110:LEU:HD13	0.43	2.12	8	2
1:A:90:GLU:CD	1:A:101:LYS:HD3	0.43	2.38	18	1
1:A:98:ILE:HB	1:A:111:ASN:CB	0.43	2.43	1	1
1:A:104:GLU:HG3	1:A:105:ARG:N	0.43	2.28	9	1
1:A:103:ASP:C	1:A:105:ARG:N	0.43	2.77	15	2
1:A:6:GLU:C	1:A:7:ILE:HD13	0.43	2.39	3	1
1:A:37:LEU:C	1:A:37:LEU:HD22	0.43	2.38	12	2
1:A:32:VAL:CG2	1:A:57:TRP:CE3	0.43	2.98	8	1
1:A:17:PRO:C	1:A:39:PHE:CE2	0.43	2.97	13	1
1:A:15:LEU:CB	1:A:95:MET:HA	0.43	2.44	3	2
1:A:28:GLY:H	1:A:56:ARG:C	0.43	2.20	4	1
1:A:69:PHE:O	1:A:70:PHE:HB2	0.43	2.12	20	3
1:A:9:ILE:HG23	1:A:75:ALA:CB	0.43	2.42	11	1
1:A:14:THR:CG2	1:A:15:LEU:HD12	0.43	2.44	13	1
1:A:27:SER:H	1:A:56:ARG:HG3	0.43	1.74	13	1
1:A:5:LYS:HB3	1:A:85:CYS:O	0.43	2.14	2	1
1:A:6:GLU:HG3	1:A:48:LYS:HB3	0.43	1.90	4	2
1:A:58:ASN:OD1	1:A:74:GLU:HA	0.43	2.13	5	1
1:A:30:THR:H	1:A:57:TRP:CD1	0.43	2.32	12	1
1:A:88:ARG:HD3	1:A:89:TYR:H	0.43	1.72	12	1
1:A:70:PHE:H	1:A:114:ARG:CB	0.43	2.26	14	1
1:A:75:ALA:O	1:A:88:ARG:HD2	0.43	2.14	17	1
1:A:100:PHE:CZ	1:A:102:MET:HE3	0.43	2.49	17	1
1:A:27:SER:HB2	1:A:58:ASN:HB2	0.43	1.90	12	2
1:A:15:LEU:CD2	1:A:94:ARG:HB2	0.43	2.43	12	1
1:A:103:ASP:CB	1:A:106:PRO:HB2	0.43	2.43	12	1
1:A:68:LYS:O	1:A:114:ARG:HB3	0.43	2.14	13	1
1:A:114:ARG:O	1:A:115:SER:HB2	0.43	2.14	7	1
1:A:13:ASN:HB3	1:A:21:LEU:HD21	0.43	1.90	16	1
1:A:35:GLN:NE2	1:A:43:ARG:HD2	0.43	2.29	19	1
1:A:76:TYR:HB2	1:A:88:ARG:CD	0.43	2.44	19	1
1:A:76:TYR:CB	1:A:88:ARG:HD3	0.43	2.44	19	1
1:A:27:SER:HB2	1:A:58:ASN:HB3	0.43	1.91	8	1
1:A:62:ARG:CD	1:A:70:PHE:HB2	0.43	2.44	11	1
1:A:13:ASN:HA	1:A:37:LEU:HD11	0.43	1.91	13	1
1:A:23:TYR:OH	1:A:43:ARG:NE	0.43	2.48	18	1
1:A:35:GLN:CG	1:A:36:TYR:H	0.43	2.26	18	1
1:A:47:PHE:O	1:A:48:LYS:HB2	0.42	2.14	7	1
1:A:6:GLU:HG3	1:A:48:LYS:HB2	0.42	1.90	8	2
1:A:30:THR:HG22	1:A:32:VAL:HG12	0.42	1.91	11	1
1:A:24:HIS:HB2	1:A:34:VAL:HG13	0.42	1.91	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD13	1:A:61:PHE:CD2	0.42	2.49	1	1
1:A:68:LYS:O	1:A:69:PHE:HB2	0.42	2.14	19	2
1:A:37:LEU:HB3	1:A:43:ARG:HB2	0.42	1.91	6	1
1:A:27:SER:HB2	1:A:57:TRP:C	0.42	2.39	9	1
1:A:18:SER:N	1:A:39:PHE:CD2	0.42	2.88	13	1
1:A:34:VAL:CG1	1:A:35:GLN:N	0.42	2.75	18	1
1:A:76:TYR:HB2	1:A:88:ARG:HD3	0.42	1.90	19	1
1:A:7:ILE:HG23	1:A:88:ARG:H	0.42	1.74	14	1
1:A:75:ALA:O	1:A:88:ARG:NE	0.42	2.52	18	1
1:A:23:TYR:CD2	1:A:25:CYS:SG	0.42	3.13	6	1
1:A:37:LEU:HB3	1:A:43:ARG:CG	0.42	2.43	12	1
1:A:27:SER:HB3	1:A:57:TRP:HA	0.42	1.91	1	1
1:A:61:PHE:HB2	1:A:71:THR:CG2	0.42	2.44	2	1
1:A:10:VAL:O	1:A:90:GLU:HG2	0.42	2.14	3	1
1:A:70:PHE:N	1:A:114:ARG:HA	0.42	2.30	11	1
1:A:92:SER:OG	1:A:99:TYR:HB3	0.42	2.13	11	1
1:A:89:TYR:HB3	1:A:102:MET:N	0.42	2.29	12	1
1:A:20:ILE:HD11	1:A:38:ASN:HB3	0.42	1.91	18	1
1:A:21:LEU:HB2	1:A:113:TRP:CZ3	0.42	2.49	18	1
1:A:15:LEU:CA	1:A:95:MET:HG2	0.42	2.43	19	2
1:A:31:ASN:CA	1:A:57:TRP:HB2	0.42	2.45	20	1
1:A:98:ILE:HG12	1:A:113:TRP:N	0.42	2.30	2	1
1:A:30:THR:N	1:A:57:TRP:HD1	0.42	2.12	4	1
1:A:94:ARG:HA	1:A:97:ALA:H	0.42	1.75	6	1
1:A:5:LYS:O	1:A:7:ILE:HG12	0.42	2.14	11	1
1:A:6:GLU:CB	1:A:48:LYS:HB2	0.42	2.44	20	1
1:A:30:THR:C	1:A:57:TRP:CB	0.42	2.86	4	1
1:A:30:THR:CG2	1:A:47:PHE:HE1	0.42	2.28	11	1
1:A:30:THR:HB	1:A:47:PHE:CD1	0.42	2.50	12	1
1:A:25:CYS:O	1:A:33:GLY:HA3	0.42	2.15	13	1
1:A:15:LEU:HA	1:A:95:MET:CA	0.42	2.44	19	1
1:A:89:TYR:HB3	1:A:102:MET:H	0.42	1.75	12	1
1:A:97:ALA:HB3	1:A:99:TYR:CE1	0.42	2.49	14	1
1:A:63:GLN:HE21	1:A:63:GLN:HA	0.42	1.75	15	1
1:A:90:GLU:OE1	1:A:101:LYS:HD3	0.42	2.15	17	1
1:A:28:GLY:C	1:A:30:THR:N	0.42	2.75	18	1
1:A:45:ILE:HD11	1:A:57:TRP:CE3	0.42	2.50	5	1
1:A:76:TYR:CD1	1:A:87:LYS:HD3	0.42	2.50	10	1
1:A:28:GLY:CA	1:A:56:ARG:HB2	0.42	2.44	13	1
1:A:27:SER:HB2	1:A:57:TRP:CE2	0.42	2.50	15	1
1:A:19:ARG:HE	1:A:19:ARG:H	0.42	1.57	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ARG:HA	1:A:86:GLY:HA3	0.42	1.92	17	1
1:A:64:GLY:O	1:A:65:ILE:HB	0.42	2.15	17	1
1:A:76:TYR:CD1	1:A:76:TYR:C	0.42	2.96	20	1
1:A:15:LEU:HB2	1:A:19:ARG:NE	0.42	2.30	6	1
1:A:21:LEU:HB2	1:A:113:TRP:CE3	0.42	2.50	18	1
1:A:69:PHE:HA	1:A:115:SER:H	0.42	1.75	19	1
1:A:6:GLU:H	1:A:85:CYS:HA	0.41	1.75	3	1
1:A:44:ILE:HG22	1:A:45:ILE:O	0.41	2.15	4	1
1:A:19:ARG:O	1:A:20:ILE:HD13	0.41	2.15	9	1
1:A:68:LYS:HE3	1:A:115:SER:OXT	0.41	2.14	17	1
1:A:20:ILE:CD1	1:A:38:ASN:HB3	0.41	2.45	18	1
1:A:27:SER:C	1:A:58:ASN:H	0.41	2.22	20	1
1:A:13:ASN:HD21	1:A:19:ARG:C	0.41	2.22	2	1
1:A:26:ARG:C	1:A:57:TRP:HB2	0.41	2.40	6	1
1:A:5:LYS:CB	1:A:86:GLY:HA2	0.41	2.45	15	1
1:A:13:ASN:HB3	1:A:37:LEU:HB2	0.41	1.93	17	1
1:A:56:ARG:HB2	1:A:86:GLY:CA	0.41	2.45	17	1
1:A:59:CYS:O	1:A:72:GLU:HA	0.41	2.15	17	1
1:A:32:VAL:HG21	1:A:45:ILE:HG12	0.41	1.93	4	1
1:A:101:LYS:HB2	1:A:107:PRO:HA	0.41	1.92	9	1
1:A:5:LYS:O	1:A:85:CYS:HA	0.41	2.14	15	1
1:A:7:ILE:HG22	1:A:8:GLU:N	0.41	2.31	17	1
1:A:9:ILE:HD13	1:A:87:LYS:CG	0.41	2.46	17	1
1:A:16:GLY:CA	1:A:39:PHE:CE1	0.41	3.02	18	1
1:A:35:GLN:CG	1:A:36:TYR:N	0.41	2.84	18	1
1:A:100:PHE:CG	1:A:107:PRO:CB	0.41	2.99	14	1
1:A:102:MET:HB2	1:A:107:PRO:HD3	0.41	1.93	2	1
1:A:14:THR:OG1	1:A:39:PHE:CE1	0.41	2.73	4	1
1:A:26:ARG:CA	1:A:57:TRP:HA	0.41	2.45	8	1
1:A:6:GLU:HG3	1:A:48:LYS:CB	0.41	2.45	16	1
1:A:56:ARG:HA	1:A:57:TRP:CE3	0.41	2.50	16	1
1:A:32:VAL:CG1	1:A:45:ILE:HG12	0.41	2.45	20	1
1:A:90:GLU:CD	1:A:91:LEU:HG	0.41	2.40	3	1
1:A:21:LEU:HA	1:A:63:GLN:NE2	0.41	2.30	7	1
1:A:89:TYR:CD2	1:A:102:MET:HB2	0.41	2.51	8	1
1:A:56:ARG:CG	1:A:76:TYR:HA	0.41	2.45	9	1
1:A:15:LEU:CD1	1:A:15:LEU:N	0.41	2.83	14	2
1:A:24:HIS:CE1	1:A:33:GLY:HA2	0.41	2.50	18	1
1:A:112:LYS:N	1:A:112:LYS:HD2	0.41	2.30	1	1
1:A:15:LEU:HG	1:A:95:MET:N	0.41	2.30	2	1
1:A:28:GLY:N	1:A:56:ARG:HA	0.41	2.30	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:THR:HG23	1:A:94:ARG:CG	0.41	2.45	10	1
1:A:15:LEU:HD11	1:A:94:ARG:CG	0.41	2.46	12	1
1:A:32:VAL:HB	1:A:57:TRP:CH2	0.41	2.51	13	1
1:A:56:ARG:HG3	1:A:56:ARG:O	0.41	2.15	13	1
1:A:65:ILE:CG1	1:A:66:ASN:N	0.41	2.84	3	2
1:A:106:PRO:HB3	1:A:107:PRO:HD2	0.41	1.93	12	1
1:A:14:THR:OG1	1:A:39:PHE:HA	0.41	2.16	18	1
1:A:29:ASN:HB3	1:A:76:TYR:HB3	0.41	1.92	4	1
1:A:69:PHE:C	1:A:114:ARG:HB2	0.41	2.41	7	1
1:A:13:ASN:ND2	1:A:19:ARG:HB3	0.41	2.30	8	1
1:A:27:SER:HB2	1:A:30:THR:CB	0.41	2.46	16	1
1:A:47:PHE:HB2	1:A:87:LYS:HE3	0.41	1.93	17	1
1:A:26:ARG:NE	1:A:26:ARG:HA	0.41	2.30	18	1
1:A:99:TYR:CD1	1:A:99:TYR:N	0.41	2.89	18	1
1:A:15:LEU:HA	1:A:95:MET:N	0.41	2.31	19	1
1:A:17:PRO:HA	1:A:19:ARG:NH1	0.41	2.31	19	1
1:A:8:GLU:N	1:A:88:ARG:HG2	0.41	2.28	20	1
1:A:8:GLU:HG2	1:A:46:LYS:HB3	0.41	1.92	3	1
1:A:114:ARG:O	1:A:115:SER:HB3	0.41	2.16	4	2
1:A:13:ASN:HD22	1:A:21:LEU:HB2	0.41	1.76	5	1
1:A:73:VAL:CG1	1:A:91:LEU:HD13	0.41	2.46	5	1
1:A:66:ASN:C	1:A:68:LYS:N	0.41	2.78	14	1
1:A:56:ARG:HB2	1:A:76:TYR:CE2	0.41	2.51	16	1
1:A:9:ILE:HA	1:A:88:ARG:H	0.41	1.75	17	1
1:A:46:LYS:HE3	1:A:46:LYS:H	0.41	1.75	19	1
1:A:10:VAL:N	1:A:90:GLU:HB3	0.40	2.31	3	1
1:A:72:GLU:O	1:A:72:GLU:HG2	0.40	2.16	3	1
1:A:104:GLU:C	1:A:105:ARG:HG2	0.40	2.41	7	1
1:A:27:SER:N	1:A:56:ARG:HB2	0.40	2.30	12	1
1:A:36:TYR:CG	1:A:37:LEU:N	0.40	2.88	15	1
1:A:73:VAL:HG13	1:A:111:ASN:ND2	0.40	2.32	18	1
1:A:7:ILE:HD13	1:A:7:ILE:N	0.40	2.32	3	1
1:A:94:ARG:O	1:A:95:MET:C	0.40	2.64	4	1
1:A:88:ARG:HA	1:A:88:ARG:NE	0.40	2.31	5	1
1:A:113:TRP:CD1	1:A:113:TRP:H	0.40	2.34	9	1
1:A:74:GLU:CD	1:A:74:GLU:H	0.40	2.24	18	1
1:A:10:VAL:N	1:A:90:GLU:HB2	0.40	2.31	3	1
1:A:37:LEU:CG	1:A:43:ARG:HB2	0.40	2.46	5	1
1:A:94:ARG:CB	1:A:113:TRP:HE1	0.40	2.30	6	1
1:A:105:ARG:CG	1:A:106:PRO:HD3	0.40	2.47	9	1
1:A:90:GLU:N	1:A:102:MET:HB2	0.40	2.30	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:ARG:CB	1:A:39:PHE:CE1	0.40	3.04	13	1
1:A:15:LEU:N	1:A:19:ARG:HG2	0.40	2.29	16	1
1:A:15:LEU:C	1:A:95:MET:HG2	0.40	2.42	19	1
1:A:29:ASN:H	1:A:57:TRP:CA	0.40	2.29	20	1
1:A:98:ILE:HB	1:A:111:ASN:HB3	0.40	1.93	10	1
1:A:113:TRP:O	1:A:114:ARG:HG3	0.40	2.17	16	1
1:A:14:THR:HG23	1:A:94:ARG:HG2	0.40	1.93	2	1
1:A:28:GLY:N	1:A:57:TRP:N	0.40	2.70	4	1
1:A:29:ASN:C	1:A:57:TRP:CD1	0.40	2.99	4	1
1:A:46:LYS:O	1:A:47:PHE:CD1	0.40	2.75	6	1
1:A:43:ARG:HA	1:A:43:ARG:NE	0.40	2.31	10	1
1:A:57:TRP:HB3	1:A:75:ALA:HB3	0.40	1.94	14	1
1:A:9:ILE:HD13	1:A:57:TRP:CE3	0.40	2.51	18	1
1:A:108:GLN:HB2	1:A:109:PRO:CD	0.40	2.46	20	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	95/115 (83%)	74±4 (78±4%)	14±3 (15±3%)	7±3 (7±3%)	2	15
All	All	1900/2300 (83%)	1474 (78%)	289 (15%)	137 (7%)	2	15

All 37 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	95	MET	18
1	A	65	ILE	14
1	A	85	CYS	7
1	A	40	LYS	7
1	A	29	ASN	7
1	A	114	ARG	6
1	A	56	ARG	5
1	A	66	ASN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	27	SER	5
1	A	32	VAL	5
1	A	17	PRO	5
1	A	104	GLU	4
1	A	63	GLN	4
1	A	14	THR	3
1	A	68	LYS	3
1	A	33	GLY	3
1	A	97	ALA	3
1	A	109	PRO	3
1	A	105	ARG	3
1	A	106	PRO	3
1	A	18	SER	3
1	A	94	ARG	2
1	A	96	ASP	2
1	A	107	PRO	2
1	A	19	ARG	2
1	A	5	LYS	2
1	A	39	PHE	1
1	A	102	MET	1
1	A	71	THR	1
1	A	111	ASN	1
1	A	48	LYS	1
1	A	69	PHE	1
1	A	67	MET	1
1	A	86	GLY	1
1	A	6	GLU	1
1	A	7	ILE	1
1	A	28	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	87/103 (84%)	71±3 (82±3%)	16±3 (18±3%)	3	36
All	All	1740/2060 (84%)	1420 (82%)	320 (18%)	3	36

All 60 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	73	VAL	20
1	A	10	VAL	19
1	A	9	ILE	18
1	A	91	LEU	18
1	A	19	ARG	14
1	A	20	ILE	13
1	A	42	THR	13
1	A	71	THR	13
1	A	15	LEU	11
1	A	37	LEU	11
1	A	32	VAL	9
1	A	25	CYS	9
1	A	30	THR	9
1	A	8	GLU	7
1	A	21	LEU	6
1	A	5	LYS	6
1	A	43	ARG	6
1	A	46	LYS	6
1	A	56	ARG	6
1	A	112	LYS	5
1	A	14	THR	5
1	A	76	TYR	5
1	A	85	CYS	4
1	A	12	LYS	4
1	A	110	LEU	4
1	A	88	ARG	4
1	A	47	PHE	4
1	A	48	LYS	4
1	A	57	TRP	4
1	A	99	TYR	4
1	A	45	ILE	3
1	A	68	LYS	3
1	A	114	ARG	3
1	A	36	TYR	3
1	A	89	TYR	3
1	A	63	GLN	3
1	A	26	ARG	2
1	A	13	ASN	2
1	A	72	GLU	2
1	A	113	TRP	2
1	A	103	ASP	2
1	A	59	CYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	74	GLU	2
1	A	31	ASN	2
1	A	70	PHE	2
1	A	38	ASN	2
1	A	40	LYS	2
1	A	87	LYS	2
1	A	94	ARG	2
1	A	95	MET	2
1	A	7	ILE	2
1	A	98	ILE	2
1	A	61	PHE	2
1	A	39	PHE	1
1	A	107	PRO	1
1	A	24	HIS	1
1	A	92	SER	1
1	A	58	ASN	1
1	A	69	PHE	1
1	A	101	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 66% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Sph15star_03_04_18.str*

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	1096
Number of shifts mapped to atoms	1096
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	112	0.39 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	103	-0.13 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	100	0.56 ± 0.14	Should be applied
^{15}N	105	-0.42 ± 0.38	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 66%, i.e. 936 atoms were assigned a chemical shift out of a possible 1420. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	453/478 (95%)	188/194 (97%)	176/192 (92%)	89/92 (97%)
Sidechain	452/805 (56%)	296/517 (57%)	156/241 (65%)	0/47 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	31/137 (23%)	31/66 (47%)	0/67 (0%)	0/4 (0%)
Overall	936/1420 (66%)	515/777 (66%)	332/500 (66%)	89/143 (62%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 66%, i.e. 1095 atoms were assigned a chemical shift out of a possible 1662. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	542/571 (95%)	225/232 (97%)	212/230 (92%)	105/109 (96%)
Sidechain	520/946 (55%)	339/607 (56%)	181/285 (64%)	0/54 (0%)
Aromatic	33/145 (23%)	33/70 (47%)	0/69 (0%)	0/6 (0%)
Overall	1095/1662 (66%)	597/909 (66%)	393/584 (67%)	105/169 (62%)

7.1.4 Statistically unusual chemical shifts ⓘ

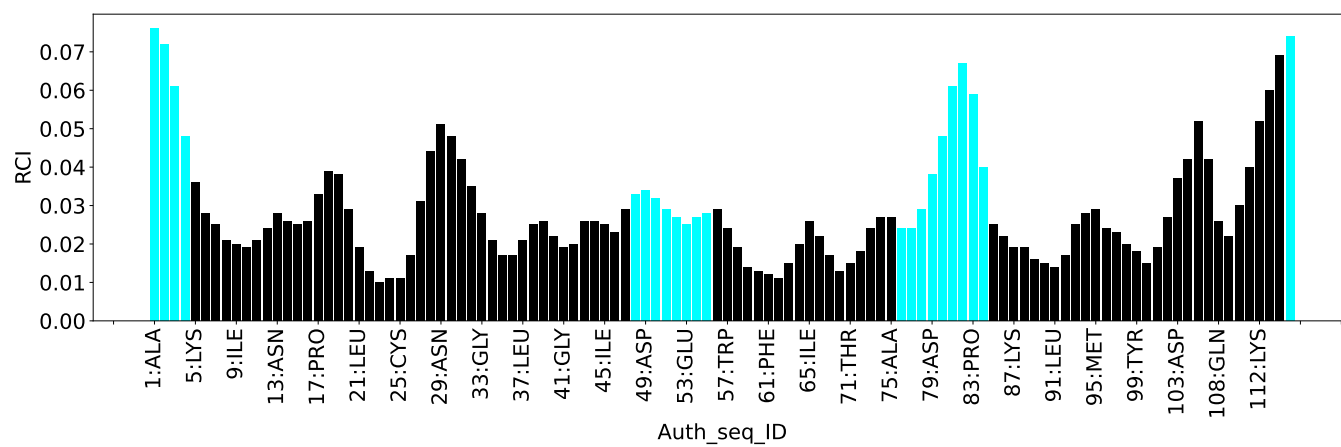
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	35	GLN	HB2	0.47	0.80 – 3.29	-6.3
1	A	35	GLN	HB3	0.47	0.71 – 3.33	-5.9
1	A	7	ILE	HB	0.20	0.35 – 3.22	-5.5
1	A	57	TRP	HE1	6.73	6.88 – 13.28	-5.2

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2671
Intra-residue ($ i-j =0$)	1434
Sequential ($ i-j =1$)	569
Medium range ($ i-j >1$ and $ i-j <5$)	68
Long range ($ i-j \geq 5$)	546
Inter-chain	0
Hydrogen bond restraints	52
Disulfide bond restraints	2
Total dihedral-angle restraints	126
Number of unmapped restraints	0
Number of restraints per residue	24.3
Number of long range restraints per residue ¹	5.2

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)	119.3	0.2
0.2-0.5 (Medium)	211.2	0.5
>0.5 (Large)	121.0	8.2

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	20.6	9.9
10.0-20.0 (Medium)	1.5	19.99
>20.0 (Large)	0.4	36.99

9 Distance violation analysis ⓘ

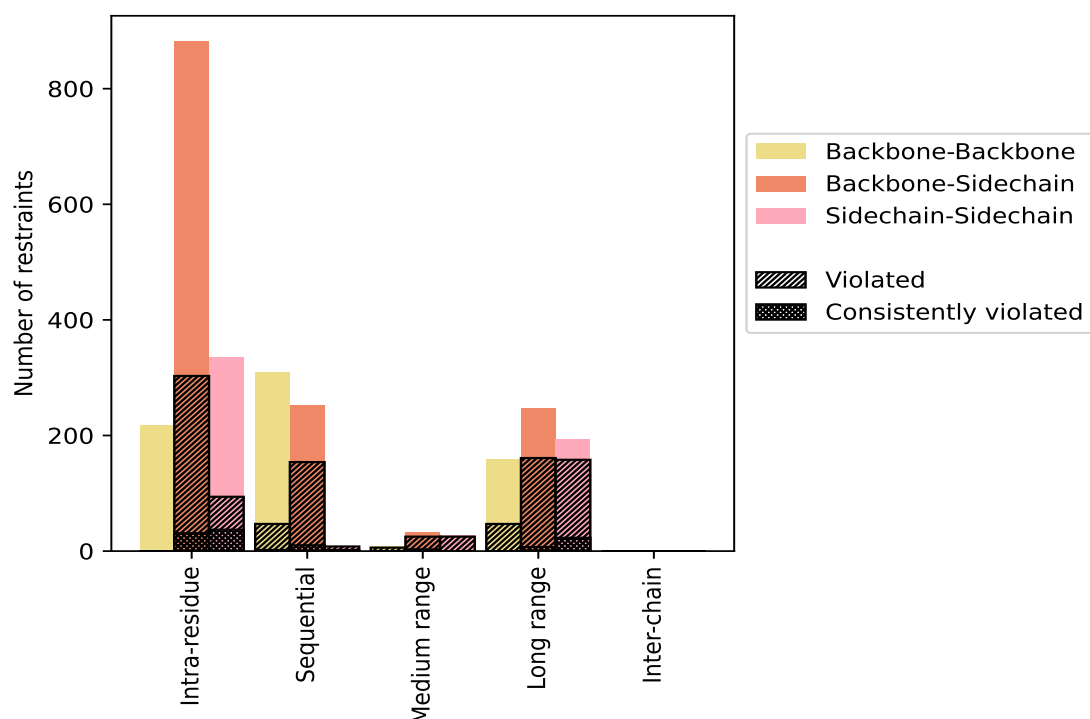
9.1 Summary of distance violations ⓘ

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)	1434	53.7	397	27.7	14.9	68	4.7	2.5
Backbone-Backbone	217	8.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	882	33.0	303	34.4	11.3	31	3.5	1.2
Sidechain-Sidechain	335	12.5	94	28.1	3.5	37	11.0	1.4
Sequential (i-j =1)	569	21.3	209	36.7	7.8	14	2.5	0.5
Backbone-Backbone	309	11.6	47	15.2	1.8	2	0.6	0.1
Backbone-Sidechain	252	9.4	154	61.1	5.8	10	4.0	0.4
Sidechain-Sidechain	8	0.3	8	100.0	0.3	2	25.0	0.1
Medium range (i-j >1 & i-j <5)	68	2.5	56	82.4	2.1	3	4.4	0.1
Backbone-Backbone	9	0.3	6	66.7	0.2	0	0.0	0.0
Backbone-Sidechain	32	1.2	25	78.1	0.9	3	9.4	0.1
Sidechain-Sidechain	27	1.0	25	92.6	0.9	0	0.0	0.0
Long range (i-j ≥5)	546	20.4	349	63.9	13.1	30	5.5	1.1
Backbone-Backbone	159	6.0	47	29.6	1.8	0	0.0	0.0
Backbone-Sidechain	195	7.3	144	73.8	5.4	7	3.6	0.3
Sidechain-Sidechain	192	7.2	158	82.3	5.9	23	12.0	0.9
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	52	1.9	17	32.7	0.6	0	0.0	0.0
Disulfide bond	2	0.1	0	0.0	0.0	0	0.0	0.0
Total	2671	100.0	1028	38.5	38.5	115	4.3	4.3
Backbone-Backbone	694	26.0	100	14.4	3.7	2	0.3	0.1
Backbone-Sidechain	1413	52.9	643	45.5	24.1	51	3.6	1.9
Sidechain-Sidechain	564	21.1	285	50.5	10.7	62	11.0	2.3

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	182	68	22	161	0	433	0.41	1.97	0.31	0.33
2	196	74	26	151	0	447	0.4	1.79	0.29	0.33
3	182	86	28	161	0	457	0.41	2.54	0.35	0.31
4	161	84	30	178	0	453	0.42	3.45	0.35	0.32
5	181	69	36	169	0	455	0.46	6.3	0.47	0.33
6	182	75	33	188	0	478	0.41	2.48	0.35	0.31
7	186	85	22	171	0	464	0.42	1.77	0.33	0.32
8	156	79	26	185	0	446	0.42	5.13	0.39	0.33
9	169	81	28	170	0	448	0.43	3.41	0.38	0.33
10	175	83	26	162	0	446	0.44	3.08	0.34	0.35

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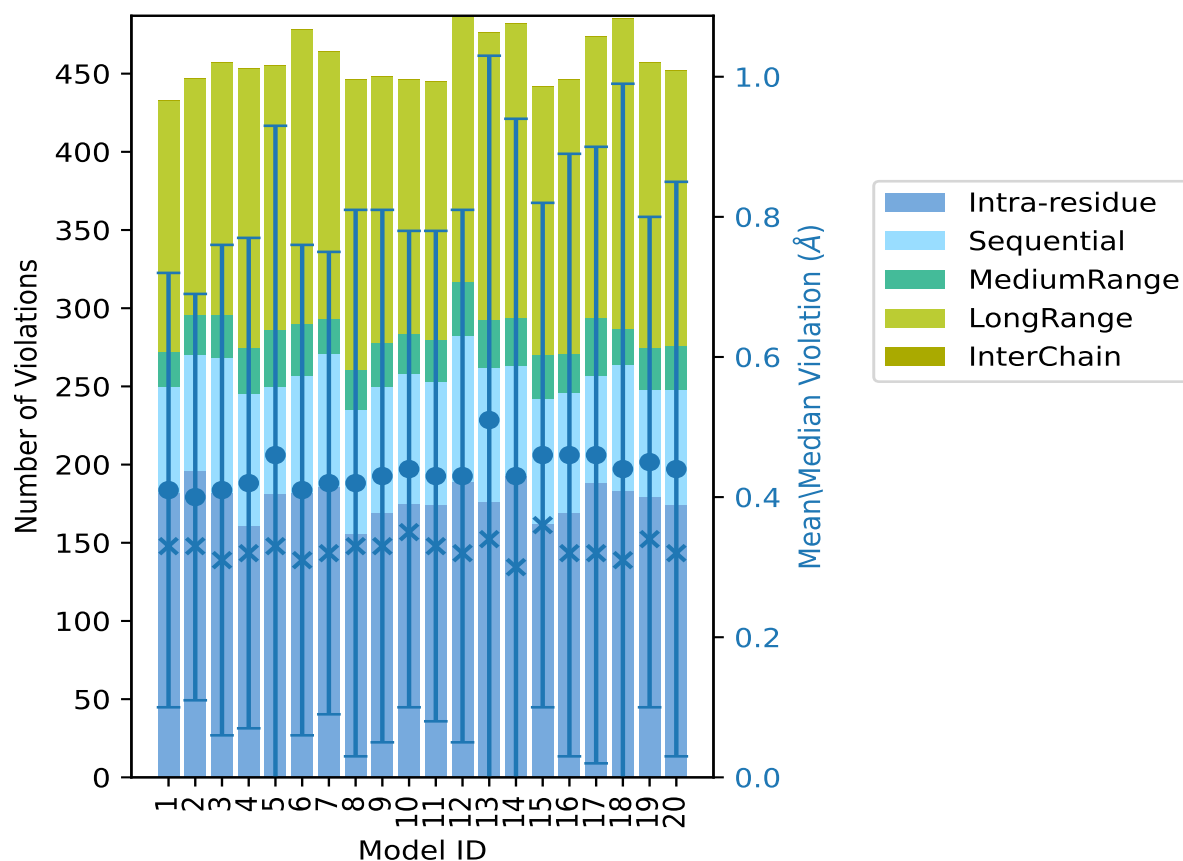
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	174	79	27	165	0	445	0.43	2.53	0.35	0.33
12	189	93	35	170	0	487	0.43	3.17	0.38	0.32
13	176	86	31	183	0	476	0.51	3.35	0.52	0.34
14	193	70	31	188	0	482	0.43	5.88	0.51	0.3
15	162	80	28	172	0	442	0.46	3.19	0.36	0.36
16	169	77	25	175	0	446	0.46	3.23	0.43	0.32
17	188	69	37	180	0	474	0.46	3.41	0.44	0.32
18	183	81	23	198	0	485	0.44	8.2	0.55	0.31
19	179	69	27	182	0	457	0.45	1.93	0.35	0.34
20	174	74	28	176	0	452	0.44	3.74	0.41	0.32

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

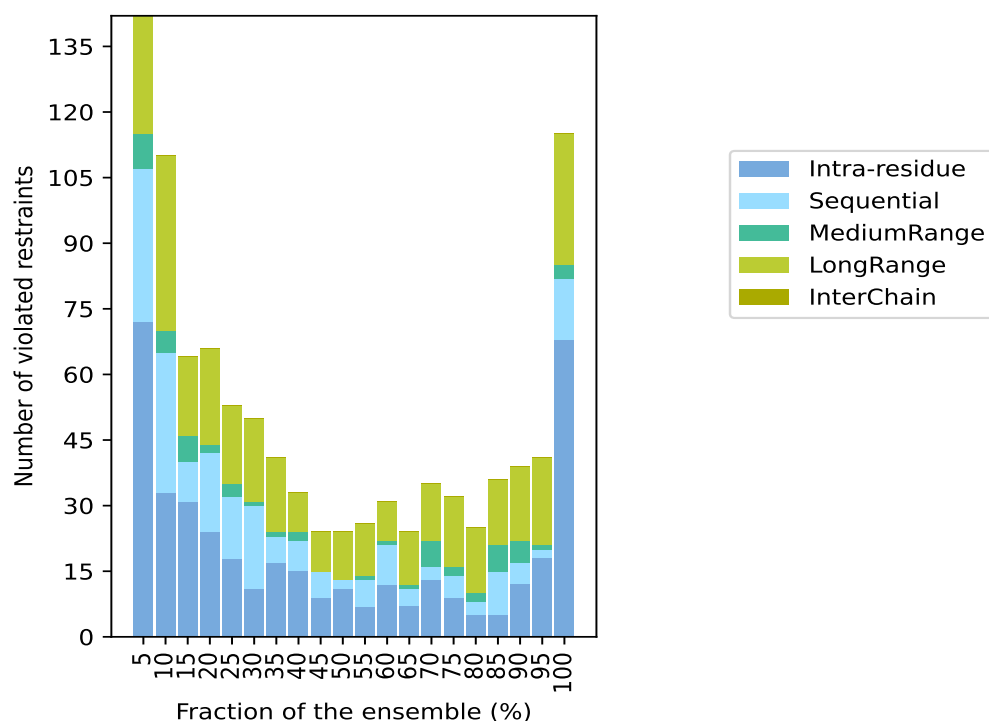
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1606(IR:1037, SQ:360, MR:12, LR:197, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
72	35	8	27	0	142	1	5.0
33	32	5	40	0	110	2	10.0
31	9	6	18	0	64	3	15.0
24	18	2	22	0	66	4	20.0
18	14	3	18	0	53	5	25.0
11	19	1	19	0	50	6	30.0
17	6	1	17	0	41	7	35.0
15	7	2	9	0	33	8	40.0
9	6	0	9	0	24	9	45.0
11	2	0	11	0	24	10	50.0
7	6	1	12	0	26	11	55.0
12	9	1	9	0	31	12	60.0
7	4	1	12	0	24	13	65.0
13	3	6	13	0	35	14	70.0
9	5	2	16	0	32	15	75.0
5	3	2	15	0	25	16	80.0
5	10	6	15	0	36	17	85.0
12	5	5	17	0	39	18	90.0
18	2	1	20	0	41	19	95.0
68	14	3	30	0	115	20	100.0

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

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

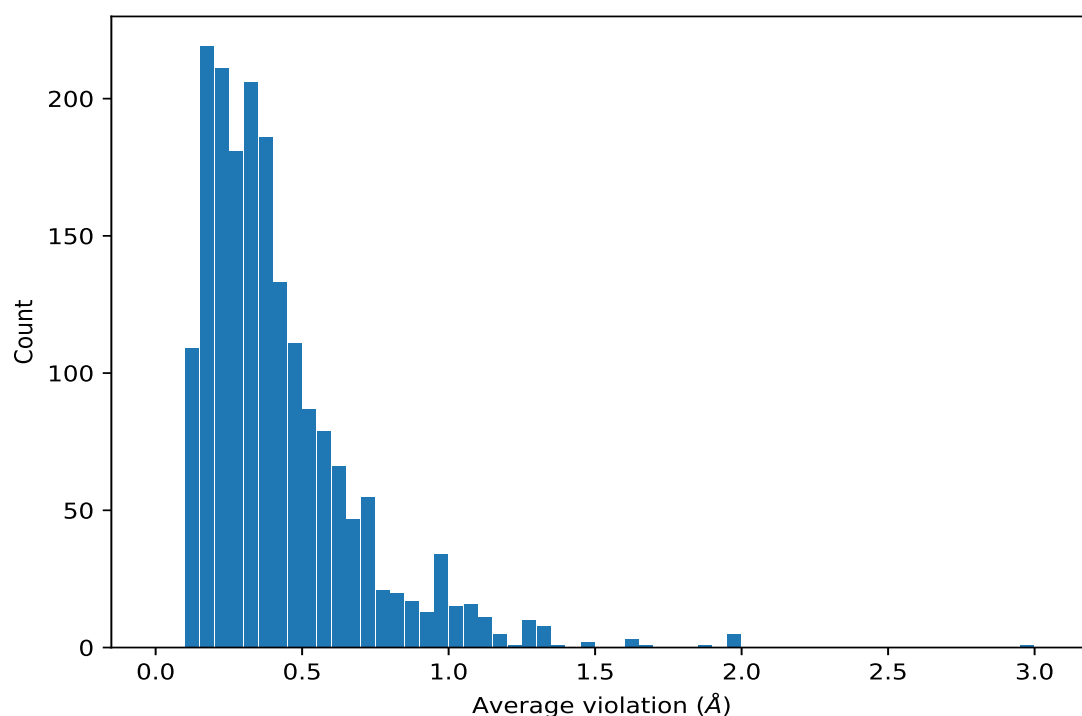
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	20	1.85	0.84	1.47
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	20	1.35	0.21	1.32
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	20	1.33	0.4	1.25
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG22	20	1.33	0.4	1.25
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG21	20	1.33	0.4	1.25
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	20	1.29	0.21	1.27
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	20	1.28	0.4	1.19
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG22	20	1.28	0.4	1.19
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG21	20	1.28	0.4	1.19
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	20	1.15	0.63	1.42
(3,248)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	20	1.15	0.63	1.42
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	20	1.12	0.32	1.13
(3,241)	1:92:A:SER:HA	1:91:A:LEU:HB3	20	1.12	0.32	1.13
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	20	1.11	0.29	1.13
(3,62)	1:104:A:GLU:HB3	1:103:A:ASP:HA	20	1.06	0.34	1.06
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HB3	20	1.06	0.34	1.06

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	20	1.06	0.34	1.06
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HA	20	1.06	0.34	1.06
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	20	1.06	0.29	1.08
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	20	1.04	0.06	1.02
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	20	1.04	0.06	1.02
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	20	1.04	0.06	1.02
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	20	1.03	0.21	1.0
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	20	1.03	0.21	1.0
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG21	20	1.03	0.21	1.0
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	20	1.03	0.21	1.0
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG23	20	1.03	0.21	1.0
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	20	1.03	0.21	1.0
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	20	0.99	0.06	0.98
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	20	0.99	0.06	0.98
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	20	0.99	0.06	0.98
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	20	0.96	0.21	0.94
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	20	0.96	0.21	0.94
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG21	20	0.96	0.21	0.94
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	20	0.96	0.21	0.94
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG23	20	0.96	0.21	0.94
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	20	0.96	0.21	0.94
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	20	0.96	0.19	0.97
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG21	20	0.96	0.19	0.97
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG21	20	0.96	0.19	0.97
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG23	20	0.96	0.19	0.97
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG22	20	0.96	0.19	0.97
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG23	20	0.96	0.19	0.97
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG22	20	0.95	0.14	0.95
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG21	20	0.95	0.14	0.95
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG22	20	0.95	0.14	0.95
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG23	20	0.95	0.14	0.95
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG21	20	0.95	0.14	0.95
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG23	20	0.95	0.14	0.95
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	20	0.94	0.22	0.91
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	20	0.94	0.22	0.91
(1,1961)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	20	0.94	0.22	0.91
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	20	0.9	0.06	0.92
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD12	20	0.9	0.06	0.92
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD13	20	0.9	0.06	0.92
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	20	0.9	0.4	0.8
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG23	20	0.9	0.4	0.8
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG21	20	0.9	0.4	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	20	0.9	0.22	0.86
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	20	0.9	0.22	0.86
(1,911)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	20	0.9	0.22	0.86
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	20	0.89	0.19	0.91
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG21	20	0.89	0.19	0.91
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG21	20	0.89	0.19	0.91
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG23	20	0.89	0.19	0.91
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG22	20	0.89	0.19	0.91
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG23	20	0.89	0.19	0.91
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD13	20	0.85	0.63	0.51
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	20	0.85	0.63	0.51
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD11	20	0.85	0.63	0.51
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB1	20	0.84	0.85	0.6
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	20	0.84	0.85	0.6
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	20	0.84	0.85	0.6
(3,8)	1:76:A:TYR:HB3	1:75:A:ALA:HB1	20	0.84	0.85	0.6
(3,8)	1:76:A:TYR:HB3	1:75:A:ALA:HB3	20	0.84	0.85	0.6
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	20	0.84	0.4	0.74
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG23	20	0.84	0.4	0.74
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG21	20	0.84	0.4	0.74
(1,1056)	1:11:A:ILE:HD12	1:11:A:ILE:HB	20	0.82	0.03	0.82
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	20	0.82	0.03	0.82
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	20	0.82	0.03	0.82
(1,1059)	1:65:A:ILE:HG23	1:65:A:ILE:HA	20	0.81	0.06	0.82
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	20	0.81	0.06	0.82
(1,1059)	1:65:A:ILE:HG21	1:65:A:ILE:HA	20	0.81	0.06	0.82
(3,106)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	20	0.78	0.62	0.67
(3,106)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	20	0.78	0.62	0.67
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	20	0.78	0.62	0.67
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	20	0.78	0.34	0.66
(3,225)	1:44:A:ILE:HD13	1:42:A:THR:HA	20	0.78	0.34	0.66
(3,225)	1:10:A:VAL:HG21	1:42:A:THR:HA	20	0.78	0.34	0.66
(3,225)	1:10:A:VAL:HG22	1:42:A:THR:HA	20	0.78	0.34	0.66
(3,225)	1:44:A:ILE:HD12	1:42:A:THR:HA	20	0.78	0.34	0.66
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	20	0.75	0.06	0.76
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD12	20	0.75	0.06	0.76
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD13	20	0.75	0.06	0.76
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG22	20	0.74	0.11	0.74
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG23	20	0.74	0.11	0.74
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	20	0.74	0.11	0.74
(1,290)	1:20:A:ILE:HD12	1:20:A:ILE:HB	20	0.71	0.27	0.8
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	20	0.71	0.27	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,290)	1:20:A:ILE:HD11	1:20:A:ILE:HB	20	0.71	0.27	0.8
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	20	0.7	0.22	0.64
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	20	0.7	0.22	0.64
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	20	0.7	0.22	0.64
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	20	0.7	0.5	0.52
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	20	0.7	0.5	0.52
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	20	0.7	0.5	0.52
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	20	0.7	0.15	0.72
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	20	0.69	0.03	0.69
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	20	0.69	0.03	0.69
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	20	0.69	0.03	0.69
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD13	20	0.67	0.65	0.4
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD11	20	0.67	0.65	0.4
(3,51)	1:18:A:SER:HB3	1:20:A:ILE:HD11	20	0.67	0.65	0.4
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD12	20	0.67	0.65	0.4
(3,51)	1:9:A:ILE:HG13	1:75:A:ALA:HA	20	0.67	0.65	0.4
(3,51)	1:11:A:ILE:HD13	1:75:A:ALA:HA	20	0.67	0.65	0.4
(3,51)	1:11:A:ILE:HD12	1:75:A:ALA:HA	20	0.67	0.65	0.4
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	20	0.66	0.06	0.68
(1,170)	1:23:A:TYR:HD2	1:23:A:TYR:HA	20	0.66	0.06	0.68
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	20	0.66	0.39	0.49
(3,40)	1:3:A:GLY:HA3	1:4:A:CYS:HA	20	0.66	0.39	0.49
(3,40)	1:15:A:LEU:HA	1:14:A:THR:HA	20	0.66	0.39	0.49
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	20	0.66	0.39	0.49
(3,39)	1:3:A:GLY:HA3	1:4:A:CYS:HA	20	0.66	0.39	0.49
(3,39)	1:15:A:LEU:HA	1:14:A:THR:HA	20	0.66	0.39	0.49
(3,39)	1:51:A:GLY:HA3	1:50:A:ASP:HA	20	0.66	0.39	0.49
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	20	0.65	0.03	0.64
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	20	0.65	0.03	0.64
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	20	0.65	0.03	0.64
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	20	0.64	0.43	0.48
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	20	0.64	0.43	0.48
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	20	0.64	0.43	0.48
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	20	0.63	0.57	0.48
(1,909)	1:10:A:VAL:HG22	1:90:A:GLU:HG2	20	0.63	0.57	0.48
(1,909)	1:10:A:VAL:HG23	1:90:A:GLU:HG2	20	0.63	0.57	0.48
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	20	0.62	0.38	0.64
(1,181)	1:61:A:PHE:HD1	1:21:A:LEU:HB2	20	0.62	0.38	0.64
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	20	0.6	0.23	0.52
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	20	0.6	0.23	0.52
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD12	20	0.6	0.23	0.52
(1,40)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	20	0.59	0.1	0.6

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	20	0.59	0.1	0.6
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	20	0.59	0.1	0.6
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	20	0.59	0.04	0.61
(1,1238)	1:11:A:ILE:HD12	1:11:A:ILE:HB	20	0.56	0.03	0.56
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	20	0.56	0.03	0.56
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	20	0.56	0.03	0.56
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	20	0.55	0.23	0.47
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	20	0.55	0.23	0.47
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD12	20	0.55	0.23	0.47
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	20	0.55	0.09	0.58
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	20	0.55	0.09	0.58
(1,1658)	1:73:A:VAL:HG22	1:74:A:GLU:H	20	0.55	0.09	0.58
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	20	0.55	0.21	0.52
(3,79)	1:113:A:TRP:H	1:113:A:TRP:HB2	20	0.55	0.21	0.52
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	20	0.55	0.21	0.52
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	20	0.54	0.01	0.55
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	20	0.54	0.01	0.55
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	20	0.53	0.09	0.56
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	20	0.53	0.09	0.56
(1,636)	1:73:A:VAL:HG22	1:74:A:GLU:H	20	0.53	0.09	0.56
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	20	0.51	0.09	0.54
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	20	0.51	0.09	0.54
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG21	20	0.51	0.09	0.54
(1,388)	1:65:A:ILE:HG23	1:65:A:ILE:HA	20	0.5	0.06	0.5
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	20	0.5	0.06	0.5
(1,388)	1:65:A:ILE:HG21	1:65:A:ILE:HA	20	0.5	0.06	0.5
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	20	0.49	0.11	0.52
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG21	20	0.49	0.11	0.52
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	20	0.49	0.11	0.52
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	20	0.49	0.08	0.49
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB2	20	0.49	0.08	0.49
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB1	20	0.49	0.08	0.49
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	20	0.47	0.11	0.5
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG21	20	0.47	0.11	0.5
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	20	0.47	0.11	0.5
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.47	0.08	0.47
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG22	20	0.47	0.08	0.47
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG23	20	0.47	0.08	0.47
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG22	20	0.46	0.06	0.48
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	20	0.46	0.06	0.48
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG23	20	0.46	0.06	0.48
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	20	0.46	0.1	0.45

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	20	0.46	0.1	0.45
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	20	0.46	0.1	0.45
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	20	0.45	0.12	0.44
(1,919)	1:70:A:PHE:HE2	1:70:A:PHE:HA	20	0.45	0.12	0.44
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG22	20	0.45	0.06	0.46
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	20	0.45	0.06	0.46
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG23	20	0.45	0.06	0.46
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	20	0.45	0.04	0.43
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	20	0.45	0.04	0.43
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB2	20	0.45	0.04	0.43
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	20	0.44	0.01	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	20	0.44	0.01	0.44
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	20	0.44	0.09	0.46
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	20	0.44	0.09	0.46
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG21	20	0.44	0.09	0.46
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	20	0.44	0.09	0.42
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	20	0.44	0.27	0.43
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD12	20	0.43	0.15	0.42
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	20	0.43	0.15	0.42
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD13	20	0.43	0.15	0.42
(1,1132)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	20	0.43	0.1	0.44
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	20	0.43	0.1	0.44
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	20	0.43	0.1	0.44
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	20	0.42	0.09	0.4
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	20	0.42	0.01	0.42
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	20	0.42	0.01	0.42
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	20	0.41	0.21	0.38
(3,78)	1:113:A:TRP:H	1:113:A:TRP:HB2	20	0.41	0.21	0.38
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	20	0.41	0.21	0.38
(1,895)	1:44:A:ILE:HG21	1:44:A:ILE:HG13	20	0.41	0.02	0.4
(1,895)	1:44:A:ILE:HG22	1:44:A:ILE:HG13	20	0.41	0.02	0.4
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	20	0.41	0.02	0.4
(1,16)	1:98:A:ILE:HD13	1:94:A:ARG:H	20	0.4	0.04	0.4
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	20	0.4	0.04	0.4
(1,16)	1:98:A:ILE:HD11	1:94:A:ARG:H	20	0.4	0.04	0.4
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG21	20	0.4	0.1	0.4
(3,257)	1:93:A:ALA:HB3	1:98:A:ILE:HG13	20	0.4	0.1	0.4
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG13	20	0.4	0.1	0.4
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	20	0.4	0.1	0.4
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG23	20	0.4	0.1	0.4
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG23	20	0.4	0.1	0.4
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG21	20	0.4	0.1	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	20	0.39	0.03	0.39
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	20	0.39	0.03	0.39
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	20	0.39	0.03	0.39
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	20	0.39	0.05	0.38
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	20	0.39	0.05	0.38
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	20	0.39	0.05	0.38
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.39	0.08	0.39
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG22	20	0.39	0.08	0.39
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG23	20	0.39	0.08	0.39
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG22	20	0.38	0.11	0.38
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG23	20	0.38	0.11	0.38
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	20	0.38	0.11	0.38
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	20	0.38	0.01	0.38
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	20	0.38	0.01	0.38
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD13	20	0.37	0.06	0.36
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	20	0.37	0.06	0.36
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	20	0.37	0.06	0.36
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	20	0.37	0.08	0.38
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD11	20	0.36	0.05	0.36
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	20	0.36	0.05	0.36
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	20	0.36	0.05	0.36
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.34	0.08	0.34
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG22	20	0.34	0.08	0.34
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG23	20	0.34	0.08	0.34
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	20	0.33	0.08	0.33
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB2	20	0.33	0.08	0.33
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB1	20	0.33	0.08	0.33
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	20	0.33	0.04	0.32
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	20	0.33	0.04	0.32
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB2	20	0.33	0.04	0.32
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	20	0.33	0.02	0.33
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	20	0.33	0.01	0.33
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	20	0.33	0.01	0.33
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	20	0.32	0.01	0.32
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	20	0.32	0.01	0.32
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	20	0.31	0.07	0.3
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	20	0.31	0.07	0.3
(1,273)	1:73:A:VAL:HG22	1:73:A:VAL:HA	20	0.31	0.07	0.3
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	20	0.31	0.06	0.32
(1,2111)	1:23:A:TYR:HD2	1:23:A:TYR:HA	20	0.31	0.06	0.32
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	20	0.31	0.01	0.31
(1,177)	1:23:A:TYR:HD1	1:23:A:TYR:HE1	20	0.31	0.01	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	20	0.31	0.1	0.3
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	20	0.31	0.1	0.3
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	20	0.31	0.1	0.3
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	20	0.29	0.04	0.3
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	20	0.29	0.04	0.3
(1,1071)	1:44:A:ILE:HD12	1:44:A:ILE:HG12	20	0.29	0.04	0.3
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	20	0.28	0.01	0.28
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	20	0.28	0.01	0.28
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	20	0.28	0.02	0.29
(1,1105)	1:98:A:ILE:HD13	1:94:A:ARG:H	20	0.26	0.05	0.26
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	20	0.26	0.05	0.26
(1,1105)	1:98:A:ILE:HD11	1:94:A:ARG:H	20	0.26	0.05	0.26
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	20	0.26	0.04	0.26
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	20	0.25	0.05	0.24
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	20	0.25	0.05	0.24
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	20	0.25	0.05	0.24
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	20	0.24	0.07	0.22
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	20	0.24	0.07	0.22
(1,2050)	1:73:A:VAL:HG22	1:73:A:VAL:HA	20	0.24	0.07	0.22
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG22	20	0.23	0.01	0.23
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	20	0.23	0.01	0.23
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	20	0.23	0.01	0.23
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	20	0.23	0.06	0.24
(1,1333)	1:23:A:TYR:HD2	1:23:A:TYR:HA	20	0.23	0.06	0.24
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG22	20	0.22	0.01	0.22
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	20	0.22	0.01	0.22
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	20	0.22	0.01	0.22
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	20	0.22	0.03	0.22
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG23	20	0.22	0.03	0.22
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG21	20	0.22	0.03	0.22
(3,92)	1:52:A:THR:HB	1:52:A:THR:HG22	20	0.22	0.03	0.22
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	20	0.2	0.03	0.2
(1,1957)	1:10:A:VAL:HG23	1:10:A:VAL:HB	20	0.2	0.03	0.2
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	20	0.2	0.03	0.2
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	20	0.2	0.01	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	20	0.2	0.01	0.2
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	20	0.18	0.02	0.18
(1,5)	1:42:A:THR:HG21	1:42:A:THR:HB	20	0.18	0.02	0.18
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	20	0.18	0.02	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD12	20	0.18	0.0	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	20	0.18	0.0	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	20	0.18	0.0	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	20	0.18	0.01	0.18
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	20	0.18	0.01	0.18
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	20	0.17	0.01	0.17
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	20	0.17	0.01	0.17
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	20	0.17	0.02	0.17
(1,908)	1:10:A:VAL:HG23	1:10:A:VAL:HB	20	0.17	0.02	0.17
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	20	0.17	0.02	0.17
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG23	20	0.14	0.01	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG21	20	0.14	0.01	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	20	0.14	0.01	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	20	0.14	0.01	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	20	0.14	0.01	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG22	20	0.13	0.01	0.13
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	20	0.13	0.01	0.13
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	20	0.13	0.01	0.13
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	20	0.11	0.01	0.11
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	19	1.25	0.79	1.8
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	19	1.25	0.79	1.8
(3,35)	1:98:A:ILE:HG21	1:61:A:PHE:HE2	19	0.7	0.18	0.75
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG21	19	0.7	0.18	0.75
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	19	0.7	0.18	0.75
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG23	19	0.7	0.18	0.75
(3,35)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	19	0.7	0.18	0.75
(3,35)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	19	0.7	0.18	0.75
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG22	19	0.7	0.18	0.75
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE1	19	0.7	0.18	0.75
(3,35)	1:98:A:ILE:HG22	1:61:A:PHE:HE1	19	0.7	0.18	0.75
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD12	19	0.66	0.06	0.67
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	19	0.66	0.06	0.67
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD11	19	0.66	0.06	0.67
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	19	0.63	0.31	0.54
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD13	19	0.63	0.31	0.54
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD11	19	0.63	0.31	0.54
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD12	19	0.58	0.06	0.59
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	19	0.58	0.06	0.59
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD11	19	0.58	0.06	0.59
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	19	0.57	0.1	0.6
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	19	0.57	0.1	0.6
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	19	0.57	0.1	0.6
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	19	0.55	0.11	0.57
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG13	19	0.55	0.11	0.57
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG12	19	0.55	0.11	0.57

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	19	0.54	0.08	0.56
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG23	19	0.54	0.08	0.56
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG21	19	0.54	0.08	0.56
(3,255)	1:93:A:ALA:HB3	1:14:A:THR:HG21	19	0.54	0.08	0.56
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD12	19	0.54	0.06	0.54
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	19	0.54	0.06	0.54
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD11	19	0.54	0.06	0.54
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	19	0.53	0.11	0.55
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG13	19	0.53	0.11	0.55
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG12	19	0.53	0.11	0.55
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	19	0.52	0.1	0.55
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	19	0.52	0.1	0.55
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	19	0.52	0.1	0.55
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	19	0.5	0.3	0.38
(3,76)	1:33:A:GLY:HA3	1:24:A:HIS:HD1	19	0.5	0.3	0.38
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	19	0.47	0.45	0.3
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD12	19	0.46	0.1	0.48
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD11	19	0.46	0.1	0.48
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	19	0.46	0.1	0.48
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	19	0.43	0.11	0.45
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	19	0.43	0.11	0.45
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD12	19	0.43	0.11	0.45
(1,21)	1:7:A:ILE:HD12	1:8:A:GLU:H	19	0.42	0.12	0.41
(1,21)	1:7:A:ILE:HD13	1:8:A:GLU:H	19	0.42	0.12	0.41
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	19	0.42	0.12	0.41
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD13	19	0.41	0.13	0.38
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	19	0.41	0.13	0.38
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD11	19	0.41	0.13	0.38
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	19	0.39	0.09	0.43
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD13	19	0.39	0.09	0.43
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD11	19	0.39	0.09	0.43
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	19	0.38	0.09	0.42
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD13	19	0.38	0.09	0.42
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD11	19	0.38	0.09	0.42
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	19	0.37	0.06	0.37
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	19	0.37	0.06	0.37
(1,1055)	1:42:A:THR:HG22	1:11:A:ILE:H	19	0.37	0.06	0.37
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	19	0.36	0.1	0.39
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	19	0.36	0.1	0.39
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	19	0.36	0.1	0.39
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	19	0.36	0.05	0.36
(1,1927)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	19	0.35	0.1	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	19	0.35	0.1	0.34
(1,1927)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	19	0.35	0.1	0.34
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG23	19	0.35	0.1	0.36
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	19	0.35	0.1	0.36
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG21	19	0.35	0.1	0.36
(1,51)	1:98:A:ILE:HG21	1:92:A:SER:H	19	0.34	0.1	0.33
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	19	0.34	0.1	0.33
(1,51)	1:98:A:ILE:HG22	1:92:A:SER:H	19	0.34	0.1	0.33
(3,319)	1:19:A:ARG:HG3	1:95:A:MET:H	19	0.33	0.08	0.33
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	19	0.33	0.08	0.33
(3,216)	1:19:A:ARG:HG3	1:95:A:MET:H	19	0.31	0.08	0.31
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	19	0.31	0.08	0.31
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	19	0.31	0.1	0.28
(3,50)	1:10:A:VAL:HA	1:10:A:VAL:HG13	19	0.31	0.1	0.28
(3,50)	1:10:A:VAL:HG21	1:10:A:VAL:HA	19	0.31	0.1	0.28
(3,50)	1:10:A:VAL:HG22	1:10:A:VAL:HA	19	0.31	0.1	0.28
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	19	0.3	0.13	0.25
(1,8)	1:10:A:VAL:HG21	1:10:A:VAL:HA	19	0.3	0.13	0.25
(1,8)	1:10:A:VAL:HG22	1:10:A:VAL:HA	19	0.3	0.13	0.25
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	19	0.3	0.06	0.28
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	19	0.3	0.06	0.28
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB2	19	0.3	0.06	0.28
(1,889)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	19	0.3	0.1	0.29
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	19	0.3	0.1	0.29
(1,889)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	19	0.3	0.1	0.29
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	19	0.29	0.08	0.28
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG22	19	0.29	0.08	0.28
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG21	19	0.29	0.08	0.28
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	19	0.28	0.08	0.25
(3,205)	1:111:A:ASN:H	1:110:A:LEU:HB2	19	0.28	0.08	0.25
(1,65)	1:34:A:VAL:HG23	1:34:A:VAL:HA	19	0.23	0.05	0.23
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	19	0.23	0.05	0.23
(1,65)	1:34:A:VAL:HG22	1:34:A:VAL:HA	19	0.23	0.05	0.23
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	19	0.22	0.04	0.23
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	19	0.22	0.04	0.23
(1,2246)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	19	0.22	0.04	0.23
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	19	0.22	0.06	0.21
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG23	19	0.22	0.06	0.21
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG22	19	0.22	0.06	0.21
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	19	0.22	0.03	0.23
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG11	19	0.22	0.03	0.23
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG13	19	0.22	0.03	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	19	0.22	0.04	0.22
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	19	0.22	0.04	0.22
(1,25)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	19	0.22	0.04	0.22
(1,1962)	1:34:A:VAL:HG23	1:34:A:VAL:HA	19	0.21	0.05	0.2
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	19	0.21	0.05	0.2
(1,1962)	1:34:A:VAL:HG22	1:34:A:VAL:HA	19	0.21	0.05	0.2
(1,1928)	1:98:A:ILE:HG21	1:98:A:ILE:HA	19	0.19	0.05	0.19
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	19	0.19	0.05	0.19
(1,1928)	1:98:A:ILE:HG22	1:98:A:ILE:HA	19	0.19	0.05	0.19
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	19	0.18	0.03	0.19
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG11	19	0.18	0.03	0.19
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG13	19	0.18	0.03	0.19
(1,255)	1:32:A:VAL:HG11	1:47:A:PHE:HE1	18	1.98	2.34	0.54
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE1	18	1.98	2.34	0.54
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE2	18	1.98	2.34	0.54
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE1	18	1.98	2.34	0.54
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE2	18	1.98	2.34	0.54
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	18	1.16	0.5	1.44
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	18	0.95	0.07	0.97
(1,1044)	1:14:A:THR:HG21	1:14:A:THR:HA	18	0.95	0.07	0.97
(1,1044)	1:14:A:THR:HG23	1:14:A:THR:HA	18	0.95	0.07	0.97
(3,231)	1:14:A:THR:HB	1:19:A:ARG:HG3	18	0.85	0.49	0.84
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	18	0.85	0.49	0.84
(3,231)	1:14:A:THR:HB	1:19:A:ARG:HG2	18	0.85	0.49	0.84
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB1	18	0.78	0.87	0.5
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	18	0.78	0.87	0.5
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	18	0.78	0.87	0.5
(3,264)	1:76:A:TYR:HB3	1:75:A:ALA:HB1	18	0.78	0.87	0.5
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	18	0.73	0.61	0.43
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG2	18	0.73	0.61	0.43
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG3	18	0.73	0.61	0.43
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	18	0.65	0.06	0.68
(1,378)	1:14:A:THR:HG21	1:14:A:THR:HA	18	0.65	0.06	0.68
(1,378)	1:14:A:THR:HG23	1:14:A:THR:HA	18	0.65	0.06	0.68
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	18	0.6	0.19	0.68
(1,2274)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	18	0.6	0.19	0.68
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	18	0.6	0.19	0.68
(1,286)	1:45:A:ILE:HG22	1:9:A:ILE:HG12	18	0.58	0.5	0.3
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	18	0.58	0.5	0.3
(1,286)	1:45:A:ILE:HG21	1:9:A:ILE:HG12	18	0.58	0.5	0.3
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	18	0.57	0.5	0.34
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	18	0.57	0.5	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	18	0.57	0.5	0.34
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	18	0.55	0.19	0.63
(1,1072)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	18	0.55	0.19	0.63
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	18	0.55	0.19	0.63
(1,2048)	1:10:A:VAL:HG21	1:90:A:GLU:H	18	0.55	0.12	0.56
(1,2048)	1:10:A:VAL:HG22	1:90:A:GLU:H	18	0.55	0.12	0.56
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	18	0.55	0.12	0.56
(3,219)	1:9:A:ILE:HG21	1:76:A:TYR:HB2	18	0.54	0.21	0.47
(3,219)	1:9:A:ILE:HG22	1:57:A:TRP:HB2	18	0.54	0.21	0.47
(3,219)	1:9:A:ILE:HG23	1:76:A:TYR:HB2	18	0.54	0.21	0.47
(3,219)	1:9:A:ILE:HG22	1:76:A:TYR:HB2	18	0.54	0.21	0.47
(3,219)	1:9:A:ILE:HG23	1:57:A:TRP:HB2	18	0.54	0.21	0.47
(3,219)	1:9:A:ILE:HG21	1:57:A:TRP:HB2	18	0.54	0.21	0.47
(3,219)	1:9:A:ILE:HG21	1:76:A:TYR:HB3	18	0.54	0.21	0.47
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	18	0.53	0.22	0.46
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG21	18	0.53	0.22	0.46
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	18	0.53	0.22	0.46
(3,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	18	0.53	0.2	0.53
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG23	18	0.53	0.2	0.53
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG21	18	0.53	0.2	0.53
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG21	18	0.53	0.2	0.53
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG23	18	0.53	0.2	0.53
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	18	0.52	0.25	0.46
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	18	0.52	0.25	0.46
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	18	0.52	0.25	0.46
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	18	0.51	0.2	0.48
(3,68)	1:1:A:ALA:HB3	1:84:A:LEU:HA	18	0.51	0.2	0.48
(3,68)	1:98:A:ILE:HB	1:111:A:ASN:HA	18	0.51	0.2	0.48
(1,19)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	18	0.47	0.49	0.26
(1,19)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	18	0.47	0.49	0.26
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	18	0.47	0.49	0.26
(1,948)	1:10:A:VAL:HG21	1:90:A:GLU:H	18	0.46	0.12	0.47
(1,948)	1:10:A:VAL:HG22	1:90:A:GLU:H	18	0.46	0.12	0.47
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	18	0.46	0.12	0.47
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD11	18	0.45	0.12	0.45
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD12	18	0.45	0.12	0.45
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	18	0.45	0.12	0.45
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD11	18	0.43	0.12	0.43
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD12	18	0.43	0.12	0.43
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	18	0.43	0.12	0.43
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG22	18	0.42	0.15	0.42
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	18	0.42	0.15	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG23	18	0.42	0.15	0.42
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	18	0.39	0.09	0.39
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	18	0.39	0.09	0.39
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD12	18	0.39	0.09	0.39
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	18	0.38	0.22	0.32
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG21	18	0.38	0.22	0.32
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	18	0.38	0.22	0.32
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	18	0.38	0.11	0.38
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	18	0.38	0.11	0.38
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	18	0.34	0.09	0.32
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	18	0.34	0.09	0.32
(1,117)	1:20:A:ILE:HD13	1:39:A:PHE:H	18	0.34	0.09	0.32
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	18	0.33	0.12	0.38
(1,298)	1:34:A:VAL:HG21	1:24:A:HIS:HE1	18	0.33	0.12	0.38
(1,298)	1:34:A:VAL:HG22	1:24:A:HIS:HE1	18	0.33	0.12	0.38
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	18	0.32	0.06	0.3
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	18	0.29	0.07	0.25
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	18	0.28	0.1	0.25
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG21	18	0.28	0.1	0.25
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG23	18	0.28	0.1	0.25
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	18	0.27	0.07	0.23
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	18	0.27	0.12	0.24
(1,1955)	1:10:A:VAL:HG21	1:10:A:VAL:HA	18	0.27	0.12	0.24
(1,1955)	1:10:A:VAL:HG22	1:10:A:VAL:HA	18	0.27	0.12	0.24
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	18	0.25	0.1	0.21
(3,327)	1:10:A:VAL:HA	1:10:A:VAL:HG13	18	0.25	0.1	0.21
(3,327)	1:10:A:VAL:HG21	1:10:A:VAL:HA	18	0.25	0.1	0.21
(3,327)	1:10:A:VAL:HG22	1:10:A:VAL:HA	18	0.25	0.1	0.21
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	18	0.19	0.08	0.16
(3,148)	1:111:A:ASN:H	1:110:A:LEU:HB2	18	0.19	0.08	0.16
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	18	0.18	0.05	0.17
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	18	0.18	0.06	0.16
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	18	0.15	0.03	0.17
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	18	0.13	0.01	0.13
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	18	0.13	0.01	0.13
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	18	0.13	0.01	0.13
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	18	0.13	0.01	0.13
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	17	1.2	0.44	1.42
(3,228)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	17	0.75	0.52	0.67
(3,228)	1:7:A:ILE:HG22	1:84:A:LEU:HB3	17	0.75	0.52	0.67
(3,228)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	17	0.75	0.52	0.67
(3,228)	1:7:A:ILE:HG23	1:84:A:LEU:HB3	17	0.75	0.52	0.67

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	17	0.73	0.33	0.75
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	17	0.73	0.33	0.75
(1,1052)	1:73:A:VAL:HG22	1:111:A:ASN:HB2	17	0.73	0.33	0.75
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	17	0.67	0.5	0.45
(3,97)	1:56:A:ARG:HB2	1:76:A:TYR:HB3	17	0.67	0.5	0.45
(3,97)	1:88:A:ARG:HB2	1:76:A:TYR:HB3	17	0.67	0.5	0.45
(3,97)	1:20:A:ILE:HG13	1:38:A:ASN:HB2	17	0.67	0.5	0.45
(3,97)	1:88:A:ARG:HB3	1:76:A:TYR:HB2	17	0.67	0.5	0.45
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	17	0.64	0.23	0.64
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG23	17	0.64	0.23	0.64
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG22	17	0.64	0.23	0.64
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	17	0.62	0.23	0.62
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG23	17	0.62	0.23	0.62
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG22	17	0.62	0.23	0.62
(3,220)	1:44:A:ILE:HG23	1:8:A:GLU:HG2	17	0.61	0.2	0.6
(3,220)	1:44:A:ILE:HG21	1:8:A:GLU:HG2	17	0.61	0.2	0.6
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG2	17	0.61	0.2	0.6
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG3	17	0.61	0.2	0.6
(3,220)	1:44:A:ILE:HG21	1:8:A:GLU:HG3	17	0.61	0.2	0.6
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	17	0.57	0.42	0.45
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	17	0.57	0.42	0.45
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	17	0.57	0.42	0.45
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	17	0.42	0.05	0.43
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	17	0.42	0.3	0.34
(3,192)	1:86:A:GLY:H	1:5:A:LYS:HB3	17	0.42	0.3	0.34
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	17	0.41	0.19	0.41
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE2	17	0.41	0.19	0.41
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	17	0.4	0.05	0.41
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	17	0.38	0.16	0.33
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD11	17	0.38	0.16	0.33
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD12	17	0.38	0.16	0.33
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	17	0.36	0.16	0.31
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD11	17	0.36	0.16	0.31
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD12	17	0.36	0.16	0.31
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	17	0.35	0.16	0.35
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	17	0.35	0.16	0.35
(1,53)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	17	0.35	0.16	0.35
(1,53)	1:76:A:TYR:HD1	1:7:A:ILE:HG21	17	0.35	0.16	0.35
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG21	17	0.35	0.16	0.35
(1,53)	1:76:A:TYR:HD1	1:7:A:ILE:HG22	17	0.35	0.16	0.35
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	17	0.35	0.07	0.35
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD2	17	0.35	0.07	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,157)	1:73:A:VAL:HG21	1:61:A:PHE:HD1	17	0.35	0.07	0.35
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	17	0.35	0.07	0.35
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD2	17	0.35	0.07	0.35
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	17	0.35	0.1	0.34
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	17	0.35	0.11	0.32
(1,156)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	17	0.35	0.11	0.32
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE2	17	0.35	0.11	0.32
(1,156)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	17	0.35	0.11	0.32
(1,156)	1:73:A:VAL:HG23	1:61:A:PHE:HE2	17	0.35	0.11	0.32
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	17	0.35	0.1	0.35
(3,134)	1:36:A:TYR:HD1	1:22:A:GLN:HA	17	0.35	0.1	0.35
(3,134)	1:36:A:TYR:HD2	1:22:A:GLN:HA	17	0.35	0.1	0.35
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	17	0.3	0.05	0.31
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD13	17	0.3	0.05	0.31
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD11	17	0.3	0.05	0.31
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	17	0.28	0.05	0.3
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD13	17	0.28	0.05	0.3
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD11	17	0.28	0.05	0.3
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	17	0.28	0.08	0.3
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG21	17	0.28	0.08	0.3
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG22	17	0.28	0.08	0.3
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG22	17	0.28	0.06	0.28
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	17	0.28	0.06	0.28
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG23	17	0.28	0.06	0.28
(3,245)	1:5:A:LYS:HA	1:5:A:LYS:HB3	17	0.27	0.17	0.2
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	17	0.27	0.17	0.2
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	17	0.26	0.08	0.28
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG21	17	0.26	0.08	0.28
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG22	17	0.26	0.08	0.28
(1,2096)	1:73:A:VAL:HG22	1:72:A:GLU:HA	17	0.25	0.08	0.24
(1,2096)	1:73:A:VAL:HG23	1:72:A:GLU:HA	17	0.25	0.08	0.24
(1,2096)	1:73:A:VAL:HG21	1:72:A:GLU:HA	17	0.25	0.08	0.24
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	17	0.25	0.07	0.25
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG23	17	0.25	0.07	0.25
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG21	17	0.25	0.07	0.25
(3,158)	1:93:A:ALA:HB3	1:14:A:THR:HG21	17	0.25	0.07	0.25
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	17	0.24	0.08	0.24
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	17	0.23	0.04	0.23
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	17	0.22	0.08	0.22
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	17	0.2	0.12	0.15
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	17	0.2	0.12	0.15
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	17	0.19	0.06	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG21	17	0.19	0.06	0.17
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG23	17	0.19	0.06	0.17
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	17	0.17	0.06	0.14
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	17	0.17	0.01	0.17
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	17	0.13	0.01	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	17	0.13	0.0	0.13
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	16	1.33	0.7	1.72
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	16	1.33	0.7	1.72
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	16	1.33	0.56	1.6
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	16	0.91	1.29	0.2
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	16	0.72	0.2	0.8
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD2	16	0.72	0.2	0.8
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	16	0.7	0.56	0.44
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	16	0.7	0.56	0.44
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	16	0.7	0.56	0.44
(3,10)	1:20:A:ILE:HG22	1:21:A:LEU:HA	16	0.47	0.13	0.46
(3,10)	1:37:A:LEU:HA	1:20:A:ILE:HG23	16	0.47	0.13	0.46
(3,10)	1:20:A:ILE:HG23	1:21:A:LEU:HA	16	0.47	0.13	0.46
(3,10)	1:37:A:LEU:HA	1:20:A:ILE:HG22	16	0.47	0.13	0.46
(3,10)	1:20:A:ILE:HG21	1:21:A:LEU:HA	16	0.47	0.13	0.46
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	16	0.43	0.12	0.48
(3,227)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	16	0.43	0.29	0.34
(3,227)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	16	0.43	0.29	0.34
(3,227)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	16	0.43	0.29	0.34
(3,227)	1:7:A:ILE:HD11	1:87:A:LYS:HB2	16	0.43	0.29	0.34
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	16	0.42	0.14	0.42
(3,289)	1:48:A:LYS:HB3	1:6:A:GLU:H	16	0.42	0.14	0.42
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	16	0.41	0.48	0.22
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	16	0.4	0.14	0.4
(3,169)	1:48:A:LYS:HB3	1:6:A:GLU:H	16	0.4	0.14	0.4
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	16	0.34	0.15	0.33
(3,33)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	16	0.34	0.15	0.33
(3,33)	1:76:A:TYR:HD1	1:7:A:ILE:HG21	16	0.34	0.15	0.33
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG21	16	0.34	0.15	0.33
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	16	0.34	0.15	0.33
(3,33)	1:76:A:TYR:HD1	1:7:A:ILE:HG22	16	0.34	0.15	0.33
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	16	0.32	0.02	0.33
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG22	16	0.32	0.02	0.33
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG23	16	0.32	0.02	0.33
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	16	0.32	0.1	0.33
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	16	0.32	0.1	0.33
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB2	16	0.32	0.1	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD13	16	0.3	0.1	0.3
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	16	0.3	0.1	0.3
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD11	16	0.3	0.1	0.3
(3,60)	1:6:A:GLU:HB2	1:48:A:LYS:HA	16	0.27	0.33	0.18
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	16	0.27	0.33	0.18
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG22	16	0.27	0.04	0.27
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	16	0.27	0.04	0.27
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG23	16	0.27	0.04	0.27
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	16	0.23	0.02	0.23
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG22	16	0.23	0.02	0.23
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG23	16	0.23	0.02	0.23
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	16	0.22	0.08	0.18
(1,1242)	1:20:A:ILE:HD12	1:39:A:PHE:H	16	0.22	0.08	0.18
(1,1242)	1:20:A:ILE:HD13	1:39:A:PHE:H	16	0.22	0.08	0.18
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	16	0.19	0.03	0.18
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	16	0.18	0.02	0.18
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG22	16	0.18	0.02	0.18
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG23	16	0.18	0.02	0.18
(3,49)	1:98:A:ILE:HG21	1:98:A:ILE:HA	16	0.18	0.04	0.16
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	16	0.18	0.04	0.16
(3,49)	1:98:A:ILE:HG22	1:98:A:ILE:HA	16	0.18	0.04	0.16
(1,890)	1:98:A:ILE:HG21	1:98:A:ILE:HA	16	0.16	0.04	0.15
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	16	0.16	0.04	0.15
(1,890)	1:98:A:ILE:HG22	1:98:A:ILE:HA	16	0.16	0.04	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	16	0.14	0.02	0.15
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG12	16	0.11	0.0	0.11
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG13	16	0.11	0.0	0.11
(3,25)	1:65:A:ILE:HD11	1:65:A:ILE:HG13	16	0.11	0.0	0.11
(3,25)	1:65:A:ILE:HD13	1:65:A:ILE:HG12	16	0.11	0.0	0.11
(3,25)	1:65:A:ILE:HD11	1:65:A:ILE:HG12	16	0.11	0.0	0.11
(3,25)	1:65:A:ILE:HD13	1:65:A:ILE:HG13	16	0.11	0.0	0.11
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	15	1.05	0.5	1.12
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	15	0.98	0.66	0.78
(3,44)	1:28:A:GLY:HA2	1:55:A:SER:HB2	15	0.98	0.66	0.78
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	15	0.72	0.19	0.75
(1,140)	1:45:A:ILE:HD11	1:9:A:ILE:HD11	15	0.72	0.19	0.75
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	15	0.72	0.19	0.75
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD12	15	0.72	0.19	0.75
(1,140)	1:45:A:ILE:HD11	1:9:A:ILE:HD13	15	0.72	0.19	0.75
(1,140)	1:45:A:ILE:HD11	1:9:A:ILE:HD12	15	0.72	0.19	0.75
(1,140)	1:45:A:ILE:HD13	1:9:A:ILE:HD11	15	0.72	0.19	0.75
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	15	0.64	0.1	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	15	0.64	0.1	0.68
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB3	15	0.64	0.1	0.68
(3,218)	1:11:A:ILE:HG21	1:59:A:CYS:HB2	15	0.61	0.38	0.47
(3,218)	1:11:A:ILE:HG23	1:37:A:LEU:HB2	15	0.61	0.38	0.47
(3,218)	1:11:A:ILE:HG22	1:37:A:LEU:HB2	15	0.61	0.38	0.47
(3,218)	1:11:A:ILE:HG21	1:37:A:LEU:HB2	15	0.61	0.38	0.47
(3,218)	1:11:A:ILE:HG22	1:59:A:CYS:HB2	15	0.61	0.38	0.47
(3,218)	1:11:A:ILE:HG23	1:59:A:CYS:HB2	15	0.61	0.38	0.47
(3,326)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	15	0.61	0.6	0.53
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	15	0.61	0.6	0.53
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	15	0.61	0.6	0.53
(3,326)	1:87:A:LYS:HB3	1:7:A:ILE:HG23	15	0.61	0.6	0.53
(3,226)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	15	0.56	0.6	0.48
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	15	0.56	0.6	0.48
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	15	0.56	0.6	0.48
(3,226)	1:87:A:LYS:HB3	1:7:A:ILE:HG23	15	0.56	0.6	0.48
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	15	0.56	0.19	0.6
(1,1293)	1:45:A:ILE:HD11	1:9:A:ILE:HD11	15	0.56	0.19	0.6
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	15	0.56	0.19	0.6
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD12	15	0.56	0.19	0.6
(1,1293)	1:45:A:ILE:HD11	1:9:A:ILE:HD13	15	0.56	0.19	0.6
(1,1293)	1:45:A:ILE:HD11	1:9:A:ILE:HD12	15	0.56	0.19	0.6
(1,1293)	1:45:A:ILE:HD13	1:9:A:ILE:HD11	15	0.56	0.19	0.6
(3,107)	1:44:A:ILE:HG23	1:8:A:GLU:HB2	15	0.55	0.19	0.55
(3,107)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	15	0.55	0.19	0.55
(3,107)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	15	0.55	0.19	0.55
(3,107)	1:44:A:ILE:HG21	1:8:A:GLU:HB2	15	0.55	0.19	0.55
(3,107)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	15	0.55	0.19	0.55
(3,107)	1:44:A:ILE:HG21	1:46:A:LYS:HB3	15	0.55	0.19	0.55
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	15	0.5	0.52	0.23
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	15	0.5	0.52	0.23
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	15	0.5	0.52	0.23
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	15	0.5	0.1	0.54
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	15	0.5	0.1	0.54
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB3	15	0.5	0.1	0.54
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	15	0.45	0.12	0.47
(1,1173)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	15	0.45	0.12	0.47
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	15	0.45	0.12	0.47
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	15	0.44	0.16	0.5
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD2	15	0.44	0.16	0.5
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	15	0.41	0.31	0.24
(1,1930)	1:98:A:ILE:HG21	1:61:A:PHE:HE2	15	0.38	0.2	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1930)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	15	0.38	0.2	0.3
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	15	0.38	0.2	0.3
(1,1930)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	15	0.38	0.2	0.3
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE1	15	0.38	0.2	0.3
(1,1930)	1:98:A:ILE:HG22	1:61:A:PHE:HE1	15	0.38	0.2	0.3
(1,1541)	1:20:A:ILE:HD11	1:38:A:ASN:H	15	0.37	0.17	0.39
(1,1541)	1:20:A:ILE:HD12	1:38:A:ASN:H	15	0.37	0.17	0.39
(1,1541)	1:20:A:ILE:HD13	1:38:A:ASN:H	15	0.37	0.17	0.39
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	15	0.37	0.38	0.28
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	15	0.37	0.38	0.28
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG22	15	0.36	0.14	0.34
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG23	15	0.36	0.14	0.34
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	15	0.36	0.14	0.34
(1,1037)	1:73:A:VAL:HG21	1:91:A:LEU:HB3	15	0.35	0.14	0.37
(1,1037)	1:73:A:VAL:HG22	1:91:A:LEU:HB3	15	0.35	0.14	0.37
(1,1037)	1:73:A:VAL:HG23	1:91:A:LEU:HB3	15	0.35	0.14	0.37
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD13	15	0.34	0.22	0.3
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	15	0.34	0.22	0.3
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	15	0.34	0.22	0.3
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	15	0.32	0.06	0.31
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG23	15	0.32	0.06	0.31
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG22	15	0.32	0.06	0.31
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	15	0.3	0.38	0.22
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	15	0.3	0.03	0.31
(3,317)	1:47:A:PHE:H	1:8:A:GLU:HG3	15	0.3	0.1	0.28
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	15	0.3	0.1	0.28
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	15	0.28	0.15	0.21
(3,246)	1:5:A:LYS:HG3	1:5:A:LYS:HA	15	0.28	0.15	0.21
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	15	0.25	0.09	0.26
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	15	0.25	0.09	0.26
(1,1143)	1:98:A:ILE:HG21	1:92:A:SER:H	15	0.24	0.08	0.21
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	15	0.24	0.08	0.21
(1,1143)	1:98:A:ILE:HG22	1:92:A:SER:H	15	0.24	0.08	0.21
(1,1097)	1:10:A:VAL:HG23	1:10:A:VAL:HA	15	0.22	0.12	0.18
(1,1097)	1:10:A:VAL:HG21	1:10:A:VAL:HA	15	0.22	0.12	0.18
(1,1097)	1:10:A:VAL:HG22	1:10:A:VAL:HA	15	0.22	0.12	0.18
(1,982)	1:73:A:VAL:HG22	1:72:A:GLU:HA	15	0.21	0.08	0.19
(1,982)	1:73:A:VAL:HG23	1:72:A:GLU:HA	15	0.21	0.08	0.19
(1,982)	1:73:A:VAL:HG21	1:72:A:GLU:HA	15	0.21	0.08	0.19
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	15	0.2	0.07	0.18
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG23	15	0.18	0.08	0.15
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG22	15	0.18	0.08	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	15	0.18	0.08	0.15
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	15	0.14	0.02	0.14
(1,1113)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	15	0.14	0.02	0.14
(1,1113)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	15	0.14	0.02	0.14
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	14	1.48	0.34	1.62
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	14	1.33	0.5	1.33
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	14	1.29	0.33	1.38
(1,264)	1:42:A:THR:HG21	1:12:A:LYS:HG2	14	1.29	0.33	1.38
(1,264)	1:42:A:THR:HG22	1:12:A:LYS:HG2	14	1.29	0.33	1.38
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	14	1.05	0.45	1.12
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	14	1.04	0.4	1.17
(3,160)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	14	1.04	0.4	1.17
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	14	0.62	0.56	0.38
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	14	0.62	0.56	0.38
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	14	0.62	0.56	0.38
(1,45)	1:9:A:ILE:HD13	1:7:A:ILE:HG22	14	0.47	0.22	0.42
(1,45)	1:9:A:ILE:HD13	1:7:A:ILE:HG21	14	0.47	0.22	0.42
(1,45)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	14	0.47	0.22	0.42
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	14	0.47	0.22	0.42
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG22	14	0.47	0.22	0.42
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG23	14	0.47	0.22	0.42
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	14	0.46	0.19	0.46
(3,174)	1:19:A:ARG:HG3	1:19:A:ARG:H	14	0.46	0.19	0.46
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG22	14	0.45	0.14	0.46
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	14	0.45	0.14	0.46
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG21	14	0.45	0.14	0.46
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	14	0.44	0.14	0.49
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD2	14	0.44	0.14	0.49
(1,1107)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	14	0.44	0.52	0.17
(1,1107)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	14	0.44	0.52	0.17
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	14	0.44	0.52	0.17
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG22	14	0.43	0.14	0.44
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	14	0.43	0.14	0.44
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG21	14	0.43	0.14	0.44
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	14	0.41	0.16	0.42
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	14	0.41	0.1	0.44
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	14	0.4	0.16	0.34
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG3	14	0.4	0.16	0.34
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	14	0.39	0.08	0.41
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	14	0.37	0.09	0.41
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	14	0.37	0.08	0.39
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	14	0.37	0.12	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,310)	1:105:A:ARG:H	1:103:A:ASP:HB2	14	0.37	0.12	0.4
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	14	0.35	0.12	0.39
(3,203)	1:105:A:ARG:H	1:103:A:ASP:HB2	14	0.35	0.12	0.39
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	14	0.35	0.14	0.35
(1,1547)	1:39:A:PHE:HD1	1:39:A:PHE:H	14	0.35	0.14	0.35
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG3	14	0.34	0.44	0.21
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	14	0.34	0.44	0.21
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	14	0.33	0.11	0.34
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG21	14	0.33	0.11	0.34
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG23	14	0.33	0.11	0.34
(1,153)	1:61:A:PHE:HD1	1:71:A:THR:HG22	14	0.33	0.11	0.34
(1,153)	1:61:A:PHE:HD1	1:71:A:THR:HG21	14	0.33	0.11	0.34
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG22	14	0.32	0.09	0.3
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG23	14	0.32	0.09	0.3
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG21	14	0.32	0.09	0.3
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG22	14	0.31	0.13	0.29
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG23	14	0.31	0.13	0.29
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG21	14	0.31	0.13	0.29
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD13	14	0.31	0.22	0.26
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	14	0.31	0.22	0.26
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	14	0.31	0.22	0.26
(3,65)	1:6:A:GLU:HG2	1:48:A:LYS:HA	14	0.3	0.16	0.29
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	14	0.3	0.16	0.29
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	14	0.28	0.12	0.24
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG22	14	0.28	0.12	0.24
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG22	14	0.28	0.12	0.24
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG23	14	0.28	0.12	0.24
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG21	14	0.28	0.12	0.24
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG23	14	0.28	0.12	0.24
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG21	14	0.24	0.11	0.22
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	14	0.24	0.11	0.22
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG22	14	0.24	0.11	0.22
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	14	0.22	0.17	0.18
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	14	0.2	0.01	0.2
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG21	14	0.18	0.02	0.18
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG23	14	0.18	0.02	0.18
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG22	14	0.18	0.02	0.18
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	14	0.16	0.05	0.14
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG21	14	0.16	0.05	0.14
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG23	14	0.16	0.05	0.14
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG21	14	0.15	0.03	0.15
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG23	14	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG22	14	0.15	0.03	0.15
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	14	0.13	0.01	0.14
(1,262)	1:93:A:ALA:HB2	1:13:A:ASN:HB2	13	0.71	0.61	0.37
(1,262)	1:93:A:ALA:HB3	1:13:A:ASN:HB2	13	0.71	0.61	0.37
(1,262)	1:93:A:ALA:HB1	1:13:A:ASN:HB2	13	0.71	0.61	0.37
(3,108)	1:44:A:ILE:HG23	1:8:A:GLU:HB2	13	0.5	0.19	0.48
(3,108)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	13	0.5	0.19	0.48
(3,108)	1:9:A:ILE:HG23	1:88:A:ARG:HB3	13	0.5	0.19	0.48
(3,108)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	13	0.5	0.19	0.48
(3,108)	1:44:A:ILE:HG21	1:8:A:GLU:HB2	13	0.5	0.19	0.48
(3,108)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	13	0.5	0.19	0.48
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG22	13	0.48	0.09	0.5
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG23	13	0.48	0.09	0.5
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG21	13	0.48	0.09	0.5
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	13	0.46	0.33	0.39
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	13	0.4	0.15	0.33
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG3	13	0.4	0.15	0.33
(1,525)	1:20:A:ILE:HD11	1:38:A:ASN:H	13	0.39	0.15	0.45
(1,525)	1:20:A:ILE:HD12	1:38:A:ASN:H	13	0.39	0.15	0.45
(1,525)	1:20:A:ILE:HD13	1:38:A:ASN:H	13	0.39	0.15	0.45
(1,94)	1:9:A:ILE:HG21	1:75:A:ALA:HA	13	0.38	0.22	0.29
(1,94)	1:9:A:ILE:HG22	1:75:A:ALA:HA	13	0.38	0.22	0.29
(1,94)	1:9:A:ILE:HG23	1:75:A:ALA:HA	13	0.38	0.22	0.29
(1,892)	1:98:A:ILE:HG21	1:61:A:PHE:HE2	13	0.36	0.19	0.34
(1,892)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	13	0.36	0.19	0.34
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	13	0.36	0.19	0.34
(1,892)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	13	0.36	0.19	0.34
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE1	13	0.36	0.19	0.34
(1,892)	1:98:A:ILE:HG22	1:61:A:PHE:HE1	13	0.36	0.19	0.34
(1,1137)	1:9:A:ILE:HD13	1:7:A:ILE:HG22	13	0.35	0.21	0.28
(1,1137)	1:9:A:ILE:HD13	1:7:A:ILE:HG21	13	0.35	0.21	0.28
(1,1137)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	13	0.35	0.21	0.28
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	13	0.35	0.21	0.28
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG22	13	0.35	0.21	0.28
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG23	13	0.35	0.21	0.28
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	13	0.35	0.1	0.33
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	13	0.35	0.1	0.33
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	13	0.35	0.1	0.33
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	13	0.35	0.13	0.34
(1,531)	1:39:A:PHE:HD1	1:39:A:PHE:H	13	0.35	0.13	0.34
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	13	0.35	0.15	0.38
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	13	0.35	0.16	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	13	0.35	0.16	0.42
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	13	0.35	0.16	0.42
(3,73)	1:45:A:ILE:HB	1:9:A:ILE:HD11	13	0.35	0.16	0.42
(1,1408)	1:10:A:VAL:HG21	1:10:A:VAL:H	13	0.34	0.12	0.37
(1,1408)	1:10:A:VAL:HG22	1:10:A:VAL:H	13	0.34	0.12	0.37
(1,1408)	1:10:A:VAL:HG23	1:10:A:VAL:H	13	0.34	0.12	0.37
(1,413)	1:10:A:VAL:HG21	1:10:A:VAL:H	13	0.32	0.12	0.35
(1,413)	1:10:A:VAL:HG22	1:10:A:VAL:H	13	0.32	0.12	0.35
(1,413)	1:10:A:VAL:HG23	1:10:A:VAL:H	13	0.32	0.12	0.35
(1,1243)	1:20:A:ILE:HD12	1:20:A:ILE:HB	13	0.31	0.09	0.34
(1,1243)	1:20:A:ILE:HD13	1:20:A:ILE:HB	13	0.31	0.09	0.34
(1,1243)	1:20:A:ILE:HD11	1:20:A:ILE:HB	13	0.31	0.09	0.34
(3,212)	1:47:A:PHE:H	1:8:A:GLU:HG3	13	0.3	0.08	0.27
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	13	0.3	0.08	0.27
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	13	0.29	0.16	0.24
(1,209)	1:32:A:VAL:HG21	1:32:A:VAL:HA	13	0.29	0.16	0.24
(1,209)	1:32:A:VAL:HG23	1:32:A:VAL:HA	13	0.29	0.16	0.24
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	13	0.22	0.11	0.2
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	13	0.22	0.11	0.2
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	13	0.22	0.11	0.2
(1,145)	1:42:A:THR:HG21	1:12:A:LYS:HA	13	0.21	0.04	0.23
(1,145)	1:42:A:THR:HG23	1:12:A:LYS:HA	13	0.21	0.04	0.23
(1,145)	1:42:A:THR:HG22	1:12:A:LYS:HA	13	0.21	0.04	0.23
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	13	0.19	0.07	0.18
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	13	0.17	0.06	0.14
(1,1160)	1:34:A:VAL:HG23	1:34:A:VAL:HA	13	0.16	0.04	0.14
(1,1160)	1:34:A:VAL:HG21	1:34:A:VAL:HA	13	0.16	0.04	0.14
(1,1160)	1:34:A:VAL:HG22	1:34:A:VAL:HA	13	0.16	0.04	0.14
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	13	0.12	0.02	0.11
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	12	1.33	0.57	1.26
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	12	1.05	0.97	0.6
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB2	12	1.05	0.97	0.6
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	12	1.05	0.97	0.6
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG13	12	1.01	0.21	1.02
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG11	12	1.01	0.21	1.02
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG12	12	1.01	0.21	1.02
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG13	12	0.99	0.21	1.0
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG11	12	0.99	0.21	1.0
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG12	12	0.99	0.21	1.0
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	12	0.87	0.6	0.58
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB2	12	0.87	0.6	0.58
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	12	0.87	0.6	0.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,98)	1:11:A:ILE:HG12	1:59:A:CYS:HB3	12	0.87	0.6	0.58
(3,179)	1:29:A:ASN:H	1:56:A:ARG:HA	12	0.72	0.49	0.66
(3,179)	1:55:A:SER:HB2	1:29:A:ASN:H	12	0.72	0.49	0.66
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	12	0.63	0.52	0.45
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	12	0.63	0.52	0.45
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	12	0.63	0.52	0.45
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	12	0.58	0.15	0.64
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	12	0.57	0.15	0.62
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	12	0.44	0.33	0.37
(1,106)	1:9:A:ILE:HD13	1:9:A:ILE:HA	12	0.43	0.15	0.48
(1,106)	1:9:A:ILE:HD12	1:9:A:ILE:HA	12	0.43	0.15	0.48
(1,106)	1:9:A:ILE:HD11	1:9:A:ILE:HA	12	0.43	0.15	0.48
(1,913)	1:15:A:LEU:HD11	1:19:A:ARG:HB3	12	0.41	0.33	0.24
(1,913)	1:15:A:LEU:HD12	1:19:A:ARG:HB3	12	0.41	0.33	0.24
(1,913)	1:15:A:LEU:HD13	1:19:A:ARG:HB3	12	0.41	0.33	0.24
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	12	0.4	0.14	0.4
(3,154)	1:19:A:ARG:HG3	1:19:A:ARG:H	12	0.4	0.14	0.4
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG11	12	0.39	0.1	0.44
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG13	12	0.39	0.1	0.44
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG12	12	0.39	0.1	0.44
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG11	12	0.38	0.1	0.42
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG13	12	0.38	0.1	0.42
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG12	12	0.38	0.1	0.42
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG22	12	0.35	0.05	0.35
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG23	12	0.35	0.05	0.35
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG21	12	0.35	0.05	0.35
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	12	0.33	0.13	0.35
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	12	0.32	0.04	0.33
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	12	0.31	0.13	0.33
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	12	0.31	0.04	0.31
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD12	12	0.3	0.17	0.21
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD13	12	0.3	0.17	0.21
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD11	12	0.3	0.17	0.21
(1,1145)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	12	0.3	0.13	0.25
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	12	0.3	0.13	0.25
(1,1145)	1:76:A:TYR:HD1	1:7:A:ILE:HG21	12	0.3	0.13	0.25
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	12	0.3	0.13	0.25
(1,1145)	1:76:A:TYR:HD1	1:7:A:ILE:HG22	12	0.3	0.13	0.25
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD12	12	0.28	0.18	0.2
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD13	12	0.28	0.18	0.2
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD11	12	0.28	0.18	0.2
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	12	0.27	0.11	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,23)	1:9:A:ILE:HD13	1:75:A:ALA:HB3	12	0.27	0.11	0.25
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	12	0.27	0.11	0.25
(1,23)	1:9:A:ILE:HD13	1:75:A:ALA:HB1	12	0.27	0.11	0.25
(1,23)	1:9:A:ILE:HD13	1:75:A:ALA:HB2	12	0.27	0.11	0.25
(1,23)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	12	0.27	0.11	0.25
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD13	12	0.22	0.09	0.22
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD12	12	0.22	0.09	0.22
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD11	12	0.22	0.09	0.22
(1,47)	1:20:A:ILE:HG22	1:21:A:LEU:H	12	0.2	0.08	0.2
(1,47)	1:20:A:ILE:HG21	1:21:A:LEU:H	12	0.2	0.08	0.2
(1,47)	1:20:A:ILE:HG23	1:21:A:LEU:H	12	0.2	0.08	0.2
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	12	0.2	0.02	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	12	0.2	0.01	0.2
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	12	0.17	0.05	0.15
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	12	0.16	0.02	0.16
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	12	0.13	0.03	0.12
(3,224)	1:92:A:SER:HB3	1:99:A:TYR:HB3	11	0.66	0.29	0.67
(3,224)	1:92:A:SER:HB2	1:99:A:TYR:HB3	11	0.66	0.29	0.67
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	11	0.61	0.47	0.67
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	11	0.61	0.47	0.67
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	11	0.61	0.47	0.67
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	11	0.57	0.7	0.18
(3,161)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	11	0.57	0.48	0.29
(3,161)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	11	0.57	0.48	0.29
(3,161)	1:7:A:ILE:HG23	1:84:A:LEU:HB3	11	0.57	0.48	0.29
(3,161)	1:7:A:ILE:HG22	1:84:A:LEU:HB3	11	0.57	0.48	0.29
(1,2255)	1:73:A:VAL:HG22	1:59:A:CYS:HB3	11	0.51	0.48	0.33
(1,2255)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	11	0.51	0.48	0.33
(1,2255)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	11	0.51	0.48	0.33
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	11	0.49	0.66	0.18
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	11	0.47	0.2	0.49
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	11	0.47	0.2	0.49
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG22	11	0.47	0.2	0.49
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG21	11	0.46	0.28	0.38
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG23	11	0.46	0.28	0.38
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG22	11	0.46	0.28	0.38
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG23	11	0.46	0.28	0.38
(1,14)	1:98:A:ILE:HD12	1:71:A:THR:HG22	11	0.46	0.28	0.38
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG21	11	0.46	0.28	0.38
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG22	11	0.46	0.28	0.38
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	11	0.42	0.2	0.44
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	11	0.42	0.2	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG22	11	0.42	0.2	0.44
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	11	0.42	0.09	0.44
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	11	0.4	0.09	0.42
(1,74)	1:1:A:ALA:HB2	1:83:A:PRO:HA	11	0.37	0.21	0.31
(1,74)	1:1:A:ALA:HB3	1:83:A:PRO:HA	11	0.37	0.21	0.31
(1,74)	1:1:A:ALA:HB1	1:83:A:PRO:HA	11	0.37	0.21	0.31
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	11	0.32	0.11	0.33
(3,315)	1:104:A:GLU:H	1:104:A:GLU:HG2	11	0.32	0.11	0.33
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG2	11	0.31	0.08	0.31
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	11	0.31	0.08	0.31
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	11	0.3	0.11	0.31
(3,209)	1:104:A:GLU:H	1:104:A:GLU:HG2	11	0.3	0.11	0.31
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG2	11	0.29	0.08	0.29
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	11	0.29	0.08	0.29
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	11	0.27	0.14	0.22
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG23	11	0.27	0.11	0.26
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG22	11	0.27	0.11	0.26
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG21	11	0.27	0.11	0.26
(1,489)	1:30:A:THR:H	1:30:A:THR:HG23	11	0.25	0.11	0.24
(1,489)	1:30:A:THR:H	1:30:A:THR:HG22	11	0.25	0.11	0.24
(1,489)	1:30:A:THR:H	1:30:A:THR:HG21	11	0.25	0.11	0.24
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG22	11	0.23	0.07	0.26
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG21	11	0.23	0.07	0.26
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG23	11	0.23	0.07	0.26
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE2	11	0.22	0.09	0.23
(1,2237)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	11	0.22	0.09	0.23
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	11	0.22	0.09	0.23
(1,2237)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	11	0.22	0.09	0.23
(1,2237)	1:73:A:VAL:HG23	1:61:A:PHE:HE2	11	0.22	0.09	0.23
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	11	0.18	0.06	0.16
(1,2236)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	11	0.16	0.06	0.14
(1,2236)	1:73:A:VAL:HG22	1:61:A:PHE:HD2	11	0.16	0.06	0.14
(1,2236)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	11	0.16	0.06	0.14
(1,2236)	1:73:A:VAL:HG21	1:61:A:PHE:HD1	11	0.16	0.06	0.14
(1,2236)	1:73:A:VAL:HG23	1:61:A:PHE:HD2	11	0.16	0.06	0.14
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	11	0.15	0.02	0.14
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	11	0.14	0.04	0.12
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG13	11	0.11	0.01	0.11
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG12	11	0.11	0.01	0.11
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG11	11	0.11	0.01	0.11
(3,256)	1:32:A:VAL:HG22	1:45:A:ILE:HG12	10	1.09	1.03	0.64
(3,256)	1:32:A:VAL:HG22	1:45:A:ILE:HG13	10	1.09	1.03	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,256)	1:32:A:VAL:HG23	1:45:A:ILE:HG13	10	1.09	1.03	0.64
(3,256)	1:32:A:VAL:HG23	1:45:A:ILE:HG12	10	1.09	1.03	0.64
(3,256)	1:32:A:VAL:HG21	1:45:A:ILE:HG12	10	1.09	1.03	0.64
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	10	0.96	1.0	0.5
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	10	0.96	1.0	0.5
(3,145)	1:29:A:ASN:H	1:56:A:ARG:HA	10	0.69	0.47	0.82
(3,145)	1:55:A:SER:HB2	1:29:A:ASN:H	10	0.69	0.47	0.82
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	10	0.66	0.51	0.42
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	10	0.66	0.51	0.42
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	10	0.66	0.51	0.42
(1,1061)	1:73:A:VAL:HG22	1:59:A:CYS:HB3	10	0.47	0.49	0.25
(1,1061)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	10	0.47	0.49	0.25
(1,1061)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	10	0.47	0.49	0.25
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	10	0.47	0.31	0.43
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD11	10	0.45	0.17	0.51
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD13	10	0.45	0.17	0.51
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD12	10	0.45	0.17	0.51
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	10	0.36	0.13	0.42
(3,15)	1:84:A:LEU:HA	1:85:A:CYS:HB3	10	0.36	0.27	0.32
(3,15)	1:85:A:CYS:HB3	1:4:A:CYS:HA	10	0.36	0.27	0.32
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	10	0.35	0.13	0.4
(1,1230)	1:9:A:ILE:HD13	1:9:A:ILE:HA	10	0.33	0.1	0.34
(1,1230)	1:9:A:ILE:HD12	1:9:A:ILE:HA	10	0.33	0.1	0.34
(1,1230)	1:9:A:ILE:HD11	1:9:A:ILE:HA	10	0.33	0.1	0.34
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD12	10	0.29	0.18	0.2
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD13	10	0.29	0.18	0.2
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD11	10	0.29	0.18	0.2
(1,43)	1:7:A:ILE:HD12	1:7:A:ILE:HG21	10	0.27	0.19	0.22
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	10	0.27	0.19	0.22
(1,43)	1:7:A:ILE:HD12	1:7:A:ILE:HG23	10	0.27	0.19	0.22
(1,43)	1:7:A:ILE:HD12	1:7:A:ILE:HG22	10	0.27	0.19	0.22
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	10	0.27	0.19	0.22
(1,144)	1:95:A:MET:H	1:14:A:THR:HG22	10	0.26	0.1	0.28
(1,144)	1:95:A:MET:H	1:14:A:THR:HG23	10	0.26	0.1	0.28
(1,144)	1:95:A:MET:H	1:14:A:THR:HG21	10	0.26	0.1	0.28
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	10	0.23	0.16	0.14
(1,2223)	1:32:A:VAL:HG21	1:32:A:VAL:HA	10	0.23	0.16	0.14
(1,2223)	1:32:A:VAL:HG23	1:32:A:VAL:HA	10	0.23	0.16	0.14
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	10	0.21	0.02	0.21
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	10	0.2	0.09	0.15
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	10	0.2	0.09	0.15
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	10	0.2	0.19	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	10	0.18	0.02	0.18
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	10	0.16	0.02	0.16
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	10	0.16	0.02	0.16
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	10	0.16	0.05	0.15
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	10	0.13	0.02	0.13
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	10	0.11	0.0	0.11
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	9	1.1	0.42	0.84
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	9	1.06	0.42	0.8
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD11	9	0.83	0.26	0.95
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD12	9	0.83	0.26	0.95
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD13	9	0.83	0.26	0.95
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	9	0.57	0.43	0.54
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	9	0.56	0.7	0.18
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	9	0.55	0.43	0.52
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	9	0.49	0.44	0.24
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	9	0.48	0.34	0.32
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	9	0.48	0.34	0.32
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD11	9	0.37	0.07	0.4
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.37	0.07	0.4
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD12	9	0.37	0.07	0.4
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	9	0.34	0.11	0.29
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	9	0.3	0.07	0.32
(3,294)	1:27:A:SER:HB2	1:28:A:GLY:H	9	0.3	0.07	0.32
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	9	0.28	0.07	0.3
(3,178)	1:27:A:SER:HB2	1:28:A:GLY:H	9	0.28	0.07	0.3
(1,1171)	1:1:A:ALA:HB2	1:83:A:PRO:HA	9	0.28	0.21	0.18
(1,1171)	1:1:A:ALA:HB3	1:83:A:PRO:HA	9	0.28	0.21	0.18
(1,1171)	1:1:A:ALA:HB1	1:83:A:PRO:HA	9	0.28	0.21	0.18
(3,16)	1:26:A:ARG:HB2	1:31:A:ASN:HA	9	0.25	0.07	0.25
(3,16)	1:31:A:ASN:HA	1:26:A:ARG:HB3	9	0.25	0.07	0.25
(1,2250)	1:11:A:ILE:HD13	1:61:A:PHE:HE1	9	0.24	0.13	0.22
(1,2250)	1:11:A:ILE:HD12	1:61:A:PHE:HE1	9	0.24	0.13	0.22
(1,2250)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	9	0.24	0.13	0.22
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	9	0.22	0.08	0.19
(3,42)	1:47:A:PHE:HB2	1:47:A:PHE:HA	9	0.22	0.08	0.19
(3,94)	1:87:A:LYS:HB2	1:87:A:LYS:HA	9	0.22	0.08	0.2
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	9	0.22	0.08	0.2
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG22	9	0.2	0.08	0.19
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG21	9	0.2	0.08	0.19
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	9	0.2	0.02	0.2
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	9	0.2	0.09	0.14
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	9	0.2	0.09	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB2	9	0.18	0.04	0.2
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB1	9	0.18	0.04	0.2
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB3	9	0.18	0.04	0.2
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	9	0.17	0.02	0.17
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	9	0.15	0.05	0.13
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	9	0.13	0.01	0.13
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	9	0.12	0.02	0.12
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	8	1.49	0.86	1.37
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	8	1.16	0.05	1.15
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	8	1.14	0.06	1.13
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD13	8	0.71	0.78	0.45
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD11	8	0.71	0.78	0.45
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD12	8	0.71	0.78	0.45
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	8	0.7	0.56	0.68
(3,1)	1:57:A:TRP:HB2	1:9:A:ILE:HD11	8	0.63	0.52	0.44
(3,1)	1:76:A:TYR:HB3	1:9:A:ILE:HD12	8	0.63	0.52	0.44
(3,1)	1:76:A:TYR:HB3	1:9:A:ILE:HD13	8	0.63	0.52	0.44
(3,1)	1:57:A:TRP:HB2	1:9:A:ILE:HD13	8	0.63	0.52	0.44
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG11	8	0.62	0.1	0.67
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG12	8	0.62	0.1	0.67
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG13	8	0.62	0.1	0.67
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	8	0.61	0.1	0.66
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	8	0.61	0.1	0.66
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG13	8	0.61	0.1	0.66
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG11	8	0.6	0.1	0.65
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG12	8	0.6	0.1	0.65
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG13	8	0.6	0.1	0.65
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	8	0.51	0.35	0.53
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	8	0.47	0.34	0.32
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	8	0.47	0.34	0.32
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	8	0.47	0.42	0.32
(1,1102)	1:98:A:ILE:HD13	1:71:A:THR:HG21	8	0.46	0.24	0.44
(1,1102)	1:98:A:ILE:HD12	1:71:A:THR:HG22	8	0.46	0.24	0.44
(1,1102)	1:98:A:ILE:HD13	1:71:A:THR:HG22	8	0.46	0.24	0.44
(1,1102)	1:98:A:ILE:HD11	1:71:A:THR:HG23	8	0.46	0.24	0.44
(1,1102)	1:98:A:ILE:HD11	1:71:A:THR:HG21	8	0.46	0.24	0.44
(1,1102)	1:98:A:ILE:HD11	1:71:A:THR:HG22	8	0.46	0.24	0.44
(1,1102)	1:98:A:ILE:HD13	1:71:A:THR:HG23	8	0.46	0.24	0.44
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	8	0.44	0.1	0.5
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	8	0.44	0.1	0.5
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG13	8	0.44	0.1	0.5
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	8	0.41	0.52	0.25

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	8	0.41	0.03	0.4
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	8	0.4	0.03	0.39
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB2	8	0.37	0.13	0.43
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB3	8	0.37	0.13	0.43
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	8	0.36	0.17	0.38
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB2	8	0.35	0.13	0.4
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB3	8	0.35	0.13	0.4
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB2	8	0.34	0.13	0.38
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB1	8	0.34	0.13	0.38
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB3	8	0.34	0.13	0.38
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	8	0.34	0.17	0.36
(3,251)	1:99:A:TYR:HA	1:110:A:LEU:HB2	8	0.32	0.12	0.34
(3,251)	1:99:A:TYR:HA	1:109:A:PRO:HB3	8	0.32	0.12	0.34
(1,336)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	8	0.32	0.13	0.28
(1,336)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	8	0.32	0.13	0.28
(1,336)	1:98:A:ILE:HD12	1:61:A:PHE:HE1	8	0.32	0.13	0.28
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE1	8	0.28	0.12	0.24
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE2	8	0.28	0.12	0.24
(1,1913)	1:9:A:ILE:HD13	1:9:A:ILE:HA	8	0.27	0.06	0.25
(1,1913)	1:9:A:ILE:HD12	1:9:A:ILE:HA	8	0.27	0.06	0.25
(1,1913)	1:9:A:ILE:HD11	1:9:A:ILE:HA	8	0.27	0.06	0.25
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	8	0.23	0.06	0.22
(1,1166)	1:47:A:PHE:HD2	1:30:A:THR:HG21	8	0.23	0.1	0.21
(1,1166)	1:47:A:PHE:HD1	1:30:A:THR:HG22	8	0.23	0.1	0.21
(1,1166)	1:47:A:PHE:HD2	1:30:A:THR:HG22	8	0.23	0.1	0.21
(1,1166)	1:47:A:PHE:HD1	1:30:A:THR:HG21	8	0.23	0.1	0.21
(1,1166)	1:47:A:PHE:HD1	1:30:A:THR:HG23	8	0.23	0.1	0.21
(3,24)	1:10:A:VAL:H	1:9:A:ILE:HB	8	0.23	0.12	0.17
(3,24)	1:9:A:ILE:H	1:9:A:ILE:HB	8	0.23	0.12	0.17
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	8	0.18	0.06	0.18
(1,272)	1:52:A:THR:HG23	1:52:A:THR:HA	8	0.14	0.02	0.14
(1,272)	1:52:A:THR:HG22	1:52:A:THR:HA	8	0.14	0.02	0.14
(1,272)	1:52:A:THR:HG21	1:52:A:THR:HA	8	0.14	0.02	0.14
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	8	0.12	0.02	0.11
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	8	0.12	0.02	0.12
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	8	0.12	0.01	0.11
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB2	7	1.1	0.75	1.16
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB3	7	1.1	0.75	1.16
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB1	7	1.1	0.75	1.16
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	7	0.8	0.08	0.78
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	7	0.73	0.08	0.71
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	7	0.56	0.05	0.55

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	7	0.55	0.34	0.73
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	7	0.51	0.4	0.33
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD11	7	0.51	0.17	0.58
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD13	7	0.51	0.17	0.58
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD12	7	0.51	0.17	0.58
(1,1935)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	7	0.44	0.07	0.45
(1,1935)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	7	0.44	0.07	0.45
(1,1935)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	7	0.44	0.07	0.45
(1,75)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	7	0.4	0.07	0.42
(1,75)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	7	0.4	0.07	0.42
(1,75)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	7	0.4	0.07	0.42
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB2	7	0.36	0.11	0.4
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB3	7	0.36	0.11	0.4
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	7	0.35	0.23	0.2
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	7	0.33	0.22	0.18
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB3	7	0.32	0.16	0.24
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB2	7	0.32	0.16	0.24
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD11	7	0.32	0.1	0.31
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD12	7	0.32	0.1	0.31
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	7	0.32	0.1	0.31
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD1	7	0.31	0.14	0.32
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD2	7	0.31	0.14	0.32
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	7	0.3	0.01	0.31
(1,11)	1:73:A:VAL:HG21	1:98:A:ILE:HD13	7	0.3	0.1	0.32
(1,11)	1:73:A:VAL:HG22	1:98:A:ILE:HD12	7	0.3	0.1	0.32
(1,11)	1:73:A:VAL:HG21	1:98:A:ILE:HD12	7	0.3	0.1	0.32
(1,11)	1:73:A:VAL:HG21	1:98:A:ILE:HD11	7	0.3	0.1	0.32
(1,11)	1:73:A:VAL:HG23	1:98:A:ILE:HD13	7	0.3	0.1	0.32
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	7	0.3	0.2	0.18
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD11	7	0.3	0.1	0.3
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD12	7	0.3	0.1	0.3
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	7	0.3	0.1	0.3
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	7	0.29	0.09	0.35
(1,1172)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	7	0.28	0.07	0.29
(1,1172)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	7	0.28	0.07	0.29
(1,1172)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	7	0.28	0.07	0.29
(3,14)	1:50:A:ASP:HA	1:50:A:ASP:HB3	7	0.28	0.06	0.3
(3,14)	1:111:A:ASN:HA	1:111:A:ASN:HB2	7	0.28	0.06	0.3
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	7	0.26	0.01	0.26
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD1	7	0.25	0.14	0.21
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD2	7	0.25	0.14	0.21
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	7	0.25	0.12	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD13	7	0.24	0.1	0.2
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD11	7	0.24	0.1	0.2
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD12	7	0.24	0.1	0.2
(1,1110)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	7	0.24	0.08	0.23
(1,1110)	1:9:A:ILE:HD13	1:75:A:ALA:HB3	7	0.24	0.08	0.23
(1,1110)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	7	0.24	0.08	0.23
(1,1110)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	7	0.24	0.08	0.23
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	7	0.23	0.06	0.23
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	7	0.23	0.05	0.21
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	7	0.23	0.03	0.23
(1,1982)	1:47:A:PHE:HD2	1:30:A:THR:HB	7	0.2	0.04	0.19
(1,1982)	1:47:A:PHE:HD1	1:30:A:THR:HB	7	0.2	0.04	0.19
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD1	7	0.19	0.07	0.18
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD2	7	0.19	0.07	0.18
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	7	0.19	0.09	0.13
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG21	7	0.18	0.06	0.18
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG22	7	0.18	0.06	0.18
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG23	7	0.18	0.06	0.18
(1,1948)	1:61:A:PHE:HD1	1:71:A:THR:HG22	7	0.18	0.06	0.18
(1,1948)	1:61:A:PHE:HD1	1:71:A:THR:HG21	7	0.18	0.06	0.18
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	7	0.18	0.08	0.16
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD11	7	0.18	0.03	0.2
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD13	7	0.18	0.03	0.2
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD12	7	0.18	0.03	0.2
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	7	0.16	0.08	0.13
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	7	0.15	0.0	0.15
(1,924)	1:47:A:PHE:HD2	1:30:A:THR:HB	7	0.15	0.04	0.14
(1,924)	1:47:A:PHE:HD1	1:30:A:THR:HB	7	0.15	0.04	0.14
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	7	0.14	0.0	0.14
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	7	0.13	0.05	0.11
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB2	6	1.12	0.7	1.38
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB3	6	1.12	0.7	1.38
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB1	6	1.12	0.7	1.38
(1,242)	1:39:A:PHE:HD2	1:17:A:PRO:HA	6	0.7	0.91	0.24
(1,85)	1:74:A:GLU:HA	1:74:A:GLU:HG2	6	0.56	0.17	0.55
(1,1036)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	6	0.53	0.36	0.48
(1,1577)	1:9:A:ILE:HG12	1:46:A:LYS:H	6	0.47	0.41	0.36
(1,1177)	1:74:A:GLU:HA	1:74:A:GLU:HG2	6	0.42	0.16	0.42
(1,1310)	1:98:A:ILE:HD13	1:71:A:THR:HG21	6	0.42	0.2	0.42
(1,1310)	1:98:A:ILE:HD11	1:71:A:THR:HG23	6	0.42	0.2	0.42
(1,1310)	1:98:A:ILE:HD11	1:71:A:THR:HG21	6	0.42	0.2	0.42
(1,1310)	1:98:A:ILE:HD11	1:71:A:THR:HG22	6	0.42	0.2	0.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1310)	1:98:A:ILE:HD13	1:71:A:THR:HG23	6	0.42	0.2	0.42
(4,23)	1:21:A:LEU:H	1:37:A:LEU:O	6	0.41	0.28	0.24
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD11	6	0.41	0.13	0.45
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD13	6	0.41	0.13	0.45
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD12	6	0.41	0.13	0.45
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB2	6	0.38	0.05	0.38
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB3	6	0.38	0.05	0.38
(3,167)	1:5:A:LYS:HG2	1:6:A:GLU:H	6	0.38	0.17	0.33
(3,167)	1:5:A:LYS:HG3	1:6:A:GLU:H	6	0.38	0.17	0.33
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD12	6	0.36	0.13	0.34
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD11	6	0.36	0.13	0.34
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD13	6	0.36	0.13	0.34
(1,678)	1:87:A:LYS:HB3	1:88:A:ARG:H	6	0.35	0.36	0.22
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	6	0.33	0.12	0.37
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB2	6	0.33	0.12	0.37
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD1	6	0.32	0.12	0.3
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD2	6	0.32	0.12	0.3
(1,453)	1:20:A:ILE:H	1:19:A:ARG:HB3	6	0.31	0.2	0.25
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	6	0.31	0.12	0.35
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB2	6	0.31	0.12	0.35
(3,297)	1:47:A:PHE:HB3	1:48:A:LYS:H	6	0.28	0.12	0.27
(3,185)	1:47:A:PHE:HB3	1:48:A:LYS:H	6	0.27	0.12	0.26
(1,1135)	1:7:A:ILE:HD12	1:7:A:ILE:HG21	6	0.26	0.21	0.2
(1,1135)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	6	0.26	0.21	0.2
(1,1135)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	6	0.26	0.21	0.2
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD1	6	0.26	0.15	0.22
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD2	6	0.26	0.15	0.22
(1,391)	1:112:A:LYS:H	1:98:A:ILE:HB	6	0.26	0.28	0.12
(1,42)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	6	0.25	0.12	0.23
(1,42)	1:7:A:ILE:HD11	1:84:A:LEU:HB3	6	0.25	0.12	0.23
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE1	6	0.24	0.11	0.24
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE2	6	0.24	0.11	0.24
(1,244)	1:70:A:PHE:HD1	1:70:A:PHE:HB3	6	0.24	0.04	0.26
(1,668)	1:85:A:CYS:H	1:84:A:LEU:HA	6	0.24	0.06	0.25
(3,309)	1:103:A:ASP:HB3	1:104:A:GLU:H	6	0.24	0.15	0.18
(3,309)	1:104:A:GLU:H	1:103:A:ASP:HB2	6	0.24	0.15	0.18
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB3	6	0.23	0.1	0.2
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB1	6	0.23	0.1	0.2
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB2	6	0.23	0.1	0.2
(3,202)	1:103:A:ASP:HB3	1:104:A:GLU:H	6	0.22	0.15	0.16
(3,202)	1:104:A:GLU:H	1:103:A:ASP:HB2	6	0.22	0.15	0.16
(1,1762)	1:102:A:MET:H	1:101:A:LYS:HB2	6	0.22	0.11	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2228)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	6	0.21	0.08	0.2
(1,2228)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	6	0.21	0.08	0.2
(1,2228)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	6	0.21	0.08	0.2
(1,292)	1:43:A:ARG:HB2	1:43:A:ARG:HA	6	0.21	0.03	0.23
(1,1721)	1:57:A:TRP:H	1:76:A:TYR:H	6	0.21	0.05	0.2
(1,54)	1:7:A:ILE:HG21	1:8:A:GLU:H	6	0.21	0.08	0.22
(1,54)	1:7:A:ILE:HG22	1:8:A:GLU:H	6	0.21	0.08	0.22
(1,54)	1:7:A:ILE:HG23	1:8:A:GLU:H	6	0.21	0.08	0.22
(1,1631)	1:58:A:ASN:HB3	1:59:A:CYS:H	6	0.19	0.06	0.2
(1,695)	1:57:A:TRP:H	1:76:A:TYR:H	6	0.19	0.05	0.18
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB1	6	0.19	0.09	0.15
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB2	6	0.19	0.09	0.15
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB3	6	0.19	0.09	0.15
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG23	6	0.18	0.08	0.17
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG22	6	0.18	0.08	0.17
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG21	6	0.18	0.08	0.17
(1,1787)	1:115:A:SER:H	1:114:A:ARG:HB3	6	0.18	0.06	0.17
(1,1503)	1:30:A:THR:H	1:27:A:SER:H	6	0.18	0.06	0.18
(3,125)	1:73:A:VAL:HG12	1:73:A:VAL:HG22	6	0.18	0.06	0.17
(3,125)	1:73:A:VAL:HG11	1:73:A:VAL:HG23	6	0.18	0.06	0.17
(3,125)	1:73:A:VAL:HG12	1:73:A:VAL:HG21	6	0.18	0.06	0.17
(3,125)	1:45:A:ILE:HG21	1:45:A:ILE:HD13	6	0.18	0.06	0.17
(3,125)	1:73:A:VAL:HG11	1:73:A:VAL:HG22	6	0.18	0.06	0.17
(3,125)	1:73:A:VAL:HG13	1:73:A:VAL:HG23	6	0.18	0.06	0.17
(1,2019)	1:4:A:CYS:HB3	1:4:A:CYS:HA	6	0.17	0.04	0.18
(1,761)	1:115:A:SER:H	1:114:A:ARG:HB3	6	0.17	0.05	0.16
(1,1898)	1:89:A:TYR:H	1:10:A:VAL:H	6	0.16	0.03	0.16
(1,974)	1:39:A:PHE:HA	1:39:A:PHE:HD1	6	0.16	0.04	0.16
(1,1548)	1:39:A:PHE:HA	1:40:A:LYS:H	6	0.16	0.02	0.15
(1,804)	1:25:A:CYS:H	1:59:A:CYS:HB3	6	0.15	0.04	0.13
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD2	6	0.15	0.03	0.14
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD1	6	0.15	0.03	0.14
(1,532)	1:39:A:PHE:HA	1:40:A:LYS:H	6	0.14	0.02	0.14
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB2	6	0.13	0.01	0.14
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB1	6	0.13	0.01	0.14
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB3	6	0.13	0.01	0.14
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD2	6	0.13	0.03	0.12
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD1	6	0.13	0.03	0.12
(1,1003)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	5	0.98	0.4	1.15
(1,2276)	1:19:A:ARG:HB2	1:14:A:THR:HA	5	0.74	0.9	0.14
(1,249)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	5	0.66	0.64	0.18
(1,1019)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	5	0.6	0.41	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,288)	1:6:A:GLU:HG2	1:6:A:GLU:H	5	0.54	0.06	0.54
(1,1802)	1:56:A:ARG:H	1:56:A:ARG:HB3	5	0.53	0.26	0.64
(3,168)	1:6:A:GLU:HG2	1:6:A:GLU:H	5	0.53	0.06	0.53
(1,558)	1:9:A:ILE:HG12	1:46:A:LYS:H	5	0.52	0.41	0.54
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD13	5	0.5	0.14	0.51
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD12	5	0.5	0.14	0.51
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD11	5	0.5	0.14	0.51
(3,63)	1:104:A:GLU:HG2	1:104:A:GLU:HA	5	0.49	0.03	0.48
(3,63)	1:104:A:GLU:HG3	1:104:A:GLU:HA	5	0.49	0.03	0.48
(1,294)	1:35:A:GLN:HA	1:36:A:TYR:HD1	5	0.48	0.4	0.22
(1,1936)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	5	0.46	0.19	0.5
(1,1936)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	5	0.46	0.19	0.5
(1,352)	1:57:A:TRP:HE1	1:56:A:ARG:HA	5	0.4	0.58	0.12
(3,34)	1:11:A:ILE:HD13	1:61:A:PHE:HE1	5	0.36	0.07	0.37
(3,34)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	5	0.36	0.07	0.37
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD13	5	0.36	0.14	0.37
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD12	5	0.36	0.14	0.37
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD11	5	0.36	0.14	0.37
(3,338)	1:104:A:GLU:HG2	1:104:A:GLU:HA	5	0.34	0.03	0.32
(3,338)	1:104:A:GLU:HG3	1:104:A:GLU:HA	5	0.34	0.03	0.32
(1,1738)	1:94:A:ARG:HB3	1:96:A:ASP:H	5	0.34	0.17	0.32
(1,1058)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	5	0.3	0.09	0.28
(1,1058)	1:11:A:ILE:HD12	1:61:A:PHE:HE1	5	0.3	0.09	0.28
(3,75)	1:76:A:TYR:HA	1:76:A:TYR:HD2	5	0.3	0.05	0.28
(3,75)	1:30:A:THR:HA	1:30:A:THR:H	5	0.3	0.05	0.28
(3,75)	1:39:A:PHE:HA	1:39:A:PHE:HD1	5	0.3	0.05	0.28
(3,75)	1:76:A:TYR:HA	1:76:A:TYR:HD1	5	0.3	0.05	0.28
(1,2038)	1:7:A:ILE:HD12	1:7:A:ILE:HG21	5	0.29	0.21	0.2
(1,2038)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	5	0.29	0.21	0.2
(1,2038)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	5	0.29	0.21	0.2
(3,147)	1:5:A:LYS:HG2	1:6:A:GLU:H	5	0.29	0.16	0.3
(3,147)	1:5:A:LYS:HG3	1:6:A:GLU:H	5	0.29	0.16	0.3
(1,48)	1:37:A:LEU:H	1:20:A:ILE:HG22	5	0.28	0.1	0.25
(3,332)	1:69:A:PHE:HA	1:115:A:SER:HB3	5	0.28	0.15	0.26
(3,332)	1:69:A:PHE:HA	1:115:A:SER:HB2	5	0.28	0.15	0.26
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD12	5	0.26	0.11	0.22
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD11	5	0.26	0.11	0.22
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD13	5	0.26	0.11	0.22
(3,189)	1:74:A:GLU:HA	1:76:A:TYR:H	5	0.26	0.24	0.14
(1,1850)	1:71:A:THR:H	1:70:A:PHE:HE1	5	0.25	0.07	0.24
(1,1850)	1:71:A:THR:H	1:70:A:PHE:HE2	5	0.25	0.07	0.24
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD11	5	0.25	0.09	0.27

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD12	5	0.25	0.09	0.27
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD13	5	0.25	0.09	0.27
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG22	5	0.24	0.08	0.26
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG23	5	0.24	0.08	0.26
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG21	5	0.24	0.08	0.26
(1,817)	1:71:A:THR:H	1:70:A:PHE:HE1	5	0.23	0.07	0.22
(1,817)	1:71:A:THR:H	1:70:A:PHE:HE2	5	0.23	0.07	0.22
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG22	5	0.22	0.08	0.24
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG23	5	0.22	0.08	0.24
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG21	5	0.22	0.08	0.24
(4,13)	1:90:A:GLU:H	1:101:A:LYS:O	5	0.22	0.1	0.17
(1,736)	1:102:A:MET:H	1:101:A:LYS:HB2	5	0.22	0.11	0.19
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG22	5	0.21	0.05	0.19
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG23	5	0.21	0.05	0.19
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG21	5	0.21	0.05	0.19
(3,29)	1:115:A:SER:HA	1:69:A:PHE:HA	5	0.21	0.06	0.25
(3,29)	1:114:A:ARG:HA	1:69:A:PHE:HA	5	0.21	0.06	0.25
(1,1796)	1:32:A:VAL:H	1:26:A:ARG:HA	5	0.2	0.07	0.17
(1,608)	1:58:A:ASN:HB3	1:59:A:CYS:H	5	0.19	0.04	0.2
(1,622)	1:71:A:THR:H	1:71:A:THR:HG23	5	0.18	0.08	0.17
(1,622)	1:71:A:THR:H	1:71:A:THR:HG22	5	0.18	0.08	0.17
(1,622)	1:71:A:THR:H	1:71:A:THR:HG21	5	0.18	0.08	0.17
(1,1022)	1:73:A:VAL:HG21	1:91:A:LEU:HB2	5	0.18	0.05	0.16
(1,1022)	1:73:A:VAL:HG22	1:91:A:LEU:HB2	5	0.18	0.05	0.16
(1,1022)	1:73:A:VAL:HG23	1:91:A:LEU:HB2	5	0.18	0.05	0.16
(1,1826)	1:9:A:ILE:H	1:9:A:ILE:HB	5	0.17	0.02	0.17
(1,349)	1:85:A:CYS:H	1:84:A:LEU:HA	5	0.16	0.03	0.15
(1,796)	1:9:A:ILE:H	1:9:A:ILE:HB	5	0.16	0.02	0.15
(1,1163)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	5	0.16	0.06	0.14
(1,1163)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	5	0.16	0.06	0.14
(1,1163)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	5	0.16	0.06	0.14
(1,798)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.16	0.07	0.14
(3,31)	1:92:A:SER:HB3	1:92:A:SER:H	5	0.15	0.05	0.13
(3,265)	1:26:A:ARG:HB2	1:31:A:ASN:HA	5	0.15	0.07	0.12
(3,265)	1:31:A:ASN:HA	1:26:A:ARG:HB3	5	0.15	0.07	0.12
(1,860)	1:89:A:TYR:H	1:10:A:VAL:H	5	0.15	0.03	0.15
(1,154)	1:98:A:ILE:HG13	1:113:A:TRP:H	5	0.14	0.02	0.14
(1,2150)	1:62:A:ARG:HA	1:70:A:PHE:HB3	5	0.14	0.02	0.14
(1,1545)	1:38:A:ASN:HB3	1:39:A:PHE:H	5	0.14	0.01	0.14
(1,1991)	1:115:A:SER:HB2	1:115:A:SER:HA	5	0.13	0.01	0.13
(1,529)	1:38:A:ASN:HB3	1:39:A:PHE:H	5	0.12	0.01	0.12
(1,1812)	1:113:A:TRP:H	1:113:A:TRP:HB2	5	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,131)	1:38:A:ASN:HB2	1:38:A:ASN:HA	5	0.11	0.01	0.11
(3,131)	1:89:A:TYR:HB2	1:89:A:TYR:HA	5	0.11	0.01	0.11
(1,1086)	1:42:A:THR:HG22	1:42:A:THR:HB	5	0.1	0.0	0.1
(1,1086)	1:42:A:THR:HG21	1:42:A:THR:HB	5	0.1	0.0	0.1
(1,1086)	1:42:A:THR:HG23	1:42:A:THR:HB	5	0.1	0.0	0.1
(1,1265)	1:15:A:LEU:HA	1:94:A:ARG:HA	4	2.98	0.38	3.15
(1,2051)	1:101:A:LYS:HB2	1:107:A:PRO:HA	4	1.67	2.43	0.3
(1,950)	1:101:A:LYS:HB2	1:107:A:PRO:HA	4	1.62	2.43	0.24
(4,10)	1:95:A:MET:H	1:14:A:THR:O	4	0.85	1.05	0.3
(1,2176)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	4	0.66	0.4	0.62
(1,775)	1:56:A:ARG:H	1:56:A:ARG:HB3	4	0.61	0.17	0.66
(1,1816)	1:113:A:TRP:H	1:112:A:LYS:HB2	4	0.52	0.01	0.52
(1,786)	1:113:A:TRP:H	1:112:A:LYS:HB2	4	0.5	0.01	0.5
(1,896)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	4	0.5	0.1	0.52
(1,896)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	4	0.5	0.1	0.52
(1,1699)	1:7:A:ILE:HD11	1:87:A:LYS:H	4	0.48	0.22	0.44
(1,1699)	1:7:A:ILE:HD13	1:87:A:LYS:H	4	0.48	0.22	0.44
(1,677)	1:7:A:ILE:HD11	1:87:A:LYS:H	4	0.47	0.23	0.42
(1,677)	1:7:A:ILE:HD13	1:87:A:LYS:H	4	0.47	0.23	0.42
(1,1389)	1:85:A:CYS:HB2	1:5:A:LYS:H	4	0.44	0.03	0.44
(1,397)	1:85:A:CYS:HB2	1:5:A:LYS:H	4	0.43	0.03	0.42
(1,1005)	1:97:A:ALA:HB3	1:109:A:PRO:HB2	4	0.43	0.16	0.44
(1,1005)	1:97:A:ALA:HB1	1:109:A:PRO:HB2	4	0.43	0.16	0.44
(1,1731)	1:94:A:ARG:HB3	1:95:A:MET:H	4	0.39	0.27	0.3
(1,229)	1:112:A:LYS:HB3	1:112:A:LYS:HA	4	0.39	0.0	0.39
(1,39)	1:45:A:ILE:HA	1:45:A:ILE:HG12	4	0.38	0.14	0.44
(1,711)	1:94:A:ARG:HB3	1:96:A:ASP:H	4	0.38	0.15	0.36
(1,340)	1:87:A:LYS:HB3	1:88:A:ARG:H	4	0.37	0.38	0.16
(1,704)	1:94:A:ARG:HB3	1:95:A:MET:H	4	0.37	0.27	0.28
(1,1732)	1:95:A:MET:HB3	1:95:A:MET:H	4	0.34	0.03	0.34
(1,705)	1:95:A:MET:HB3	1:95:A:MET:H	4	0.33	0.03	0.32
(1,734)	1:102:A:MET:H	1:102:A:MET:HG2	4	0.33	0.23	0.23
(1,1356)	1:98:A:ILE:HD11	1:71:A:THR:HG23	4	0.31	0.13	0.32
(1,1356)	1:98:A:ILE:HD11	1:71:A:THR:HG21	4	0.31	0.13	0.32
(1,1356)	1:98:A:ILE:HD11	1:71:A:THR:HG22	4	0.31	0.13	0.32
(1,1356)	1:98:A:ILE:HD13	1:71:A:THR:HG23	4	0.31	0.13	0.32
(1,1168)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	4	0.29	0.1	0.32
(1,1168)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	4	0.29	0.1	0.32
(3,287)	1:4:A:CYS:HB2	1:5:A:LYS:H	4	0.29	0.03	0.29
(3,287)	1:4:A:CYS:HB3	1:5:A:LYS:H	4	0.29	0.03	0.29
(1,1501)	1:29:A:ASN:HB2	1:30:A:THR:H	4	0.28	0.06	0.3
(1,1998)	1:32:A:VAL:HG22	1:32:A:VAL:HA	4	0.27	0.13	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,165)	1:4:A:CYS:HB2	1:5:A:LYS:H	4	0.27	0.03	0.26
(3,165)	1:4:A:CYS:HB3	1:5:A:LYS:H	4	0.27	0.03	0.26
(1,306)	1:30:A:THR:HB	1:47:A:PHE:HE2	4	0.26	0.06	0.24
(1,306)	1:30:A:THR:HB	1:47:A:PHE:HE1	4	0.26	0.06	0.24
(1,488)	1:29:A:ASN:HB2	1:30:A:THR:H	4	0.26	0.06	0.28
(3,4)	1:45:A:ILE:HG13	1:45:A:ILE:HB	4	0.24	0.03	0.24
(1,1211)	1:32:A:VAL:HG22	1:32:A:VAL:HA	4	0.23	0.13	0.2
(1,299)	1:23:A:TYR:HE2	1:45:A:ILE:HD13	4	0.23	0.11	0.2
(1,299)	1:23:A:TYR:HE2	1:45:A:ILE:HD11	4	0.23	0.11	0.2
(1,2126)	1:23:A:TYR:HE1	1:36:A:TYR:HA	4	0.22	0.11	0.18
(1,427)	1:14:A:THR:H	1:93:A:ALA:HB1	4	0.21	0.09	0.22
(1,427)	1:14:A:THR:H	1:93:A:ALA:HB3	4	0.21	0.09	0.22
(1,769)	1:32:A:VAL:H	1:26:A:ARG:HA	4	0.2	0.06	0.18
(1,1839)	1:57:A:TRP:H	1:56:A:ARG:HB3	4	0.19	0.02	0.18
(3,197)	1:91:A:LEU:H	1:91:A:LEU:HB2	4	0.19	0.04	0.19
(1,1308)	1:109:A:PRO:HA	1:97:A:ALA:HB2	4	0.19	0.04	0.18
(1,1308)	1:109:A:PRO:HA	1:97:A:ALA:HB1	4	0.19	0.04	0.18
(1,1308)	1:109:A:PRO:HA	1:97:A:ALA:HB3	4	0.19	0.04	0.18
(1,809)	1:57:A:TRP:H	1:56:A:ARG:HB3	4	0.18	0.03	0.18
(1,2063)	1:73:A:VAL:HG22	1:73:A:VAL:HA	4	0.18	0.09	0.13
(1,2063)	1:73:A:VAL:HG21	1:73:A:VAL:HA	4	0.18	0.09	0.13
(1,2063)	1:73:A:VAL:HG23	1:73:A:VAL:HA	4	0.18	0.09	0.13
(1,621)	1:70:A:PHE:H	1:114:A:ARG:H	4	0.18	0.05	0.16
(1,1765)	1:104:A:GLU:H	1:104:A:GLU:HB2	4	0.18	0.08	0.15
(1,1140)	1:20:A:ILE:HG23	1:21:A:LEU:H	4	0.18	0.06	0.16
(1,1140)	1:20:A:ILE:HG21	1:21:A:LEU:H	4	0.18	0.06	0.16
(1,1140)	1:20:A:ILE:HG22	1:21:A:LEU:H	4	0.18	0.06	0.16
(1,2)	1:30:A:THR:HA	1:30:A:THR:HG22	4	0.17	0.07	0.15
(1,2)	1:30:A:THR:HA	1:30:A:THR:HG21	4	0.17	0.07	0.15
(1,2)	1:30:A:THR:HA	1:30:A:THR:HG23	4	0.17	0.07	0.15
(1,1918)	1:11:A:ILE:HG22	1:11:A:ILE:HD11	4	0.17	0.05	0.18
(1,1918)	1:11:A:ILE:HG23	1:11:A:ILE:HD11	4	0.17	0.05	0.18
(1,1918)	1:11:A:ILE:HG23	1:11:A:ILE:HD12	4	0.17	0.05	0.18
(1,1918)	1:11:A:ILE:HG22	1:11:A:ILE:HD12	4	0.17	0.05	0.18
(1,979)	1:90:A:GLU:HA	1:90:A:GLU:HG2	4	0.17	0.09	0.13
(3,311)	1:105:A:ARG:HG3	1:105:A:ARG:H	4	0.17	0.06	0.16
(3,311)	1:105:A:ARG:HG2	1:105:A:ARG:H	4	0.17	0.06	0.16
(1,1452)	1:19:A:ARG:HB3	1:19:A:ARG:H	4	0.17	0.03	0.18
(1,2071)	1:35:A:GLN:HG3	1:35:A:GLN:HA	4	0.16	0.05	0.16
(1,1828)	1:9:A:ILE:H	1:9:A:ILE:HG12	4	0.16	0.07	0.14
(1,381)	1:70:A:PHE:HE1	1:70:A:PHE:HA	4	0.16	0.06	0.14
(1,935)	1:4:A:CYS:HB3	1:4:A:CYS:HA	4	0.16	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,928)	1:69:A:PHE:HA	1:115:A:SER:HB3	4	0.15	0.03	0.14
(1,1608)	1:52:A:THR:H	1:50:A:ASP:HA	4	0.15	0.06	0.12
(1,448)	1:19:A:ARG:HB3	1:19:A:ARG:H	4	0.15	0.03	0.16
(1,1908)	1:111:A:ASN:H	1:110:A:LEU:HB3	4	0.14	0.01	0.15
(1,2148)	1:70:A:PHE:HB2	1:62:A:ARG:HA	4	0.14	0.03	0.14
(1,38)	1:45:A:ILE:HD11	1:45:A:ILE:HG13	4	0.14	0.03	0.13
(1,38)	1:45:A:ILE:HD13	1:45:A:ILE:HG13	4	0.14	0.03	0.13
(1,2020)	1:4:A:CYS:HB3	1:4:A:CYS:HA	4	0.13	0.02	0.12
(1,870)	1:111:A:ASN:H	1:110:A:LEU:HB3	4	0.13	0.02	0.13
(1,1298)	1:42:A:THR:HG21	1:12:A:LYS:HA	4	0.13	0.01	0.12
(1,1298)	1:42:A:THR:HG22	1:12:A:LYS:HA	4	0.13	0.01	0.12
(1,980)	1:12:A:LYS:HB2	1:92:A:SER:HA	4	0.12	0.02	0.12
(1,848)	1:45:A:ILE:H	1:44:A:ILE:HG12	4	0.12	0.02	0.11
(1,887)	1:98:A:ILE:HB	1:98:A:ILE:HG22	4	0.11	0.01	0.11
(1,887)	1:98:A:ILE:HB	1:98:A:ILE:HG21	4	0.11	0.01	0.11
(1,546)	1:43:A:ARG:H	1:44:A:ILE:HG13	4	0.11	0.01	0.11
(1,127)	1:45:A:ILE:H	1:45:A:ILE:HG13	3	0.97	0.02	0.96
(1,1260)	1:45:A:ILE:H	1:45:A:ILE:HG13	3	0.82	0.02	0.81
(1,1018)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	3	0.75	0.31	0.56
(1,254)	1:23:A:TYR:HB2	1:61:A:PHE:HD2	3	0.72	0.05	0.69
(1,254)	1:23:A:TYR:HB2	1:61:A:PHE:HD1	3	0.72	0.05	0.69
(1,1958)	1:11:A:ILE:H	1:10:A:VAL:HG22	3	0.53	0.4	0.31
(1,1958)	1:11:A:ILE:H	1:10:A:VAL:HG23	3	0.53	0.4	0.31
(1,1958)	1:11:A:ILE:H	1:10:A:VAL:HG21	3	0.53	0.4	0.31
(1,253)	1:23:A:TYR:HB2	1:61:A:PHE:HE2	3	0.49	0.06	0.51
(1,253)	1:23:A:TYR:HB2	1:61:A:PHE:HE1	3	0.49	0.06	0.51
(1,910)	1:11:A:ILE:H	1:10:A:VAL:HG22	3	0.48	0.4	0.26
(1,910)	1:11:A:ILE:H	1:10:A:VAL:HG23	3	0.48	0.4	0.26
(1,910)	1:11:A:ILE:H	1:10:A:VAL:HG21	3	0.48	0.4	0.26
(3,258)	1:57:A:TRP:HB2	1:75:A:ALA:HB3	3	0.42	0.13	0.45
(3,258)	1:76:A:TYR:HB3	1:75:A:ALA:HB3	3	0.42	0.13	0.45
(3,258)	1:57:A:TRP:HB2	1:75:A:ALA:HB1	3	0.42	0.13	0.45
(1,37)	1:75:A:ALA:HB2	1:9:A:ILE:HG22	3	0.41	0.16	0.39
(1,37)	1:75:A:ALA:HB2	1:9:A:ILE:HG21	3	0.41	0.16	0.39
(1,847)	1:7:A:ILE:H	1:48:A:LYS:HA	3	0.36	0.17	0.35
(1,1129)	1:45:A:ILE:HA	1:45:A:ILE:HG12	3	0.35	0.05	0.36
(3,284)	1:69:A:PHE:HA	1:115:A:SER:HB2	3	0.34	0.1	0.34
(3,284)	1:69:A:PHE:HA	1:115:A:SER:HB3	3	0.34	0.1	0.34
(1,644)	1:76:A:TYR:H	1:74:A:GLU:HB3	3	0.33	0.3	0.15
(1,963)	1:80:A:LEU:HA	1:80:A:LEU:HB2	3	0.31	0.01	0.31
(3,119)	1:90:A:GLU:HB2	1:10:A:VAL:HG12	3	0.31	0.07	0.33
(3,119)	1:11:A:ILE:HD12	1:59:A:CYS:HB2	3	0.31	0.07	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,119)	1:90:A:GLU:HB2	1:10:A:VAL:HG13	3	0.31	0.07	0.33
(3,27)	1:5:A:LYS:HG3	1:5:A:LYS:HA	3	0.3	0.17	0.22
(3,27)	1:5:A:LYS:HG2	1:5:A:LYS:HA	3	0.3	0.17	0.22
(1,293)	1:47:A:PHE:HA	1:47:A:PHE:HD2	3	0.3	0.08	0.27
(1,293)	1:47:A:PHE:HA	1:47:A:PHE:HD1	3	0.3	0.08	0.27
(3,272)	1:92:A:SER:HB3	1:93:A:ALA:H	3	0.3	0.08	0.27
(1,30)	1:45:A:ILE:HD11	1:45:A:ILE:HB	3	0.3	0.01	0.3
(1,30)	1:45:A:ILE:HD13	1:45:A:ILE:HB	3	0.3	0.01	0.3
(3,48)	1:45:A:ILE:HA	1:45:A:ILE:HG13	3	0.28	0.0	0.28
(1,1956)	1:10:A:VAL:HG23	1:42:A:THR:HB	3	0.27	0.07	0.24
(1,1956)	1:10:A:VAL:HG21	1:42:A:THR:HB	3	0.27	0.07	0.24
(1,15)	1:98:A:ILE:HD12	1:61:A:PHE:HE1	3	0.27	0.02	0.26
(1,15)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	3	0.27	0.02	0.26
(1,15)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	3	0.27	0.02	0.26
(1,370)	1:102:A:MET:H	1:102:A:MET:HG2	3	0.27	0.21	0.13
(3,118)	1:90:A:GLU:HB2	1:10:A:VAL:HG12	3	0.26	0.07	0.23
(3,118)	1:73:A:VAL:HG22	1:59:A:CYS:HB2	3	0.26	0.07	0.23
(3,118)	1:90:A:GLU:HB2	1:10:A:VAL:HG13	3	0.26	0.07	0.23
(3,303)	1:88:A:ARG:HB3	1:88:A:ARG:H	3	0.26	0.05	0.29
(3,195)	1:88:A:ARG:HB3	1:88:A:ARG:H	3	0.25	0.05	0.27
(1,1247)	1:20:A:ILE:HA	1:20:A:ILE:HD12	3	0.24	0.08	0.28
(1,1247)	1:20:A:ILE:HA	1:20:A:ILE:HD13	3	0.24	0.08	0.28
(1,1247)	1:20:A:ILE:HA	1:20:A:ILE:HD11	3	0.24	0.08	0.28
(1,124)	1:45:A:ILE:HG21	1:45:A:ILE:HD12	3	0.23	0.08	0.29
(1,124)	1:45:A:ILE:HG23	1:45:A:ILE:HD11	3	0.23	0.08	0.29
(1,124)	1:45:A:ILE:HG21	1:45:A:ILE:HD13	3	0.23	0.08	0.29
(1,1134)	1:7:A:ILE:HD11	1:84:A:LEU:HB3	3	0.23	0.08	0.23
(1,1134)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	3	0.23	0.08	0.23
(1,490)	1:30:A:THR:H	1:27:A:SER:H	3	0.22	0.01	0.22
(1,305)	1:61:A:PHE:HD2	1:23:A:TYR:HA	3	0.22	0.0	0.22
(1,2263)	1:37:A:LEU:HA	1:37:A:LEU:HB2	3	0.22	0.03	0.23
(1,1941)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	3	0.21	0.13	0.14
(1,1941)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	3	0.21	0.13	0.14
(1,907)	1:10:A:VAL:HG23	1:42:A:THR:HB	3	0.21	0.07	0.18
(1,907)	1:10:A:VAL:HG21	1:42:A:THR:HB	3	0.21	0.07	0.18
(1,1397)	1:108:A:GLN:HG2	1:108:A:GLN:H	3	0.21	0.04	0.23
(1,291)	1:73:A:VAL:HG21	1:71:A:THR:HG22	3	0.21	0.02	0.19
(1,291)	1:73:A:VAL:HG23	1:71:A:THR:HG22	3	0.21	0.02	0.19
(1,291)	1:73:A:VAL:HG23	1:71:A:THR:HG23	3	0.21	0.02	0.19
(1,1141)	1:37:A:LEU:H	1:20:A:ILE:HG22	3	0.2	0.07	0.24
(1,1118)	1:45:A:ILE:HD11	1:45:A:ILE:HB	3	0.2	0.02	0.2
(1,1118)	1:45:A:ILE:HD13	1:45:A:ILE:HB	3	0.2	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1152)	1:15:A:LEU:HA	1:15:A:LEU:HD12	3	0.2	0.05	0.19
(1,1152)	1:15:A:LEU:HA	1:15:A:LEU:HD13	3	0.2	0.05	0.19
(1,1600)	1:50:A:ASP:H	1:49:A:ASP:HB2	3	0.19	0.03	0.18
(1,404)	1:108:A:GLN:HG2	1:108:A:GLN:H	3	0.19	0.04	0.21
(1,739)	1:104:A:GLU:H	1:104:A:GLU:HB2	3	0.19	0.07	0.15
(1,9)	1:98:A:ILE:HD11	1:98:A:ILE:HA	3	0.18	0.04	0.18
(1,9)	1:98:A:ILE:HD13	1:98:A:ILE:HA	3	0.18	0.04	0.18
(1,580)	1:50:A:ASP:H	1:49:A:ASP:HB2	3	0.17	0.03	0.16
(3,204)	1:105:A:ARG:HG3	1:105:A:ARG:H	3	0.17	0.06	0.18
(3,204)	1:105:A:ARG:HG2	1:105:A:ARG:H	3	0.17	0.06	0.18
(1,1064)	1:37:A:LEU:HA	1:37:A:LEU:HB2	3	0.17	0.03	0.18
(1,1430)	1:14:A:THR:H	1:93:A:ALA:H	3	0.16	0.05	0.17
(1,877)	1:11:A:ILE:HG22	1:11:A:ILE:HD11	3	0.16	0.03	0.15
(1,877)	1:11:A:ILE:HG23	1:11:A:ILE:HD11	3	0.16	0.03	0.15
(1,877)	1:11:A:ILE:HG23	1:11:A:ILE:HD12	3	0.16	0.03	0.15
(1,1892)	1:30:A:THR:H	1:27:A:SER:H	3	0.16	0.01	0.16
(3,262)	1:45:A:ILE:HG13	1:45:A:ILE:HB	3	0.16	0.02	0.16
(1,1976)	1:112:A:LYS:HA	1:97:A:ALA:HB1	3	0.16	0.04	0.14
(1,1976)	1:112:A:LYS:HA	1:97:A:ALA:HB3	3	0.16	0.04	0.14
(1,1103)	1:98:A:ILE:HD12	1:61:A:PHE:HE1	3	0.15	0.02	0.14
(1,1103)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	3	0.15	0.02	0.14
(1,1103)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	3	0.15	0.02	0.14
(1,2070)	1:35:A:GLN:HA	1:35:A:GLN:HG2	3	0.15	0.02	0.16
(3,295)	1:36:A:TYR:H	1:35:A:GLN:HB2	3	0.15	0.03	0.13
(3,295)	1:35:A:GLN:HB3	1:36:A:TYR:H	3	0.15	0.03	0.13
(1,245)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	3	0.14	0.05	0.11
(1,1618)	1:54:A:ARG:H	1:52:A:THR:HB	3	0.14	0.01	0.15
(1,2007)	1:78:A:PRO:HA	1:78:A:PRO:HB2	3	0.13	0.03	0.12
(3,56)	1:85:A:CYS:HB3	1:85:A:CYS:HA	3	0.13	0.02	0.13
(3,181)	1:36:A:TYR:H	1:35:A:GLN:HB2	3	0.13	0.03	0.12
(3,181)	1:35:A:GLN:HB3	1:36:A:TYR:H	3	0.13	0.03	0.12
(3,222)	1:92:A:SER:HB3	1:12:A:LYS:HB2	3	0.13	0.0	0.13
(1,2239)	1:73:A:VAL:HG21	1:71:A:THR:HG22	3	0.13	0.02	0.12
(1,2239)	1:73:A:VAL:HG23	1:71:A:THR:HG22	3	0.13	0.02	0.12
(1,2239)	1:73:A:VAL:HG23	1:71:A:THR:HG23	3	0.13	0.02	0.12
(1,392)	1:112:A:LYS:H	1:112:A:LYS:HB2	3	0.12	0.01	0.12
(1,2075)	1:56:A:ARG:HB3	1:56:A:ARG:HA	3	0.12	0.01	0.12
(3,210)	1:44:A:ILE:H	1:44:A:ILE:HG23	3	0.12	0.01	0.11
(3,210)	1:44:A:ILE:H	1:44:A:ILE:HG21	3	0.12	0.01	0.11
(4,24)	1:37:A:LEU:H	1:21:A:LEU:O	2	1.62	0.06	1.62
(1,1074)	1:19:A:ARG:HB2	1:14:A:THR:HA	2	1.62	0.76	1.62
(1,2001)	1:39:A:PHE:HD2	1:17:A:PRO:HA	2	1.26	0.93	1.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,310)	1:39:A:PHE:HD1	1:14:A:THR:HA	2	1.19	0.7	1.19
(1,1054)	1:10:A:VAL:HG22	1:42:A:THR:HG22	2	1.0	0.52	1.0
(4,49)	1:21:A:LEU:O	1:37:A:LEU:N	2	0.98	0.1	0.98
(4,31)	1:89:A:TYR:O	1:10:A:VAL:N	2	0.8	0.7	0.8
(1,237)	1:62:A:ARG:HA	1:70:A:PHE:HA	2	0.78	0.13	0.78
(1,1678)	1:80:A:LEU:HB2	1:80:A:LEU:H	2	0.7	0.02	0.7
(1,656)	1:80:A:LEU:HB2	1:80:A:LEU:H	2	0.69	0.02	0.69
(1,1666)	1:76:A:TYR:H	1:75:A:ALA:HB2	2	0.68	0.01	0.68
(1,1666)	1:76:A:TYR:H	1:75:A:ALA:HB1	2	0.68	0.01	0.68
(1,645)	1:76:A:TYR:H	1:75:A:ALA:HB2	2	0.67	0.01	0.67
(1,645)	1:76:A:TYR:H	1:75:A:ALA:HB1	2	0.67	0.01	0.67
(4,9)	1:14:A:THR:H	1:93:A:ALA:O	2	0.62	0.5	0.62
(1,2257)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	2	0.58	0.29	0.58
(3,300)	1:53:A:GLU:HG2	1:53:A:GLU:H	2	0.57	0.04	0.57
(3,300)	1:53:A:GLU:HG3	1:53:A:GLU:H	2	0.57	0.04	0.57
(1,1729)	1:95:A:MET:HG2	1:95:A:MET:H	2	0.57	0.36	0.57
(3,188)	1:53:A:GLU:HG2	1:53:A:GLU:H	2	0.56	0.05	0.56
(3,188)	1:53:A:GLU:HG3	1:53:A:GLU:H	2	0.56	0.05	0.56
(1,186)	1:48:A:LYS:HA	1:6:A:GLU:HA	2	0.56	0.14	0.56
(1,1361)	1:35:A:GLN:HA	1:36:A:TYR:HD1	2	0.55	0.04	0.55
(1,702)	1:95:A:MET:HG2	1:95:A:MET:H	2	0.55	0.36	0.55
(1,1969)	1:62:A:ARG:HA	1:70:A:PHE:HA	2	0.53	0.13	0.53
(1,330)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	2	0.51	0.15	0.51
(1,330)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	2	0.51	0.15	0.51
(1,1954)	1:90:A:GLU:HA	1:10:A:VAL:HG21	2	0.5	0.04	0.5
(1,1954)	1:90:A:GLU:HA	1:10:A:VAL:HG23	2	0.5	0.04	0.5
(1,930)	1:12:A:LYS:HB3	1:92:A:SER:HB3	2	0.46	0.06	0.46
(1,2121)	1:36:A:TYR:HA	1:20:A:ILE:HG22	2	0.46	0.02	0.46
(1,2121)	1:36:A:TYR:HA	1:20:A:ILE:HG23	2	0.46	0.02	0.46
(4,43)	1:37:A:LEU:O	1:21:A:LEU:N	2	0.44	0.04	0.44
(1,906)	1:90:A:GLU:HA	1:10:A:VAL:HG21	2	0.44	0.04	0.44
(1,906)	1:90:A:GLU:HA	1:10:A:VAL:HG23	2	0.44	0.04	0.44
(1,72)	1:109:A:PRO:HB3	1:97:A:ALA:HB3	2	0.43	0.09	0.43
(1,72)	1:109:A:PRO:HB3	1:97:A:ALA:HB2	2	0.43	0.09	0.43
(1,1817)	1:112:A:LYS:H	1:111:A:ASN:HB2	2	0.4	0.24	0.4
(1,1479)	1:24:A:HIS:H	1:60:A:LEU:HB2	2	0.4	0.07	0.4
(1,788)	1:112:A:LYS:H	1:111:A:ASN:HB2	2	0.39	0.25	0.39
(1,469)	1:24:A:HIS:H	1:60:A:LEU:HB2	2	0.38	0.07	0.38
(1,1560)	1:42:A:THR:H	1:41:A:GLY:HA3	2	0.38	0.02	0.38
(1,2072)	1:35:A:GLN:HA	1:36:A:TYR:HD1	2	0.38	0.04	0.38
(1,175)	1:36:A:TYR:HA	1:22:A:GLN:HA	2	0.38	0.02	0.38
(4,33)	1:26:A:ARG:O	1:58:A:ASN:N	2	0.37	0.11	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,542)	1:42:A:THR:H	1:41:A:GLY:HA3	2	0.36	0.02	0.36
(3,137)	1:11:A:ILE:H	1:11:A:ILE:HD12	2	0.36	0.13	0.36
(1,1277)	1:1:A:ALA:HB1	1:83:A:PRO:HA	2	0.36	0.21	0.36
(1,1277)	1:1:A:ALA:HB3	1:83:A:PRO:HA	2	0.36	0.21	0.36
(1,2147)	1:62:A:ARG:HA	1:70:A:PHE:HA	2	0.32	0.13	0.32
(1,1406)	1:8:A:GLU:HG2	1:8:A:GLU:H	2	0.32	0.15	0.32
(1,867)	1:14:A:THR:H	1:19:A:ARG:HB3	2	0.31	0.14	0.31
(1,2144)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	2	0.31	0.18	0.31
(1,2144)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	2	0.31	0.18	0.31
(1,2229)	1:75:A:ALA:HB2	1:9:A:ILE:HG22	2	0.31	0.11	0.31
(1,232)	1:104:A:GLU:HA	1:104:A:GLU:HB2	2	0.3	0.18	0.3
(1,2123)	1:36:A:TYR:HA	1:22:A:GLN:HA	2	0.3	0.01	0.3
(1,411)	1:8:A:GLU:HG2	1:8:A:GLU:H	2	0.3	0.15	0.3
(1,1524)	1:36:A:TYR:H	1:36:A:TYR:HD1	2	0.3	0.01	0.3
(1,198)	1:92:A:SER:HA	1:92:A:SER:HB3	2	0.29	0.0	0.29
(1,2024)	1:48:A:LYS:HA	1:6:A:GLU:HA	2	0.29	0.14	0.29
(1,319)	1:90:A:GLU:HA	1:10:A:VAL:H	2	0.28	0.01	0.28
(1,1923)	1:23:A:TYR:HE2	1:11:A:ILE:HG21	2	0.28	0.1	0.28
(1,1923)	1:23:A:TYR:HE2	1:11:A:ILE:HG22	2	0.28	0.1	0.28
(1,510)	1:36:A:TYR:H	1:36:A:TYR:HD1	2	0.28	0.01	0.28
(1,2134)	1:15:A:LEU:H	1:95:A:MET:HA	2	0.28	0.07	0.28
(1,248)	1:36:A:TYR:HD1	1:36:A:TYR:HB2	2	0.27	0.16	0.27
(1,712)	1:96:A:ASP:H	1:95:A:MET:HB3	2	0.26	0.04	0.26
(1,1883)	1:113:A:TRP:HB3	1:114:A:ARG:H	2	0.26	0.07	0.26
(1,1698)	1:86:A:GLY:H	1:85:A:CYS:HB2	2	0.25	0.04	0.25
(1,1719)	1:57:A:TRP:H	1:56:A:ARG:HA	2	0.24	0.02	0.24
(1,2074)	1:113:A:TRP:HA	1:71:A:THR:HG23	2	0.24	0.1	0.24
(1,2074)	1:113:A:TRP:HA	1:71:A:THR:HG21	2	0.24	0.1	0.24
(1,676)	1:86:A:GLY:H	1:85:A:CYS:HB2	2	0.24	0.03	0.24
(1,850)	1:113:A:TRP:HB3	1:114:A:ARG:H	2	0.24	0.07	0.24
(1,995)	1:23:A:TYR:HE1	1:36:A:TYR:HA	2	0.24	0.09	0.24
(1,693)	1:57:A:TRP:H	1:56:A:ARG:HA	2	0.23	0.02	0.23
(1,1785)	1:115:A:SER:H	1:114:A:ARG:HA	2	0.23	0.12	0.23
(1,1596)	1:49:A:ASP:HB3	1:49:A:ASP:H	2	0.22	0.07	0.22
(1,182)	1:61:A:PHE:HE2	1:93:A:ALA:HB1	2	0.22	0.02	0.22
(1,250)	1:61:A:PHE:HB3	1:61:A:PHE:HD2	2	0.22	0.06	0.22
(1,139)	1:25:A:CYS:HB3	1:45:A:ILE:HD11	2	0.22	0.1	0.22
(1,139)	1:25:A:CYS:HB3	1:45:A:ILE:HD12	2	0.22	0.1	0.22
(1,883)	1:23:A:TYR:HE2	1:11:A:ILE:HG21	2	0.21	0.1	0.21
(1,883)	1:23:A:TYR:HE2	1:11:A:ILE:HG22	2	0.21	0.1	0.21
(1,169)	1:61:A:PHE:HA	1:61:A:PHE:HD1	2	0.2	0.03	0.2
(1,169)	1:61:A:PHE:HA	1:61:A:PHE:HD2	2	0.2	0.03	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,576)	1:49:A:ASP:HB3	1:49:A:ASP:H	2	0.2	0.08	0.2
(1,999)	1:15:A:LEU:H	1:95:A:MET:HA	2	0.19	0.08	0.19
(1,1257)	1:45:A:ILE:HG23	1:45:A:ILE:HD11	2	0.19	0.0	0.19
(1,1257)	1:45:A:ILE:HG21	1:45:A:ILE:HD13	2	0.19	0.0	0.19
(1,1644)	1:70:A:PHE:H	1:69:A:PHE:HA	2	0.19	0.07	0.19
(1,1910)	1:7:A:ILE:HD11	1:84:A:LEU:HB3	2	0.19	0.05	0.19
(1,1910)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	2	0.19	0.05	0.19
(1,194)	1:71:A:THR:HB	1:71:A:THR:HA	2	0.18	0.06	0.18
(1,1472)	1:22:A:GLN:HG3	1:23:A:TYR:H	2	0.18	0.04	0.18
(1,2234)	1:30:A:THR:HA	1:30:A:THR:HG22	2	0.18	0.05	0.18
(1,587)	1:52:A:THR:H	1:50:A:ASP:HA	2	0.18	0.06	0.18
(1,429)	1:14:A:THR:H	1:93:A:ALA:H	2	0.18	0.03	0.18
(1,619)	1:70:A:PHE:H	1:69:A:PHE:HA	2	0.18	0.06	0.18
(1,327)	1:7:A:ILE:HD12	1:8:A:GLU:H	2	0.17	0.06	0.17
(1,2043)	1:8:A:GLU:HB3	1:8:A:GLU:HA	2	0.17	0.06	0.17
(1,463)	1:22:A:GLN:HG3	1:23:A:TYR:H	2	0.17	0.04	0.17
(1,1146)	1:7:A:ILE:HG23	1:8:A:GLU:H	2	0.17	0.04	0.17
(1,1146)	1:7:A:ILE:HG21	1:8:A:GLU:H	2	0.17	0.04	0.17
(3,159)	1:57:A:TRP:HB2	1:75:A:ALA:HB3	2	0.17	0.05	0.17
(3,159)	1:57:A:TRP:HB2	1:75:A:ALA:HB1	2	0.17	0.05	0.17
(3,329)	1:6:A:GLU:HA	1:6:A:GLU:HG3	2	0.17	0.01	0.17
(3,329)	1:6:A:GLU:HG2	1:6:A:GLU:HA	2	0.17	0.01	0.17
(1,2161)	1:71:A:THR:HB	1:71:A:THR:HA	2	0.16	0.06	0.16
(1,962)	1:35:A:GLN:HG3	1:35:A:GLN:HA	2	0.16	0.02	0.16
(3,17)	1:87:A:LYS:HB2	1:87:A:LYS:HA	2	0.16	0.02	0.16
(1,301)	1:23:A:TYR:HD1	1:36:A:TYR:HA	2	0.16	0.06	0.16
(1,1396)	1:108:A:GLN:HG2	1:108:A:GLN:H	2	0.16	0.01	0.16
(1,1672)	1:79:A:ASP:H	1:78:A:PRO:HA	2	0.16	0.01	0.16
(1,1431)	1:15:A:LEU:H	1:14:A:THR:H	2	0.15	0.05	0.15
(1,302)	1:23:A:TYR:HD2	1:59:A:CYS:HB3	2	0.15	0.03	0.15
(1,2278)	1:15:A:LEU:HA	1:15:A:LEU:HD12	2	0.15	0.03	0.15
(1,2278)	1:15:A:LEU:HA	1:15:A:LEU:HD13	2	0.15	0.03	0.15
(1,1147)	1:61:A:PHE:HD2	1:71:A:THR:HG22	2	0.14	0.03	0.14
(1,1147)	1:61:A:PHE:HD1	1:71:A:THR:HG21	2	0.14	0.03	0.14
(1,650)	1:79:A:ASP:H	1:78:A:PRO:HA	2	0.14	0.01	0.14
(1,1917)	1:9:A:ILE:H	1:9:A:ILE:HD11	2	0.14	0.02	0.14
(1,364)	1:113:A:TRP:H	1:112:A:LYS:HB3	2	0.13	0.01	0.13
(1,594)	1:54:A:ARG:H	1:52:A:THR:HB	2	0.13	0.0	0.13
(1,1667)	1:57:A:TRP:H	1:76:A:TYR:H	2	0.13	0.02	0.13
(3,232)	1:6:A:GLU:HA	1:6:A:GLU:HG3	2	0.13	0.01	0.13
(3,232)	1:6:A:GLU:HG2	1:6:A:GLU:HA	2	0.13	0.01	0.13
(1,1390)	1:85:A:CYS:HB3	1:5:A:LYS:H	2	0.12	0.02	0.12

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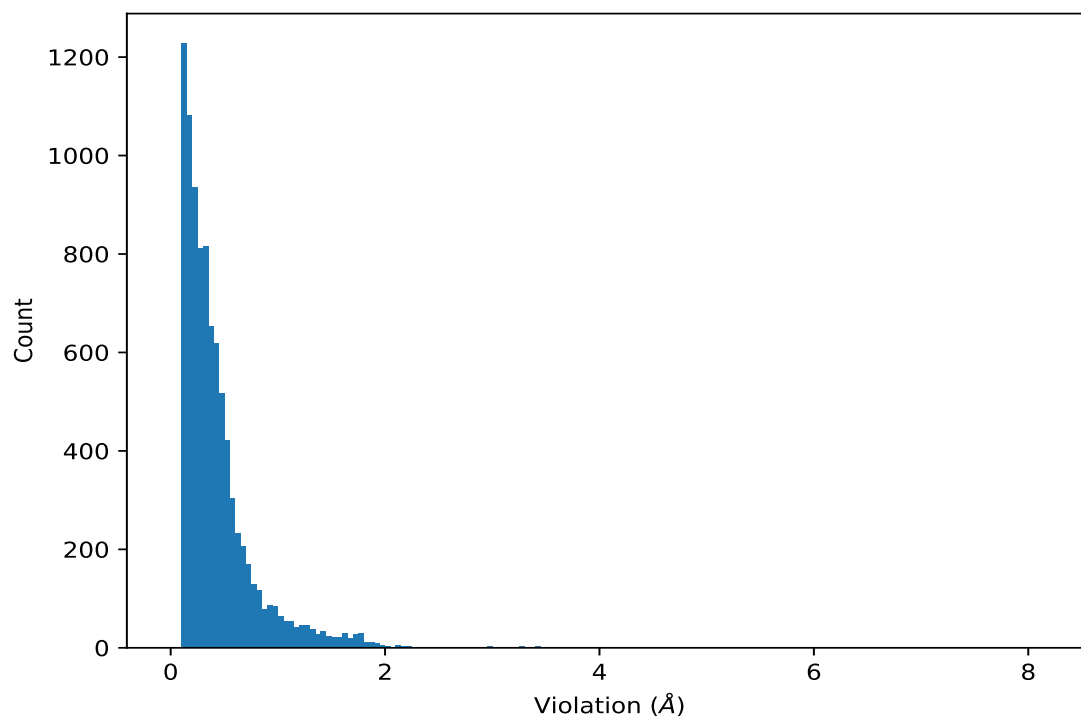
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1640)	1:65:A:ILE:H	1:65:A:ILE:HB	2	0.12	0.01	0.12
(1,1755)	1:99:A:TYR:HB3	1:100:A:PHE:H	2	0.12	0.02	0.12
(1,638)	1:75:A:ALA:H	1:58:A:ASN:HA	2	0.12	0.01	0.12
(1,1661)	1:75:A:ALA:H	1:58:A:ASN:HA	2	0.12	0.01	0.12
(1,176)	1:100:A:PHE:HA	1:91:A:LEU:HA	2	0.12	0.02	0.12
(1,78)	1:74:A:GLU:HA	1:74:A:GLU:HB3	2	0.11	0.0	0.11
(1,671)	1:85:A:CYS:H	1:84:A:LEU:HB2	2	0.11	0.0	0.11
(1,1693)	1:85:A:CYS:H	1:84:A:LEU:HB2	2	0.11	0.0	0.11
(1,1801)	1:56:A:ARG:H	1:55:A:SER:H	2	0.11	0.01	0.11
(1,615)	1:65:A:ILE:H	1:65:A:ILE:HB	2	0.11	0.0	0.11
(1,1979)	1:112:A:LYS:HB3	1:112:A:LYS:HA	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE2	18	8.2
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE2	5	6.3
(1,2051)	1:101:A:LYS:HB2	1:107:A:PRO:HA	14	5.88
(1,950)	1:101:A:LYS:HB2	1:107:A:PRO:HA	14	5.83
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE2	8	5.13
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	20	3.74
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	20	3.49
(1,255)	1:32:A:VAL:HG11	1:47:A:PHE:HE1	4	3.45
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	14	3.43
(3,8)	1:76:A:TYR:HB3	1:75:A:ALA:HB1	9	3.41
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	17	3.41
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	18	3.4
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	13	3.35
(3,264)	1:76:A:TYR:HB3	1:75:A:ALA:HB1	9	3.29
(1,1265)	1:15:A:LEU:HA	1:94:A:ARG:HA	14	3.29
(1,1265)	1:15:A:LEU:HA	1:94:A:ARG:HA	17	3.27
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	16	3.23
(3,256)	1:32:A:VAL:HG22	1:45:A:ILE:HG12	18	3.21
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE1	15	3.19
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	12	3.17
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	17	3.12
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	16	3.11
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	10	3.08
(1,1265)	1:15:A:LEU:HA	1:94:A:ARG:HA	12	3.03
(3,256)	1:32:A:VAL:HG21	1:45:A:ILE:HG12	13	3.0
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	20	2.98
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	5	2.97
(1,909)	1:10:A:VAL:HG22	1:90:A:GLU:HG2	13	2.96
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	9	2.94
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	16	2.76
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD13	17	2.74
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	16	2.71
(1,242)	1:39:A:PHE:HD2	1:17:A:PRO:HA	18	2.67
(4,10)	1:95:A:MET:H	1:14:A:THR:O	18	2.66
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	13	2.64
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG21	13	2.61
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	5	2.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG21	13	2.55
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	3	2.54
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	11	2.53
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	6	2.48
(1,2276)	1:19:A:ARG:HB2	1:14:A:THR:HA	13	2.43
(3,51)	1:11:A:ILE:HD12	1:75:A:ALA:HA	18	2.41
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	13	2.39
(1,1074)	1:19:A:ARG:HB2	1:14:A:THR:HA	13	2.37
(1,1265)	1:15:A:LEU:HA	1:94:A:ARG:HA	6	2.34
(1,2049)	1:10:A:VAL:HG21	1:12:A:LYS:H	13	2.31
(4,34)	1:14:A:THR:O	1:95:A:MET:N	18	2.26
(3,51)	1:9:A:ILE:HG13	1:75:A:ALA:HA	13	2.25
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE1	17	2.24
(1,949)	1:10:A:VAL:HG21	1:12:A:LYS:H	13	2.23
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG2	9	2.22
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	11	2.2
(1,2001)	1:39:A:PHE:HD2	1:17:A:PRO:HA	18	2.19
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	18	2.18
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	8	2.15
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	16	2.14
(3,248)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	13	2.12
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	18	2.12
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	16	2.12
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	16	2.1
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	18	2.05
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	3	2.02
(1,262)	1:93:A:ALA:HB1	1:13:A:ASN:HB2	13	2.02
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	13	2.0
(3,1)	1:76:A:TYR:HB3	1:9:A:ILE:HD13	6	2.0
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	11	1.99
(3,228)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	17	1.97
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	3	1.97
(1,255)	1:32:A:VAL:HG11	1:47:A:PHE:HE1	1	1.97
(1,255)	1:32:A:VAL:HG11	1:47:A:PHE:HE1	13	1.96
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	1	1.95
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	4	1.94
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB3	11	1.94
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD11	19	1.93
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	3	1.92
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	15	1.92
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	4	1.92
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	14	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	13	1.91
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	19	1.91
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	18	1.9
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	16	1.89
(1,310)	1:39:A:PHE:HD1	1:14:A:THR:HA	13	1.89
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB2	19	1.89
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	5	1.88
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	19	1.88
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG3	13	1.87
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	5	1.87
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	20	1.87
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	18	1.86
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB1	16	1.86
(3,51)	1:11:A:ILE:HD13	1:75:A:ALA:HA	19	1.85
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	12	1.84
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	6	1.83
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	17	1.83
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	6	1.82
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	13	1.82
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	6	1.81
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	5	1.81
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	16	1.81
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	10	1.8
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	13	1.8
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB3	11	1.8
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD13	16	1.8
(3,248)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	2	1.79
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	2	1.79
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	3	1.79
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	15	1.79
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG21	8	1.79
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	11	1.78
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	14	1.78
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	18	1.78
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	16	1.77
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	18	1.77
(3,98)	1:11:A:ILE:HG12	1:59:A:CYS:HB3	20	1.77
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	7	1.77
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	8	1.77
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	19	1.77
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	12	1.77
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	19	1.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG2	3	1.76
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	20	1.76
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	5	1.76
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	19	1.76
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	6	1.76
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	20	1.76
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	12	1.76
(3,225)	1:44:A:ILE:HD13	1:42:A:THR:HA	3	1.75
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG22	4	1.75
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	10	1.75
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB2	19	1.75
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	7	1.75
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	8	1.75
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	17	1.75
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	7	1.74
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	19	1.74
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	12	1.74
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG21	8	1.74
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	6	1.74
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	17	1.74
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	7	1.73
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	17	1.73
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	14	1.73
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	12	1.72
(3,97)	1:20:A:ILE:HG13	1:38:A:ASN:HB2	18	1.72
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	5	1.72
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	8	1.72
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB1	16	1.72
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	12	1.72
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	5	1.72
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	17	1.71
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	15	1.71
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	17	1.71
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	15	1.71
(4,8)	1:91:A:LEU:H	1:10:A:VAL:O	3	1.7
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	7	1.7
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	4	1.7
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG22	4	1.7
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	10	1.7
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	5	1.7
(1,249)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	17	1.7
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	11	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD13	7	1.69
(4,24)	1:37:A:LEU:H	1:21:A:LEU:O	15	1.68
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	4	1.68
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	5	1.68
(3,231)	1:14:A:THR:HB	1:19:A:ARG:HG2	20	1.68
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	10	1.68
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	5	1.68
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	8	1.68
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	19	1.68
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	17	1.67
(1,181)	1:61:A:PHE:HD1	1:21:A:LEU:HB2	3	1.67
(3,225)	1:44:A:ILE:HD12	1:42:A:THR:HA	13	1.66
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	20	1.66
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	13	1.66
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	15	1.66
(3,160)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	13	1.65
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	16	1.65
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	15	1.65
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	1	1.64
(3,140)	1:48:A:LYS:HB2	1:47:A:PHE:H	20	1.64
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	7	1.64
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	4	1.64
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	9	1.64
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	5	1.63
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	10	1.63
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	7	1.63
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD11	12	1.63
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	15	1.63
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	20	1.63
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	18	1.63
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	15	1.62
(3,241)	1:92:A:SER:HA	1:91:A:LEU:HB3	8	1.62
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG22	6	1.62
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	2	1.62
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	13	1.62
(3,228)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	8	1.61
(1,2255)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	17	1.61
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	15	1.61
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	10	1.61
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	7	1.61
(3,228)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	13	1.6
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG22	14	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	9	1.6
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	17	1.6
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	17	1.6
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	20	1.6
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD13	12	1.6
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	12	1.59
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	15	1.59
(1,262)	1:93:A:ALA:HB2	1:13:A:ASN:HB2	4	1.59
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	3	1.58
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	14	1.58
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	11	1.58
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	6	1.58
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	9	1.58
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	5	1.58
(3,179)	1:29:A:ASN:H	1:56:A:ARG:HA	14	1.57
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG22	6	1.57
(4,24)	1:37:A:LEU:H	1:21:A:LEU:O	10	1.56
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	11	1.56
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	11	1.56
(1,352)	1:57:A:TRP:HE1	1:56:A:ARG:HA	15	1.56
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	6	1.56
(3,161)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	17	1.55
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	5	1.55
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG22	14	1.55
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	14	1.55
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	14	1.55
(3,218)	1:11:A:ILE:HG22	1:37:A:LEU:HB2	12	1.54
(3,62)	1:104:A:GLU:HB3	1:103:A:ASP:HA	1	1.54
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	9	1.54
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	19	1.54
(1,1061)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	17	1.54
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	7	1.53
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	1	1.53
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	5	1.53
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	19	1.52
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	7	1.52
(4,31)	1:89:A:TYR:O	1:10:A:VAL:N	11	1.51
(3,39)	1:15:A:LEU:HA	1:14:A:THR:HA	12	1.51
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	18	1.51
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	16	1.51
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	10	1.51
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	14	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1054)	1:10:A:VAL:HG22	1:42:A:THR:HG22	13	1.51
(1,59)	1:10:A:VAL:HG12	1:10:A:VAL:H	13	1.51
(3,40)	1:15:A:LEU:HA	1:14:A:THR:HA	12	1.5
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	20	1.5
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	4	1.5
(1,264)	1:42:A:THR:HG21	1:12:A:LYS:HG2	11	1.5
(3,179)	1:55:A:SER:HB2	1:29:A:ASN:H	10	1.49
(3,40)	1:15:A:LEU:HA	1:14:A:THR:HA	17	1.49
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	1	1.49
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	10	1.49
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	14	1.49
(3,227)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	12	1.48
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	9	1.48
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	3	1.48
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	9	1.47
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	12	1.47
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	9	1.47
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	1	1.47
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	13	1.47
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	1	1.47
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	19	1.47
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	3	1.47
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	3	1.46
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	18	1.46
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	2	1.46
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	2	1.46
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	16	1.46
(3,39)	1:51:A:GLY:HA3	1:50:A:ASP:HA	17	1.45
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	1	1.45
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	7	1.44
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	13	1.44
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	18	1.44
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	3	1.44
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	17	1.44
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	20	1.44
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	8	1.44
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	19	1.44
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	20	1.44
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	2	1.44
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	1	1.44
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	2	1.44
(3,241)	1:92:A:SER:HA	1:91:A:LEU:HB3	15	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,145)	1:29:A:ASN:H	1:56:A:ARG:HA	14	1.43
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	15	1.43
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	16	1.43
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	5	1.43
(3,40)	1:3:A:GLY:HA3	1:4:A:CYS:HA	6	1.42
(3,39)	1:3:A:GLY:HA3	1:4:A:CYS:HA	6	1.42
(1,2255)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	5	1.42
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	14	1.42
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	3	1.42
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	20	1.42
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	16	1.41
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	5	1.41
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG23	13	1.41
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	9	1.41
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	16	1.41
(1,264)	1:42:A:THR:HG22	1:12:A:LYS:HG2	10	1.41
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	20	1.4
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	17	1.4
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	16	1.4
(1,264)	1:42:A:THR:HG22	1:12:A:LYS:HG2	17	1.4
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	12	1.4
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	20	1.39
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	14	1.39
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	9	1.38
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	17	1.38
(1,1961)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	12	1.38
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	13	1.38
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	18	1.38
(1,262)	1:93:A:ALA:HB3	1:13:A:ASN:HB2	20	1.38
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	11	1.38
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	9	1.37
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	6	1.37
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	2	1.37
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	7	1.37
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	8	1.37
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	18	1.37
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	7	1.37
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	15	1.37
(1,264)	1:42:A:THR:HG21	1:12:A:LYS:HG2	19	1.37
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	3	1.36
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	16	1.36
(3,145)	1:55:A:SER:HB2	1:29:A:ASN:H	10	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	18	1.35
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	10	1.35
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	20	1.35
(1,1061)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	5	1.35
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	5	1.35
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG23	13	1.35
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	6	1.34
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	4	1.34
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	18	1.34
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	1	1.34
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	8	1.34
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	3	1.34
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	3	1.34
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	17	1.34
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	7	1.34
(3,160)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	2	1.33
(3,106)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	19	1.33
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HB3	2	1.33
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	15	1.33
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	13	1.33
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	6	1.33
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	17	1.33
(1,911)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	12	1.33
(3,40)	1:3:A:GLY:HA3	1:4:A:CYS:HA	14	1.32
(3,39)	1:3:A:GLY:HA3	1:4:A:CYS:HA	14	1.32
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	4	1.32
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	13	1.32
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	9	1.32
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	13	1.32
(1,1019)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	20	1.32
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	18	1.32
(1,286)	1:45:A:ILE:HG22	1:9:A:ILE:HG12	19	1.32
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	19	1.31
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	13	1.31
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	7	1.31
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	8	1.31
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	16	1.31
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	13	1.31
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	13	1.31
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	17	1.3
(1,1003)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	9	1.3
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	3	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	7	1.3
(1,264)	1:42:A:THR:HG21	1:12:A:LYS:HG2	14	1.3
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	7	1.29
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HA	12	1.29
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	14	1.29
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	16	1.29
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	2	1.29
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	12	1.29
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	10	1.29
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	20	1.29
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	8	1.29
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	7	1.28
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	12	1.28
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	11	1.28
(1,1577)	1:9:A:ILE:HG12	1:46:A:LYS:H	12	1.28
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	5	1.28
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	18	1.28
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	1	1.28
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	9	1.28
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	8	1.28
(1,264)	1:42:A:THR:HG22	1:12:A:LYS:HG2	20	1.28
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	10	1.27
(1,2176)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	20	1.27
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	5	1.27
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG13	13	1.27
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	4	1.27
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD13	14	1.27
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	15	1.27
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	11	1.26
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	15	1.26
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	13	1.26
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	10	1.26
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	11	1.26
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	4	1.26
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	13	1.26
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	9	1.26
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG13	13	1.26
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	5	1.26
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	19	1.25
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	2	1.25
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	12	1.25
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	11	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG21	17	1.25
(1,1003)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	15	1.25
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	19	1.25
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	13	1.25
(1,558)	1:9:A:ILE:HG12	1:46:A:LYS:H	12	1.25
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	14	1.25
(3,231)	1:14:A:THR:HB	1:19:A:ARG:HG2	19	1.24
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	15	1.24
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	6	1.24
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	11	1.24
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	11	1.24
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	17	1.24
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	4	1.24
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	10	1.24
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	5	1.24
(3,218)	1:11:A:ILE:HG21	1:37:A:LEU:HB2	20	1.23
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	11	1.23
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	1	1.23
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	4	1.23
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	14	1.23
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	16	1.23
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	4	1.23
(1,286)	1:45:A:ILE:HG22	1:9:A:ILE:HG12	18	1.23
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	12	1.22
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	4	1.22
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	5	1.22
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	1	1.22
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	15	1.22
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	19	1.22
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG12	8	1.22
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	13	1.22
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	12	1.22
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	11	1.22
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	2	1.22
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	2	1.22
(1,262)	1:93:A:ALA:HB2	1:13:A:ASN:HB2	1	1.22
(1,239)	1:14:A:THR:HB	1:39:A:PHE:HD1	13	1.22
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	5	1.21
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	14	1.21
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	17	1.21
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	7	1.21
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	5	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	4	1.21
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG12	8	1.21
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	8	1.21
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	13	1.2
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG11	17	1.2
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	19	1.2
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	10	1.2
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	11	1.2
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	11	1.2
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	14	1.2
(3,161)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	8	1.19
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG23	8	1.19
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	4	1.19
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	13	1.19
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	5	1.19
(1,1018)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	20	1.19
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	2	1.19
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	12	1.19
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	11	1.19
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG21	17	1.19
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	13	1.19
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	1	1.18
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	10	1.18
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	13	1.18
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	15	1.18
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	6	1.18
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG11	17	1.18
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	16	1.18
(3,161)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	13	1.17
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	15	1.17
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	7	1.17
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	3	1.17
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	1	1.17
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	1	1.17
(3,228)	1:7:A:ILE:HG23	1:84:A:LEU:HB3	16	1.16
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	15	1.16
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG23	8	1.16
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	15	1.16
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	5	1.16
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	20	1.16
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	17	1.16
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	15	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB2	6	1.16
(3,218)	1:11:A:ILE:HG21	1:37:A:LEU:HB2	6	1.15
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG21	7	1.15
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	6	1.15
(1,1003)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	11	1.15
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	5	1.15
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	19	1.15
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	3	1.15
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	2	1.15
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	13	1.15
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	10	1.14
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG21	16	1.14
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	2	1.14
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	8	1.14
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	20	1.14
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	11	1.14
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	10	1.14
(1,678)	1:87:A:LYS:HB3	1:88:A:ARG:H	14	1.14
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	17	1.14
(3,241)	1:92:A:SER:HA	1:91:A:LEU:HB3	2	1.13
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	13	1.13
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	12	1.13
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	7	1.13
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	12	1.13
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	4	1.13
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	7	1.13
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG23	8	1.13
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	4	1.13
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	6	1.13
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	16	1.13
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	11	1.13
(1,249)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	5	1.13
(4,9)	1:14:A:THR:H	1:93:A:ALA:O	13	1.12
(3,241)	1:92:A:SER:HA	1:91:A:LEU:HB3	4	1.12
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG3	7	1.12
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	3	1.12
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	13	1.12
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG22	1	1.12
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	16	1.12
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	13	1.12
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG22	2	1.12
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	8	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	5	1.12
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	13	1.12
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	20	1.12
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	1	1.12
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	7	1.12
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	13	1.11
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	5	1.11
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	20	1.11
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	4	1.11
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	6	1.11
(1,225)	1:24:A:HIS:HA	1:34:A:VAL:HA	18	1.11
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	10	1.11
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	1	1.1
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	8	1.1
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG22	4	1.1
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG21	13	1.1
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	19	1.1
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	4	1.1
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	10	1.1
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG11	3	1.1
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	5	1.1
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	15	1.1
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	5	1.09
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	7	1.09
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	15	1.09
(1,1958)	1:11:A:ILE:H	1:10:A:VAL:HG21	13	1.09
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG23	16	1.09
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	5	1.09
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	7	1.09
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	10	1.09
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG11	16	1.09
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG21	7	1.09
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	8	1.09
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG11	3	1.09
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD11	3	1.09
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	20	1.08
(3,256)	1:32:A:VAL:HG23	1:45:A:ILE:HG12	17	1.08
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	17	1.08
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG21	20	1.08
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	1	1.08
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	11	1.08
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	19	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	17	1.08
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	20	1.08
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	3	1.08
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	12	1.08
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	2	1.08
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	17	1.08
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	12	1.08
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	10	1.08
(1,181)	1:61:A:PHE:HD1	1:21:A:LEU:HB2	11	1.08
(4,49)	1:21:A:LEU:O	1:37:A:LEU:N	15	1.07
(3,62)	1:104:A:GLU:HB3	1:103:A:ASP:HA	20	1.07
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	3	1.07
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	13	1.07
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	16	1.07
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	7	1.07
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG22	2	1.07
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	13	1.07
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	10	1.07
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG11	16	1.07
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	15	1.07
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG3	4	1.06
(3,62)	1:104:A:GLU:HB3	1:103:A:ASP:HA	10	1.06
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HA	19	1.06
(3,15)	1:84:A:LEU:HA	1:85:A:CYS:HB3	15	1.06
(1,1529)	1:36:A:TYR:H	1:35:A:GLN:HG3	15	1.06
(1,1052)	1:73:A:VAL:HG22	1:111:A:ASN:HB2	8	1.06
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	13	1.06
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	12	1.06
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	16	1.06
(3,225)	1:10:A:VAL:HG21	1:42:A:THR:HA	12	1.05
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	7	1.05
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	8	1.05
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	4	1.05
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	7	1.05
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	5	1.04
(3,179)	1:55:A:SER:HB2	1:29:A:ASN:H	19	1.04
(3,44)	1:28:A:GLY:HA2	1:55:A:SER:HB2	17	1.04
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG23	18	1.04
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG22	18	1.04
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	9	1.04
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	16	1.04
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG11	12	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:15:A:LEU:HD11	1:19:A:ARG:HB3	1	1.04
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	15	1.04
(1,910)	1:11:A:ILE:H	1:10:A:VAL:HG21	13	1.04
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	5	1.04
(1,515)	1:36:A:TYR:H	1:35:A:GLN:HG3	15	1.04
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	13	1.04
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	6	1.04
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HA	17	1.03
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG21	3	1.03
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	20	1.03
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	4	1.03
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG21	19	1.03
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG21	13	1.03
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	17	1.03
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	5	1.03
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB2	6	1.03
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	19	1.03
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	17	1.03
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG23	16	1.03
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	3	1.03
(1,340)	1:87:A:LYS:HB3	1:88:A:ARG:H	14	1.03
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD11	16	1.03
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	17	1.02
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG22	3	1.02
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	16	1.02
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	14	1.02
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	19	1.02
(1,1036)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	19	1.02
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	7	1.02
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	1	1.02
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	11	1.02
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	20	1.02
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG11	12	1.02
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG21	19	1.01
(1,1992)	1:24:A:HIS:HB3	1:34:A:VAL:HA	9	1.01
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG22	9	1.01
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	2	1.01
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	3	1.01
(1,1044)	1:14:A:THR:HG23	1:14:A:THR:HA	7	1.01
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	9	1.01
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	5	1.01
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	2	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:35:A:GLN:HA	1:36:A:TYR:HD1	10	1.01
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	3	1.01
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD13	5	1.01
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	10	1.0
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	11	1.0
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	15	1.0
(1,1052)	1:73:A:VAL:HG22	1:111:A:ASN:HB2	4	1.0
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	8	1.0
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	11	1.0
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	9	1.0
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	5	1.0
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	8	1.0
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	9	1.0
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	7	1.0
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	2	1.0
(3,224)	1:92:A:SER:HB2	1:99:A:TYR:HB3	7	0.99
(3,179)	1:55:A:SER:HB2	1:29:A:ASN:H	9	0.99
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	6	0.99
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG13	1	0.99
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG11	18	0.99
(1,1044)	1:14:A:THR:HG21	1:14:A:THR:HA	20	0.99
(1,1003)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	3	0.99
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	7	0.99
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG22	18	0.99
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	16	0.99
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	17	0.99
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	7	0.99
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	12	0.99
(1,127)	1:45:A:ILE:H	1:45:A:ILE:HG13	5	0.99
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD13	7	0.99
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	17	0.98
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	3	0.98
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	15	0.98
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	10	0.98
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	20	0.98
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG12	5	0.98
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	7	0.98
(1,1044)	1:14:A:THR:HG21	1:14:A:THR:HA	14	0.98
(1,1044)	1:14:A:THR:HG21	1:14:A:THR:HA	15	0.98
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	4	0.98
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG21	13	0.98
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	14	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:20:A:ILE:HD11	1:20:A:ILE:HB	12	0.98
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	12	0.98
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	1	0.98
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD13	12	0.98
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	9	0.98
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	19	0.97
(3,179)	1:55:A:SER:HB2	1:29:A:ASN:H	16	0.97
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG23	13	0.97
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	8	0.97
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	16	0.97
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG21	2	0.97
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG21	6	0.97
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	6	0.97
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	20	0.97
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	2	0.97
(1,1044)	1:14:A:THR:HG23	1:14:A:THR:HA	10	0.97
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG21	19	0.97
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	2	0.97
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	19	0.97
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG13	1	0.97
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG11	18	0.97
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	7	0.97
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	4	0.97
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	6	0.97
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	14	0.96
(3,224)	1:92:A:SER:HB2	1:99:A:TYR:HB3	13	0.96
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	14	0.96
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	4	0.96
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG21	2	0.96
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	11	0.96
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	6	0.96
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	10	0.96
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	16	0.96
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG12	5	0.96
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	16	0.96
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	6	0.96
(1,127)	1:45:A:ILE:H	1:45:A:ILE:HG13	1	0.96
(1,74)	1:1:A:ALA:HB3	1:83:A:PRO:HA	15	0.96
(3,224)	1:92:A:SER:HB2	1:99:A:TYR:HB3	9	0.95
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HA	9	0.95
(1,1961)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	3	0.95
(1,1961)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	19	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	5	0.95
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	1	0.95
(1,1919)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	18	0.95
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	10	0.95
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	1	0.95
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	16	0.95
(1,929)	1:24:A:HIS:HB3	1:34:A:VAL:HA	9	0.95
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG22	9	0.95
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG23	11	0.95
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	15	0.95
(1,290)	1:20:A:ILE:HD12	1:20:A:ILE:HB	3	0.95
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	6	0.95
(1,290)	1:20:A:ILE:HD11	1:20:A:ILE:HB	9	0.95
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	8	0.95
(1,127)	1:45:A:ILE:H	1:45:A:ILE:HG13	7	0.95
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD11	19	0.95
(3,225)	1:10:A:VAL:HG21	1:42:A:THR:HA	9	0.94
(3,179)	1:55:A:SER:HB2	1:29:A:ASN:H	17	0.94
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG21	9	0.94
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	6	0.94
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	10	0.94
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	2	0.94
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	4	0.94
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG23	14	0.94
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG12	4	0.94
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	15	0.94
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	10	0.94
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	3	0.94
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	12	0.94
(1,140)	1:45:A:ILE:HD11	1:9:A:ILE:HD13	14	0.94
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD12	9	0.94
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD12	11	0.94
(1,94)	1:9:A:ILE:HG22	1:75:A:ALA:HA	2	0.94
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	4	0.94
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG23	17	0.94
(3,79)	1:113:A:TRP:H	1:113:A:TRP:HB2	2	0.93
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD12	17	0.93
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	11	0.93
(1,1729)	1:95:A:MET:HG2	1:95:A:MET:H	12	0.93
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	16	0.93
(1,1044)	1:14:A:THR:HG23	1:14:A:THR:HA	17	0.93
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	19	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	10	0.93
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	20	0.93
(1,294)	1:35:A:GLN:HA	1:36:A:TYR:HD1	15	0.93
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	15	0.93
(1,264)	1:42:A:THR:HG21	1:12:A:LYS:HG2	9	0.93
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	10	0.93
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	14	0.93
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	15	0.93
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	14	0.93
(3,219)	1:9:A:ILE:HG22	1:57:A:TRP:HB2	2	0.92
(3,79)	1:113:A:TRP:H	1:113:A:TRP:HB2	13	0.92
(3,35)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	14	0.92
(1,2276)	1:19:A:ARG:HB2	1:14:A:THR:HA	1	0.92
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	13	0.92
(1,1059)	1:65:A:ILE:HG23	1:65:A:ILE:HA	14	0.92
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	5	0.92
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	6	0.92
(1,913)	1:15:A:LEU:HD11	1:19:A:ARG:HB3	13	0.92
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	6	0.92
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG12	4	0.92
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	19	0.92
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD13	13	0.92
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	20	0.92
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	8	0.91
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	2	0.91
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	16	0.91
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	15	0.91
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	4	0.91
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	8	0.91
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	16	0.91
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG21	2	0.91
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG21	6	0.91
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	6	0.91
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG23	14	0.91
(1,702)	1:95:A:MET:HG2	1:95:A:MET:H	12	0.91
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	12	0.91
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	17	0.91
(1,237)	1:62:A:ARG:HA	1:70:A:PHE:HA	11	0.91
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	6	0.91
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD12	11	0.91
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD12	2	0.91
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD13	3	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	4	0.91
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD12	17	0.91
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	17	0.91
(3,145)	1:55:A:SER:HB2	1:29:A:ASN:H	19	0.9
(3,79)	1:113:A:TRP:H	1:113:A:TRP:HB2	9	0.9
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG21	5	0.9
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG22	11	0.9
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	12	0.9
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.9
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	7	0.9
(1,911)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	3	0.9
(1,911)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	19	0.9
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG21	1	0.9
(1,879)	1:11:A:ILE:HG12	1:11:A:ILE:HG22	18	0.9
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	5	0.9
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	6	0.9
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	14	0.9
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	17	0.9
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG2	10	0.89
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	14	0.89
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG22	6	0.89
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	20	0.89
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.89
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD12	14	0.89
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	20	0.89
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG12	15	0.89
(1,1059)	1:65:A:ILE:HG23	1:65:A:ILE:HA	18	0.89
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	10	0.89
(1,913)	1:15:A:LEU:HD13	1:19:A:ARG:HB3	8	0.89
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	4	0.89
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	5	0.89
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	2	0.89
(4,49)	1:21:A:LEU:O	1:37:A:LEU:N	10	0.88
(3,224)	1:92:A:SER:HB3	1:99:A:TYR:HB3	8	0.88
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	18	0.88
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG22	14	0.88
(3,7)	1:11:A:ILE:H	1:11:A:ILE:HG21	17	0.88
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	5	0.88
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	6	0.88
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG21	9	0.88
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	3	0.88
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	8	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1059)	1:65:A:ILE:HG23	1:65:A:ILE:HA	1	0.88
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	3	0.88
(1,1036)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	11	0.88
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	6	0.88
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	2	0.88
(1,391)	1:112:A:LYS:H	1:98:A:ILE:HB	3	0.88
(1,290)	1:20:A:ILE:HD12	1:20:A:ILE:HB	19	0.88
(1,279)	1:60:A:LEU:HB2	1:24:A:HIS:HB2	6	0.88
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD13	19	0.88
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD13	9	0.88
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG21	20	0.88
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG21	18	0.88
(3,224)	1:92:A:SER:HB3	1:99:A:TYR:HB3	10	0.87
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG21	15	0.87
(1,2257)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	17	0.87
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG23	19	0.87
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.87
(1,1059)	1:65:A:ILE:HG21	1:65:A:ILE:HA	11	0.87
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	11	0.87
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG12	15	0.87
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	9	0.87
(1,262)	1:93:A:ALA:HB1	1:13:A:ASN:HB2	16	0.87
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	8	0.87
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	12	0.87
(4,23)	1:21:A:LEU:H	1:37:A:LEU:O	15	0.86
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	10	0.86
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	8	0.86
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG23	7	0.86
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	1	0.86
(1,1074)	1:19:A:ARG:HB2	1:14:A:THR:HA	1	0.86
(1,1056)	1:11:A:ILE:HD12	1:11:A:ILE:HB	3	0.86
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG22	19	0.86
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	4	0.85
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG2	20	0.85
(3,145)	1:55:A:SER:HB2	1:29:A:ASN:H	9	0.85
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG23	7	0.85
(1,1961)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	16	0.85
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	1	0.85
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG23	12	0.85
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD13	5	0.85
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	2	0.85
(1,1056)	1:11:A:ILE:HD12	1:11:A:ILE:HB	5	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	9	0.85
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	13	0.85
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	15	0.85
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	19	0.85
(1,1044)	1:14:A:THR:HG22	1:14:A:THR:HA	12	0.85
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	13	0.85
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.85
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD12	14	0.85
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	20	0.85
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	4	0.85
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	13	0.85
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD11	8	0.85
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG23	17	0.85
(3,220)	1:44:A:ILE:HG21	1:8:A:GLU:HG3	9	0.84
(3,219)	1:9:A:ILE:HG21	1:76:A:TYR:HB2	15	0.84
(3,219)	1:9:A:ILE:HG22	1:76:A:TYR:HB2	17	0.84
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD13	20	0.84
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	2	0.84
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	1	0.84
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG23	2	0.84
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	9	0.84
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG21	4	0.84
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG22	20	0.84
(1,1731)	1:94:A:ARG:HB3	1:95:A:MET:H	12	0.84
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	12	0.84
(1,1260)	1:45:A:ILE:H	1:45:A:ILE:HG13	5	0.84
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	7	0.84
(1,1059)	1:65:A:ILE:HG21	1:65:A:ILE:HA	4	0.84
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	6	0.84
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	7	0.84
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	10	0.84
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	1	0.84
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.84
(1,290)	1:20:A:ILE:HD12	1:20:A:ILE:HB	1	0.84
(3,248)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	19	0.83
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	14	0.83
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	4	0.83
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG23	10	0.83
(3,145)	1:55:A:SER:HB2	1:29:A:ASN:H	16	0.83
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	20	0.83
(3,68)	1:98:A:ILE:HB	1:111:A:ASN:HA	13	0.83
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	4	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG21	15	0.83
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG21	14	0.83
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	17	0.83
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	20	0.83
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	17	0.83
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	2	0.83
(1,1699)	1:7:A:ILE:HD11	1:87:A:LYS:H	19	0.83
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	12	0.83
(1,1171)	1:1:A:ALA:HB3	1:83:A:PRO:HA	15	0.83
(1,1102)	1:98:A:ILE:HD13	1:71:A:THR:HG23	17	0.83
(1,1059)	1:65:A:ILE:HG23	1:65:A:ILE:HA	16	0.83
(1,1059)	1:65:A:ILE:HG21	1:65:A:ILE:HA	17	0.83
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	4	0.83
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	6	0.83
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	12	0.83
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	20	0.83
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	9	0.83
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	16	0.83
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	7	0.83
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	6	0.82
(3,225)	1:10:A:VAL:HG22	1:42:A:THR:HA	19	0.82
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG3	6	0.82
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG3	8	0.82
(3,107)	1:44:A:ILE:HG21	1:46:A:LYS:HB3	19	0.82
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	1	0.82
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE1	17	0.82
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	19	0.82
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG21	9	0.82
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	12	0.82
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	18	0.82
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	4	0.82
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	1	0.82
(1,1059)	1:65:A:ILE:HG21	1:65:A:ILE:HA	12	0.82
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	13	0.82
(1,1056)	1:11:A:ILE:HD12	1:11:A:ILE:HB	1	0.82
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	11	0.82
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG21	9	0.82
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	3	0.82
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.82
(1,704)	1:94:A:ARG:HB3	1:95:A:MET:H	12	0.82
(1,677)	1:7:A:ILE:HD11	1:87:A:LYS:H	19	0.82
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	2	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD11	1	0.82
(1,85)	1:74:A:GLU:HA	1:74:A:GLU:HG2	18	0.82
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	8	0.82
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	13	0.81
(3,219)	1:9:A:ILE:HG21	1:76:A:TYR:HB3	20	0.81
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	10	0.81
(3,145)	1:55:A:SER:HB2	1:29:A:ASN:H	17	0.81
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG22	19	0.81
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	12	0.81
(1,1930)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	2	0.81
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	6	0.81
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	13	0.81
(1,1802)	1:56:A:ARG:H	1:56:A:ARG:HB3	7	0.81
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	6	0.81
(1,1260)	1:45:A:ILE:H	1:45:A:ILE:HG13	1	0.81
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	5	0.81
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	5	0.81
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	1	0.81
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG23	19	0.81
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG22	20	0.81
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	12	0.81
(1,242)	1:39:A:PHE:HD2	1:17:A:PRO:HA	16	0.81
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	6	0.81
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD12	6	0.81
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD12	18	0.81
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	11	0.81
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	15	0.81
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	18	0.81
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	19	0.81
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	19	0.81
(3,225)	1:10:A:VAL:HG22	1:42:A:THR:HA	11	0.8
(3,106)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	2	0.8
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG21	6	0.8
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	12	0.8
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	16	0.8
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	10	0.8
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG22	15	0.8
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG23	17	0.8
(1,1260)	1:45:A:ILE:H	1:45:A:ILE:HG13	7	0.8
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	2	0.8
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	15	0.8
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	14	0.8
(1,911)	1:34:A:VAL:HG22	1:24:A:HIS:HB3	16	0.8
(1,254)	1:23:A:TYR:HB2	1:61:A:PHE:HD1	18	0.8
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	7	0.8
(3,106)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	6	0.79
(3,78)	1:113:A:TRP:H	1:113:A:TRP:HB2	2	0.79
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	12	0.79
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	7	0.79
(3,35)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	8	0.79
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG21	10	0.79
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	17	0.79
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	8	0.79
(1,1293)	1:45:A:ILE:HD11	1:9:A:ILE:HD13	14	0.79
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD12	11	0.79
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	10	0.79
(1,1056)	1:11:A:ILE:HD11	1:11:A:ILE:HB	12	0.79
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	18	0.79
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	20	0.79
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG23	7	0.79
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	20	0.79
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	1	0.79
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG23	12	0.79
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	13	0.79
(1,775)	1:56:A:ARG:H	1:56:A:ARG:HB3	7	0.79
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	15	0.79
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	20	0.79
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG2	11	0.78
(3,108)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	14	0.78
(3,97)	1:88:A:ARG:HB2	1:76:A:TYR:HB3	11	0.78
(3,78)	1:113:A:TRP:H	1:113:A:TRP:HB2	13	0.78
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	12	0.78
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	10	0.78
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	12	0.78
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	16	0.78
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG21	3	0.78
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG21	15	0.78
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	20	0.78
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	14	0.78
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG22	3	0.78
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	1	0.78
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	11	0.78
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	14	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD12	9	0.78
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	10	0.78
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	14	0.78
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	15	0.78
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	7	0.78
(1,1059)	1:65:A:ILE:HG23	1:65:A:ILE:HA	19	0.78
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	1	0.78
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG23	2	0.78
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG21	4	0.78
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	2	0.78
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG22	15	0.78
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG23	17	0.78
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	4	0.78
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	14	0.77
(3,107)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	14	0.77
(3,106)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	14	0.77
(3,68)	1:98:A:ILE:HB	1:111:A:ASN:HA	15	0.77
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	16	0.77
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	4	0.77
(3,35)	1:98:A:ILE:HG21	1:61:A:PHE:HE2	1	0.77
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG22	15	0.77
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	5	0.77
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	7	0.77
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	10	0.77
(1,1059)	1:65:A:ILE:HG23	1:65:A:ILE:HA	8	0.77
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	6	0.77
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG21	14	0.77
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	17	0.77
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	17	0.77
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	17	0.77
(1,290)	1:20:A:ILE:HD12	1:20:A:ILE:HB	10	0.77
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	2	0.77
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	1	0.77
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	14	0.76
(3,241)	1:92:A:SER:HA	1:91:A:LEU:HB3	6	0.76
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG23	2	0.76
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG23	12	0.76
(3,78)	1:113:A:TRP:H	1:113:A:TRP:HB2	9	0.76
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG21	2	0.76
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	12	0.76
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG21	13	0.76
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	3	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	15	0.76
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	8	0.76
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	4	0.76
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	11	0.76
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG22	16	0.76
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD12	11	0.76
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD12	2	0.76
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	4	0.76
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD13	13	0.76
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	20	0.76
(1,1102)	1:98:A:ILE:HD11	1:71:A:THR:HG21	18	0.76
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	16	0.76
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG21	9	0.76
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG22	17	0.76
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	9	0.76
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	12	0.76
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG22	18	0.76
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	6	0.76
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	14	0.76
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	2	0.76
(3,255)	1:93:A:ALA:HB3	1:14:A:THR:HG21	18	0.75
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG22	11	0.75
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	19	0.75
(3,108)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	16	0.75
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	19	0.75
(3,35)	1:98:A:ILE:HG22	1:61:A:PHE:HE1	18	0.75
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	6	0.75
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	19	0.75
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG23	18	0.75
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	19	0.75
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	18	0.75
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	16	0.75
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	15	0.75
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD13	3	0.75
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD12	17	0.75
(1,1059)	1:65:A:ILE:HG21	1:65:A:ILE:HA	9	0.75
(1,1059)	1:65:A:ILE:HG21	1:65:A:ILE:HA	20	0.75
(1,1056)	1:11:A:ILE:HD13	1:11:A:ILE:HB	17	0.75
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	20	0.75
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	10	0.75
(1,892)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	2	0.75
(1,644)	1:76:A:TYR:H	1:74:A:GLU:HB3	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	17	0.75
(1,170)	1:23:A:TYR:HD2	1:23:A:TYR:HA	2	0.75
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	9	0.75
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD12	16	0.75
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	10	0.75
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD11	18	0.75
(3,326)	1:87:A:LYS:HB3	1:7:A:ILE:HG23	9	0.74
(3,256)	1:32:A:VAL:HG23	1:45:A:ILE:HG12	11	0.74
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	16	0.74
(3,107)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	16	0.74
(3,107)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	17	0.74
(3,106)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	16	0.74
(3,106)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	17	0.74
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	18	0.74
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	16	0.74
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	2	0.74
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	5	0.74
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	8	0.74
(1,1921)	1:61:A:PHE:HD2	1:11:A:ILE:HG23	14	0.74
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	2	0.74
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	10	0.74
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	16	0.74
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG21	6	0.74
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	12	0.74
(1,1044)	1:14:A:THR:HG21	1:14:A:THR:HA	6	0.74
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	11	0.74
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	19	0.74
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	1	0.74
(1,170)	1:23:A:TYR:HD2	1:23:A:TYR:HA	3	0.74
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	19	0.74
(1,123)	1:45:A:ILE:HA	1:45:A:ILE:HD13	16	0.74
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	12	0.74
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	15	0.74
(4,23)	1:21:A:LEU:H	1:37:A:LEU:O	10	0.73
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	5	0.73
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	15	0.73
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	16	0.73
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	17	0.73
(3,225)	1:10:A:VAL:HG21	1:42:A:THR:HA	8	0.73
(3,225)	1:10:A:VAL:HG22	1:42:A:THR:HA	10	0.73
(3,219)	1:9:A:ILE:HG23	1:57:A:TRP:HB2	11	0.73
(3,218)	1:11:A:ILE:HG21	1:37:A:LEU:HB2	17	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,189)	1:74:A:GLU:HA	1:76:A:TYR:H	11	0.73
(3,161)	1:7:A:ILE:HG23	1:84:A:LEU:HB3	16	0.73
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	11	0.73
(3,68)	1:98:A:ILE:HB	1:111:A:ASN:HA	19	0.73
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	10	0.73
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG23	7	0.73
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG21	3	0.73
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	7	0.73
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	14	0.73
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	4	0.73
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	14	0.73
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	11	0.73
(1,1961)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	5	0.73
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	13	0.73
(1,1949)	1:61:A:PHE:HE2	1:71:A:THR:HG21	11	0.73
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	7	0.73
(1,1921)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	11	0.73
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	10	0.73
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	12	0.73
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	10	0.73
(1,1036)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	12	0.73
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	14	0.73
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	15	0.73
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	8	0.73
(1,170)	1:23:A:TYR:HD2	1:23:A:TYR:HA	10	0.73
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	3	0.73
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	4	0.73
(3,228)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	4	0.72
(3,228)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	10	0.72
(3,108)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	15	0.72
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	2	0.72
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	10	0.72
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	13	0.72
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	19	0.72
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG22	6	0.72
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	3	0.72
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	17	0.72
(1,1678)	1:80:A:LEU:HB2	1:80:A:LEU:H	12	0.72
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	1	0.72
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	12	0.72
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD13	19	0.72
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG22	19	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	19	0.72
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	6	0.72
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG21	3	0.72
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG21	15	0.72
(1,1019)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	16	0.72
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	7	0.72
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	3	0.72
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG22	3	0.72
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG21	1	0.72
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	10	0.72
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	9	0.72
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	20	0.72
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	5	0.72
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	17	0.72
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	9	0.72
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	9	0.72
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	14	0.72
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	4	0.72
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	11	0.72
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG22	14	0.72
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	3	0.71
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG23	20	0.71
(3,174)	1:19:A:ARG:HG3	1:19:A:ARG:H	15	0.71
(3,107)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	15	0.71
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	15	0.71
(1,2038)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	19	0.71
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	11	0.71
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	1	0.71
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG23	14	0.71
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	7	0.71
(1,1802)	1:56:A:ARG:H	1:56:A:ARG:HB3	5	0.71
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	13	0.71
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	7	0.71
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	3	0.71
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	6	0.71
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	15	0.71
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	19	0.71
(1,1059)	1:65:A:ILE:HG22	1:65:A:ILE:HA	2	0.71
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	5	0.71
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	20	0.71
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG22	16	0.71
(1,734)	1:102:A:MET:H	1:102:A:MET:HG2	19	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,656)	1:80:A:LEU:HB2	1:80:A:LEU:H	12	0.71
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	5	0.71
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	3	0.71
(1,378)	1:14:A:THR:HG23	1:14:A:THR:HA	7	0.71
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	8	0.71
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	10	0.71
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD11	19	0.71
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	19	0.71
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD12	1	0.71
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	4	0.7
(3,228)	1:7:A:ILE:HG22	1:84:A:LEU:HB3	9	0.7
(3,108)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	7	0.7
(3,68)	1:98:A:ILE:HB	1:111:A:ASN:HA	11	0.7
(3,8)	1:76:A:TYR:HB3	1:75:A:ALA:HB1	7	0.7
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG23	10	0.7
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG11	6	0.7
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG12	7	0.7
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	4	0.7
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	12	0.7
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	18	0.7
(1,1666)	1:76:A:TYR:H	1:75:A:ALA:HB2	16	0.7
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD11	8	0.7
(1,1215)	1:24:A:HIS:HA	1:34:A:VAL:HA	18	0.7
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG23	17	0.7
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	8	0.7
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG23	14	0.7
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	5	0.7
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	8	0.7
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	16	0.7
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD13	17	0.7
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG22	10	0.7
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	3	0.7
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	13	0.7
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	17	0.7
(1,453)	1:20:A:ILE:H	1:19:A:ARG:HB3	1	0.7
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	11	0.7
(1,290)	1:20:A:ILE:HD11	1:20:A:ILE:HB	11	0.7
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	20	0.7
(1,186)	1:48:A:LYS:HA	1:6:A:GLU:HA	19	0.7
(1,170)	1:23:A:TYR:HD2	1:23:A:TYR:HA	11	0.7
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	12	0.7
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	20	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	7	0.7
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	15	0.7
(1,45)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	12	0.7
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD12	4	0.7
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	5	0.7
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD12	8	0.7
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	20	0.7
(1,21)	1:7:A:ILE:HD12	1:8:A:GLU:H	17	0.7
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	19	0.69
(3,226)	1:87:A:LYS:HB3	1:7:A:ILE:HG23	9	0.69
(3,225)	1:10:A:VAL:HG22	1:42:A:THR:HA	6	0.69
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	3	0.69
(3,107)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	7	0.69
(3,106)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	7	0.69
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	14	0.69
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	17	0.69
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG21	18	0.69
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	7	0.69
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	11	0.69
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	8	0.69
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	1	0.69
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG12	19	0.69
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	6	0.69
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	9	0.69
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	15	0.69
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	1	0.69
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	20	0.69
(1,1310)	1:98:A:ILE:HD13	1:71:A:THR:HG23	17	0.69
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	7	0.69
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	7	0.69
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	14	0.69
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG23	18	0.69
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	19	0.69
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	2	0.69
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	13	0.69
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG22	6	0.69
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	7	0.69
(1,775)	1:56:A:ARG:H	1:56:A:ARG:HB3	5	0.69
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	7	0.69
(1,378)	1:14:A:THR:HG21	1:14:A:THR:HA	20	0.69
(1,254)	1:23:A:TYR:HB2	1:61:A:PHE:HD2	14	0.69
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	6	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	7	0.69
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	19	0.69
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	8	0.69
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	9	0.69
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	13	0.69
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	5	0.69
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	11	0.69
(3,228)	1:7:A:ILE:HG23	1:84:A:LEU:HB3	6	0.68
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HA	8	0.68
(3,10)	1:37:A:LEU:HA	1:20:A:ILE:HG22	20	0.68
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	10	0.68
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG11	6	0.68
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG12	7	0.68
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG12	19	0.68
(1,2097)	1:60:A:LEU:HB3	1:72:A:GLU:HA	17	0.68
(1,2048)	1:10:A:VAL:HG22	1:90:A:GLU:H	16	0.68
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	3	0.68
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	10	0.68
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	11	0.68
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	17	0.68
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG23	18	0.68
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	13	0.68
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	13	0.68
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	17	0.68
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG21	11	0.68
(1,1678)	1:80:A:LEU:HB2	1:80:A:LEU:H	17	0.68
(1,1177)	1:74:A:GLU:HA	1:74:A:GLU:HG2	18	0.68
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	16	0.68
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	4	0.68
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	14	0.68
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	18	0.68
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	19	0.68
(1,911)	1:34:A:VAL:HG23	1:24:A:HIS:HB3	5	0.68
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	7	0.68
(1,645)	1:76:A:TYR:H	1:75:A:ALA:HB2	16	0.68
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	2	0.68
(1,378)	1:14:A:THR:HG23	1:14:A:THR:HA	10	0.68
(1,378)	1:14:A:THR:HG21	1:14:A:THR:HA	14	0.68
(1,378)	1:14:A:THR:HG21	1:14:A:THR:HA	15	0.68
(1,254)	1:23:A:TYR:HB2	1:61:A:PHE:HD2	17	0.68
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	13	0.68
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	9	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	20	0.68
(1,40)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	5	0.68
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	6	0.68
(1,40)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	14	0.68
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	18	0.68
(3,256)	1:32:A:VAL:HG22	1:45:A:ILE:HG13	5	0.67
(3,228)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	3	0.67
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	18	0.67
(3,224)	1:92:A:SER:HB3	1:99:A:TYR:HB3	1	0.67
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	10	0.67
(3,167)	1:5:A:LYS:HG3	1:6:A:GLU:H	9	0.67
(3,44)	1:28:A:GLY:HA2	1:55:A:SER:HB2	14	0.67
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD12	14	0.67
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	9	0.67
(1,2220)	1:39:A:PHE:HD1	1:14:A:THR:HG22	10	0.67
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD11	18	0.67
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG11	9	0.67
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG13	11	0.67
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	20	0.67
(1,1949)	1:61:A:PHE:HE1	1:71:A:THR:HG22	17	0.67
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	12	0.67
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD12	4	0.67
(1,1666)	1:76:A:TYR:H	1:75:A:ALA:HB1	9	0.67
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	7	0.67
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG13	6	0.67
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	15	0.67
(1,1407)	1:10:A:VAL:HG12	1:10:A:VAL:H	13	0.67
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	1	0.67
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	15	0.67
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	4	0.67
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	11	0.67
(1,902)	1:61:A:PHE:HE2	1:71:A:THR:HG21	11	0.67
(1,881)	1:61:A:PHE:HD1	1:11:A:ILE:HG23	11	0.67
(1,881)	1:61:A:PHE:HD2	1:11:A:ILE:HG23	14	0.67
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG21	11	0.67
(1,656)	1:80:A:LEU:HB2	1:80:A:LEU:H	17	0.67
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	1	0.67
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	20	0.67
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	17	0.67
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	3	0.67
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	9	0.67
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	4	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	5	0.67
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD11	12	0.67
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	4	0.67
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	2	0.67
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	16	0.67
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD12	17	0.67
(3,326)	1:87:A:LYS:HB3	1:7:A:ILE:HG23	11	0.66
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	3	0.66
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG22	3	0.66
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG23	9	0.66
(3,10)	1:20:A:ILE:HG23	1:21:A:LEU:HA	15	0.66
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG21	8	0.66
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	5	0.66
(1,2048)	1:10:A:VAL:HG22	1:90:A:GLU:H	9	0.66
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	12	0.66
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	4	0.66
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	13	0.66
(1,1969)	1:62:A:ARG:HA	1:70:A:PHE:HA	11	0.66
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	2	0.66
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	7	0.66
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD12	7	0.66
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD12	6	0.66
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD12	18	0.66
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	13	0.66
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	11	0.66
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	11	0.66
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	7	0.66
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	20	0.66
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	1	0.66
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	4	0.66
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	12	0.66
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	18	0.66
(1,645)	1:76:A:TYR:H	1:75:A:ALA:HB1	9	0.66
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	16	0.66
(1,330)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	8	0.66
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	14	0.66
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG13	11	0.66
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	18	0.66
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	15	0.66
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	13	0.66
(1,85)	1:74:A:GLU:HA	1:74:A:GLU:HG2	6	0.66
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD11	7	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	11	0.66
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	19	0.66
(3,248)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	14	0.65
(3,245)	1:5:A:LYS:HA	1:5:A:LYS:HB3	1	0.65
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG22	7	0.65
(3,225)	1:10:A:VAL:HG21	1:42:A:THR:HA	5	0.65
(3,106)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	1	0.65
(3,35)	1:61:A:PHE:HZ	1:98:A:ILE:HG23	6	0.65
(3,35)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	20	0.65
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	13	0.65
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG11	9	0.65
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG13	11	0.65
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	17	0.65
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	9	0.65
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	16	0.65
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD13	14	0.65
(1,1877)	1:7:A:ILE:H	1:7:A:ILE:HG12	19	0.65
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.65
(1,1817)	1:112:A:LYS:H	1:111:A:ASN:HB2	3	0.65
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	11	0.65
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	3	0.65
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	10	0.65
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	1	0.65
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	4	0.65
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD13	2	0.65
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	3	0.65
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	9	0.65
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	15	0.65
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG23	14	0.65
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD12	4	0.65
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG13	6	0.65
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	15	0.65
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	1	0.65
(1,237)	1:62:A:ARG:HA	1:70:A:PHE:HA	18	0.65
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	15	0.65
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	6	0.65
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	7	0.65
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	12	0.65
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD13	7	0.65
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	11	0.65
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	20	0.65
(1,106)	1:9:A:ILE:HD13	1:9:A:ILE:HA	16	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD11	6	0.65
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	3	0.65
(1,40)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	8	0.65
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	15	0.65
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD11	4	0.65
(3,288)	1:6:A:GLU:HG2	1:6:A:GLU:H	11	0.64
(3,220)	1:44:A:ILE:HG23	1:8:A:GLU:HG2	18	0.64
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	5	0.64
(3,174)	1:19:A:ARG:HG3	1:19:A:ARG:H	7	0.64
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	3	0.64
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	19	0.64
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	4	0.64
(3,10)	1:20:A:ILE:HG22	1:21:A:LEU:HA	7	0.64
(1,2277)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	6	0.64
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	1	0.64
(1,2176)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	9	0.64
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	14	0.64
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	13	0.64
(1,1963)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	14	0.64
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	19	0.64
(1,1936)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	11	0.64
(1,1936)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	20	0.64
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	12	0.64
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD11	17	0.64
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	10	0.64
(1,1802)	1:56:A:ARG:H	1:56:A:ARG:HB3	10	0.64
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	4	0.64
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	13	0.64
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD2	3	0.64
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	19	0.64
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG12	9	0.64
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	15	0.64
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	20	0.64
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	7	0.64
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	11	0.64
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	6	0.64
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	11	0.64
(1,788)	1:112:A:LYS:H	1:111:A:ASN:HB2	3	0.64
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	11	0.64
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	7	0.64
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD12	7	0.64
(1,378)	1:14:A:THR:HG23	1:14:A:THR:HA	17	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	12	0.64
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD13	18	0.64
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	13	0.64
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	19	0.63
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	12	0.63
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	1	0.63
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG22	1	0.63
(3,225)	1:10:A:VAL:HG22	1:42:A:THR:HA	15	0.63
(3,220)	1:44:A:ILE:HG23	1:8:A:GLU:HG2	20	0.63
(3,168)	1:6:A:GLU:HG2	1:6:A:GLU:H	11	0.63
(3,97)	1:88:A:ARG:HB3	1:76:A:TYR:HB2	20	0.63
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG23	12	0.63
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	8	0.63
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD12	1	0.63
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	15	0.63
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	9	0.63
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	15	0.63
(1,1658)	1:73:A:VAL:HG22	1:74:A:GLU:H	8	0.63
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	16	0.63
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	20	0.63
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	16	0.63
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG13	16	0.63
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	10	0.63
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	1	0.63
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	2	0.63
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD11	18	0.63
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	9	0.63
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	10	0.63
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	18	0.63
(1,1005)	1:97:A:ALA:HB3	1:109:A:PRO:HB2	17	0.63
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	13	0.63
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	10	0.63
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD13	11	0.63
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	3	0.63
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	10	0.63
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	17	0.63
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	13	0.63
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	8	0.63
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	17	0.63
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	16	0.63
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD13	14	0.63
(1,844)	1:7:A:ILE:H	1:7:A:ILE:HG12	19	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	4	0.63
(1,775)	1:56:A:ARG:H	1:56:A:ARG:HB3	10	0.63
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	4	0.63
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	3	0.63
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	10	0.63
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	19	0.63
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	5	0.63
(1,170)	1:23:A:TYR:HD2	1:23:A:TYR:HA	15	0.63
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	13	0.63
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD13	7	0.63
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	10	0.63
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD13	7	0.63
(3,300)	1:53:A:GLU:HG3	1:53:A:GLU:H	6	0.62
(3,256)	1:32:A:VAL:HG21	1:45:A:ILE:HG12	16	0.62
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	19	0.62
(3,245)	1:5:A:LYS:HA	1:5:A:LYS:HB3	15	0.62
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	4	0.62
(3,219)	1:9:A:ILE:HG22	1:57:A:TRP:HB2	7	0.62
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	2	0.62
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	3	0.62
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	9	0.62
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	5	0.62
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	3	0.62
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD12	4	0.62
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	5	0.62
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD12	8	0.62
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	20	0.62
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	8	0.62
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG22	9	0.62
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	12	0.62
(1,1310)	1:98:A:ILE:HD11	1:71:A:THR:HG21	18	0.62
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD11	4	0.62
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	10	0.62
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	5	0.62
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD13	9	0.62
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	20	0.62
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	3	0.62
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG23	18	0.62
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	13	0.62
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	3	0.62
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	4	0.62
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	7	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	10	0.62
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	13	0.62
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	19	0.62
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD11	17	0.62
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	10	0.62
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	13	0.62
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD2	3	0.62
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	19	0.62
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG12	9	0.62
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	5	0.62
(1,350)	1:76:A:TYR:H	1:74:A:GLU:HB3	5	0.62
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	5	0.62
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	7	0.62
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	13	0.62
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	20	0.62
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG23	9	0.62
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	3	0.62
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	18	0.61
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	18	0.61
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG21	6	0.61
(3,228)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	11	0.61
(3,227)	1:7:A:ILE:HD11	1:87:A:LYS:HB2	13	0.61
(3,226)	1:87:A:LYS:HB3	1:7:A:ILE:HG23	11	0.61
(3,220)	1:44:A:ILE:HG21	1:8:A:GLU:HG2	14	0.61
(3,218)	1:11:A:ILE:HG23	1:59:A:CYS:HB2	16	0.61
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	19	0.61
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	17	0.61
(3,188)	1:53:A:GLU:HG3	1:53:A:GLU:H	6	0.61
(3,108)	1:44:A:ILE:HG21	1:8:A:GLU:HB2	11	0.61
(3,107)	1:44:A:ILE:HG21	1:8:A:GLU:HB2	11	0.61
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	18	0.61
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB3	2	0.61
(3,7)	1:23:A:TYR:H	1:11:A:ILE:HG23	12	0.61
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	9	0.61
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	11	0.61
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	8	0.61
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG23	3	0.61
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG22	16	0.61
(1,1738)	1:94:A:ARG:HB3	1:96:A:ASP:H	4	0.61
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	2	0.61
(1,1541)	1:20:A:ILE:HD11	1:38:A:ASN:H	12	0.61
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	8	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	1	0.61
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	5	0.61
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	12	0.61
(1,1102)	1:98:A:ILE:HD11	1:71:A:THR:HG22	14	0.61
(1,1045)	1:39:A:PHE:HD1	1:14:A:THR:HG22	10	0.61
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	8	0.61
(1,983)	1:60:A:LEU:HB3	1:72:A:GLU:HA	17	0.61
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	4	0.61
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	13	0.61
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	2	0.61
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	7	0.61
(1,909)	1:10:A:VAL:HG23	1:90:A:GLU:HG2	19	0.61
(1,902)	1:61:A:PHE:HE1	1:71:A:THR:HG22	17	0.61
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	12	0.61
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	1	0.61
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	2	0.61
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	5	0.61
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	14	0.61
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	20	0.61
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	15	0.61
(1,636)	1:73:A:VAL:HG22	1:74:A:GLU:H	8	0.61
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	16	0.61
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	20	0.61
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	16	0.61
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG13	16	0.61
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	10	0.61
(1,388)	1:65:A:ILE:HG23	1:65:A:ILE:HA	14	0.61
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	4	0.61
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	13	0.61
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	4	0.61
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB1	11	0.61
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	16	0.61
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	18	0.61
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB1	8	0.61
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	2	0.61
(1,37)	1:75:A:ALA:HB2	1:9:A:ILE:HG22	8	0.61
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	5	0.61
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD13	6	0.61
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG2	3	0.6
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	9	0.6
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	16	0.6
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	4	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	5	0.6
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG23	6	0.6
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	20	0.6
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	20	0.6
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	10	0.6
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	18	0.6
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	10	0.6
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG12	3	0.6
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	12	0.6
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	9	0.6
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD12	16	0.6
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	1	0.6
(1,1075)	1:19:A:ARG:HD2	1:19:A:ARG:HB2	6	0.6
(1,948)	1:10:A:VAL:HG22	1:90:A:GLU:H	16	0.6
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	17	0.6
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	10	0.6
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	13	0.6
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	9	0.6
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	9	0.6
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	15	0.6
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG22	9	0.6
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	12	0.6
(1,290)	1:20:A:ILE:HD11	1:20:A:ILE:HB	14	0.6
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	13	0.6
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	8	0.6
(1,94)	1:9:A:ILE:HG23	1:75:A:ALA:HA	19	0.6
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	7	0.6
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD11	18	0.6
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	5	0.59
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	12	0.59
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG23	9	0.59
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	1	0.59
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	9	0.59
(3,154)	1:19:A:ARG:HG3	1:19:A:ARG:H	15	0.59
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	20	0.59
(1,2176)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	12	0.59
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	3	0.59
(1,2048)	1:10:A:VAL:HG22	1:90:A:GLU:H	12	0.59
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	2	0.59
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD12	17	0.59
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD12	5	0.59
(1,1658)	1:73:A:VAL:HG22	1:74:A:GLU:H	4	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	10	0.59
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	18	0.59
(1,1541)	1:20:A:ILE:HD13	1:38:A:ASN:H	7	0.59
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG12	19	0.59
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD1	4	0.59
(1,1361)	1:35:A:GLN:HA	1:36:A:TYR:HD1	10	0.59
(1,1255)	1:45:A:ILE:HA	1:45:A:ILE:HD13	16	0.59
(1,1238)	1:11:A:ILE:HD12	1:11:A:ILE:HB	3	0.59
(1,1238)	1:11:A:ILE:HD12	1:11:A:ILE:HB	5	0.59
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	9	0.59
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	13	0.59
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	19	0.59
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD12	1	0.59
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	14	0.59
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	1	0.59
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	8	0.59
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	15	0.59
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	16	0.59
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	12	0.59
(1,914)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	14	0.59
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	14	0.59
(1,909)	1:10:A:VAL:HG22	1:90:A:GLU:HG2	12	0.59
(1,896)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	11	0.59
(1,896)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	20	0.59
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	12	0.59
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	6	0.59
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	11	0.59
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	17	0.59
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG23	3	0.59
(1,711)	1:94:A:ARG:HB3	1:96:A:ASP:H	4	0.59
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	2	0.59
(1,525)	1:20:A:ILE:HD11	1:38:A:ASN:H	12	0.59
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	1	0.59
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	5	0.59
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE1	9	0.59
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	1	0.59
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG22	15	0.59
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG23	20	0.59
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB2	13	0.59
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD13	1	0.59
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	10	0.59
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB3	16	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	10	0.59
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	11	0.59
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD12	16	0.59
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	9	0.58
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	19	0.58
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG23	11	0.58
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	13	0.58
(3,231)	1:14:A:THR:HB	1:19:A:ARG:HG3	1	0.58
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	2	0.58
(3,225)	1:10:A:VAL:HG21	1:42:A:THR:HA	16	0.58
(3,220)	1:44:A:ILE:HG23	1:8:A:GLU:HG2	12	0.58
(3,219)	1:9:A:ILE:HG21	1:57:A:TRP:HB2	12	0.58
(3,218)	1:11:A:ILE:HG21	1:37:A:LEU:HB2	18	0.58
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	8	0.58
(3,146)	1:74:A:GLU:HA	1:76:A:TYR:H	11	0.58
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	13	0.58
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	20	0.58
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	20	0.58
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	18	0.58
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	10	0.58
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	1	0.58
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	10	0.58
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD11	7	0.58
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	11	0.58
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	16	0.58
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	16	0.58
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	3	0.58
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	10	0.58
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG21	16	0.58
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG21	20	0.58
(1,1658)	1:73:A:VAL:HG22	1:74:A:GLU:H	5	0.58
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	7	0.58
(1,1541)	1:20:A:ILE:HD12	1:38:A:ASN:H	3	0.58
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	4	0.58
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	9	0.58
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	2	0.58
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	6	0.58
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	7	0.58
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	15	0.58
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	9	0.58
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD12	4	0.58
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	5	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD12	8	0.58
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	15	0.58
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	12	0.58
(1,948)	1:10:A:VAL:HG22	1:90:A:GLU:H	9	0.58
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	15	0.58
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	19	0.58
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG22	16	0.58
(1,847)	1:7:A:ILE:H	1:48:A:LYS:HA	19	0.58
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	18	0.58
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	10	0.58
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	8	0.58
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG12	3	0.58
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	12	0.58
(1,388)	1:65:A:ILE:HG23	1:65:A:ILE:HA	18	0.58
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	18	0.58
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	5	0.58
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD11	5	0.58
(3,264)	1:76:A:TYR:HB3	1:75:A:ALA:HB1	7	0.57
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	17	0.57
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG13	17	0.57
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG23	2	0.57
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	9	0.57
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	7	0.57
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	17	0.57
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	16	0.57
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HA	11	0.57
(3,10)	1:37:A:LEU:HA	1:20:A:ILE:HG23	17	0.57
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	1	0.57
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	6	0.57
(1,2048)	1:10:A:VAL:HG22	1:90:A:GLU:H	8	0.57
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD11	6	0.57
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	11	0.57
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	3	0.57
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	5	0.57
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	12	0.57
(1,1577)	1:9:A:ILE:HG12	1:46:A:LYS:H	5	0.57
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	15	0.57
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	20	0.57
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	16	0.57
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	19	0.57
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	20	0.57
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	8	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	9	0.57
(1,636)	1:73:A:VAL:HG22	1:74:A:GLU:H	4	0.57
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	10	0.57
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	18	0.57
(1,525)	1:20:A:ILE:HD13	1:38:A:ASN:H	7	0.57
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG12	19	0.57
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD1	4	0.57
(1,388)	1:65:A:ILE:HG23	1:65:A:ILE:HA	1	0.57
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	3	0.57
(1,370)	1:102:A:MET:H	1:102:A:MET:HG2	19	0.57
(1,273)	1:73:A:VAL:HG22	1:73:A:VAL:HA	11	0.57
(1,170)	1:23:A:TYR:HD2	1:23:A:TYR:HA	14	0.57
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	1	0.57
(1,140)	1:45:A:ILE:HD11	1:9:A:ILE:HD12	15	0.57
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB1	3	0.57
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	8	0.57
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	1	0.57
(1,21)	1:7:A:ILE:HD12	1:8:A:GLU:H	4	0.57
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD13	7	0.57
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	4	0.56
(3,309)	1:103:A:ASP:HB3	1:104:A:GLU:H	2	0.56
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	14	0.56
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	18	0.56
(3,258)	1:57:A:TRP:HB2	1:75:A:ALA:HB3	4	0.56
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	14	0.56
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	16	0.56
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG21	20	0.56
(3,245)	1:5:A:LYS:HA	1:5:A:LYS:HB3	17	0.56
(3,237)	1:45:A:ILE:HA	1:44:A:ILE:HG23	18	0.56
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	18	0.56
(3,224)	1:92:A:SER:HB3	1:99:A:TYR:HB3	20	0.56
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	9	0.56
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	19	0.56
(3,160)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	17	0.56
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	12	0.56
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	15	0.56
(3,62)	1:72:A:GLU:HB3	1:71:A:THR:HA	14	0.56
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	2	0.56
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	2	0.56
(3,10)	1:20:A:ILE:HG23	1:21:A:LEU:HA	6	0.56
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG23	2	0.56
(3,1)	1:76:A:TYR:HB3	1:9:A:ILE:HD12	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	5	0.56
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	18	0.56
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	15	0.56
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	1	0.56
(1,1658)	1:73:A:VAL:HG22	1:74:A:GLU:H	18	0.56
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	6	0.56
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	15	0.56
(1,1577)	1:9:A:ILE:HG12	1:46:A:LYS:H	19	0.56
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	4	0.56
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	8	0.56
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG12	11	0.56
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG21	10	0.56
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	11	0.56
(1,1277)	1:1:A:ALA:HB3	1:83:A:PRO:HA	15	0.56
(1,1238)	1:11:A:ILE:HD12	1:11:A:ILE:HB	1	0.56
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	4	0.56
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	11	0.56
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	12	0.56
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD13	17	0.56
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	7	0.56
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	15	0.56
(1,1137)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	12	0.56
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	4	0.56
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	11	0.56
(1,1018)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	9	0.56
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	9	0.56
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	14	0.56
(1,913)	1:15:A:LEU:HD12	1:19:A:ARG:HB3	5	0.56
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	13	0.56
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD12	5	0.56
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG21	20	0.56
(1,636)	1:73:A:VAL:HG22	1:74:A:GLU:H	5	0.56
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	7	0.56
(1,525)	1:20:A:ILE:HD12	1:38:A:ASN:H	3	0.56
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	4	0.56
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	9	0.56
(1,388)	1:65:A:ILE:HG21	1:65:A:ILE:HA	11	0.56
(1,378)	1:14:A:THR:HG22	1:14:A:THR:HA	12	0.56
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	7	0.56
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB2	16	0.56
(1,106)	1:9:A:ILE:HD13	1:9:A:ILE:HA	1	0.56
(1,85)	1:74:A:GLU:HA	1:74:A:GLU:HG2	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,74)	1:1:A:ALA:HB1	1:83:A:PRO:HA	20	0.56
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	9	0.56
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	9	0.56
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD13	10	0.56
(1,40)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	1	0.56
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	16	0.56
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD13	17	0.56
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD13	11	0.56
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	18	0.55
(3,288)	1:6:A:GLU:HG2	1:6:A:GLU:H	6	0.55
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG21	17	0.55
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	16	0.55
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	17	0.55
(3,202)	1:103:A:ASP:HB3	1:104:A:GLU:H	2	0.55
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	8	0.55
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	10	0.55
(3,107)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	5	0.55
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	5	0.55
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	16	0.55
(3,97)	1:88:A:ARG:HB3	1:76:A:TYR:HB2	19	0.55
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	6	0.55
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	16	0.55
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	3	0.55
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	14	0.55
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	5	0.55
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	5	0.55
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	15	0.55
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	12	0.55
(3,10)	1:20:A:ILE:HG23	1:21:A:LEU:HA	9	0.55
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	2	0.55
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	15	0.55
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	5	0.55
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	19	0.55
(1,2048)	1:10:A:VAL:HG21	1:90:A:GLU:H	2	0.55
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG12	14	0.55
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG23	15	0.55
(1,1927)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	1	0.55
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	7	0.55
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	19	0.55
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	14	0.55
(1,1547)	1:39:A:PHE:HD1	1:39:A:PHE:H	5	0.55
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	8	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	12	0.55
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	14	0.55
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	16	0.55
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD11	19	0.55
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	3	0.55
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	15	0.55
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	13	0.55
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	5	0.55
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	20	0.55
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	2	0.55
(1,1037)	1:73:A:VAL:HG22	1:91:A:LEU:HB3	3	0.55
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	20	0.55
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	1	0.55
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	12	0.55
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	17	0.55
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	8	0.55
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	12	0.55
(1,558)	1:9:A:ILE:HG12	1:46:A:LYS:H	5	0.55
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	15	0.55
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	20	0.55
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	14	0.55
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	2	0.55
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	5	0.55
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	6	0.55
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	9	0.55
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	10	0.55
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	11	0.55
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	15	0.55
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	16	0.55
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	20	0.55
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	20	0.55
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	19	0.55
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD12	19	0.55
(1,106)	1:9:A:ILE:HD12	1:9:A:ILE:HA	12	0.55
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD11	15	0.55
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	3	0.55
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	19	0.55
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD11	13	0.55
(3,326)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	12	0.54
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	12	0.54
(3,288)	1:6:A:GLU:HG2	1:6:A:GLU:H	12	0.54
(3,257)	1:93:A:ALA:HB3	1:98:A:ILE:HG13	14	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,242)	1:90:A:GLU:HA	1:10:A:VAL:HG21	3	0.54
(3,224)	1:92:A:SER:HB2	1:99:A:TYR:HB3	3	0.54
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	13	0.54
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	14	0.54
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	18	0.54
(3,147)	1:5:A:LYS:HG3	1:6:A:GLU:H	9	0.54
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	8	0.54
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	20	0.54
(3,63)	1:104:A:GLU:HG2	1:104:A:GLU:HA	1	0.54
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD12	16	0.54
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	4	0.54
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	15	0.54
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	4	0.54
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	15	0.54
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	11	0.54
(3,27)	1:5:A:LYS:HG2	1:5:A:LYS:HA	20	0.54
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	17	0.54
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	1	0.54
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG12	14	0.54
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	17	0.54
(1,2048)	1:10:A:VAL:HG21	1:90:A:GLU:H	1	0.54
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	13	0.54
(1,1954)	1:90:A:GLU:HA	1:10:A:VAL:HG23	13	0.54
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG23	3	0.54
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	4	0.54
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG21	13	0.54
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	15	0.54
(1,1816)	1:113:A:TRP:H	1:112:A:LYS:HB2	16	0.54
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	15	0.54
(1,1541)	1:20:A:ILE:HD11	1:38:A:ASN:H	16	0.54
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG11	15	0.54
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	4	0.54
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD2	13	0.54
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	8	0.54
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	14	0.54
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	6	0.54
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	19	0.54
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	9	0.54
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	11	0.54
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	16	0.54
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD12	17	0.54
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	18	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	20	0.54
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	3	0.54
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	16	0.54
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	19	0.54
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD11	8	0.54
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	10	0.54
(1,909)	1:10:A:VAL:HG22	1:90:A:GLU:HG2	5	0.54
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD13	6	0.54
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	8	0.54
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	10	0.54
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	6	0.54
(1,636)	1:73:A:VAL:HG22	1:74:A:GLU:H	18	0.54
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	6	0.54
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	15	0.54
(1,558)	1:9:A:ILE:HG12	1:46:A:LYS:H	19	0.54
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	4	0.54
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	8	0.54
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG12	11	0.54
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG21	10	0.54
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	11	0.54
(1,388)	1:65:A:ILE:HG21	1:65:A:ILE:HA	4	0.54
(1,253)	1:23:A:TYR:HB2	1:61:A:PHE:HE1	18	0.54
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	10	0.54
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	1	0.54
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	3	0.54
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	4	0.54
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	8	0.54
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	12	0.54
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	13	0.54
(1,179)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	17	0.54
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	18	0.54
(1,170)	1:23:A:TYR:HD1	1:23:A:TYR:HA	16	0.54
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	13	0.54
(1,140)	1:45:A:ILE:HD11	1:9:A:ILE:HD11	3	0.54
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	4	0.54
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	20	0.54
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD13	15	0.54
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	13	0.54
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	1	0.54
(1,85)	1:74:A:GLU:HA	1:74:A:GLU:HG2	14	0.54
(1,44)	1:7:A:ILE:HB	1:7:A:ILE:HD11	3	0.54
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	7	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	17	0.54
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	2	0.53
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	5	0.53
(3,300)	1:53:A:GLU:HG2	1:53:A:GLU:H	2	0.53
(3,289)	1:48:A:LYS:HB3	1:6:A:GLU:H	9	0.53
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	20	0.53
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG13	3	0.53
(3,251)	1:99:A:TYR:HA	1:109:A:PRO:HB3	15	0.53
(3,228)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	1	0.53
(3,225)	1:10:A:VAL:HG23	1:42:A:THR:HA	20	0.53
(3,220)	1:44:A:ILE:HG21	1:8:A:GLU:HG2	16	0.53
(3,219)	1:9:A:ILE:HG23	1:76:A:TYR:HB2	14	0.53
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	18	0.53
(3,168)	1:6:A:GLU:HG2	1:6:A:GLU:H	6	0.53
(3,168)	1:6:A:GLU:HG2	1:6:A:GLU:H	12	0.53
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	5	0.53
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	19	0.53
(3,108)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	10	0.53
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	11	0.53
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	8	0.53
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	9	0.53
(3,10)	1:20:A:ILE:HG23	1:21:A:LEU:HA	16	0.53
(3,1)	1:57:A:TRP:HB2	1:9:A:ILE:HD13	10	0.53
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	13	0.53
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	12	0.53
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	14	0.53
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG11	2	0.53
(1,1995)	1:24:A:HIS:HA	1:34:A:VAL:HA	18	0.53
(1,1961)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	2	0.53
(1,1935)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	18	0.53
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	4	0.53
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	2	0.53
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	10	0.53
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	11	0.53
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	7	0.53
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD12	18	0.53
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.53
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG22	1	0.53
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	6	0.53
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	9	0.53
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	9	0.53
(1,1658)	1:73:A:VAL:HG22	1:74:A:GLU:H	17	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	5	0.53
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD11	18	0.53
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	19	0.53
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	6	0.53
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG21	17	0.53
(1,1238)	1:11:A:ILE:HD11	1:11:A:ILE:HB	12	0.53
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	18	0.53
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	20	0.53
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	2	0.53
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	6	0.53
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	7	0.53
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	13	0.53
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	4	0.53
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD11	6	0.53
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD11	7	0.53
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG21	15	0.53
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	3	0.53
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	18	0.53
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	3	0.53
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	16	0.53
(1,930)	1:12:A:LYS:HB3	1:92:A:SER:HB3	17	0.53
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	12	0.53
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD13	5	0.53
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	18	0.53
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	12	0.53
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	19	0.53
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	14	0.53
(1,531)	1:39:A:PHE:HD1	1:39:A:PHE:H	5	0.53
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG11	15	0.53
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	8	0.53
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	12	0.53
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	14	0.53
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	16	0.53
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD2	13	0.53
(1,388)	1:65:A:ILE:HG21	1:65:A:ILE:HA	17	0.53
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	2	0.53
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	14	0.53
(1,179)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	19	0.53
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	18	0.53
(1,156)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	15	0.53
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG23	4	0.53
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG21	16	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	10	0.53
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB2	2	0.53
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	18	0.53
(1,51)	1:98:A:ILE:HG21	1:92:A:SER:H	1	0.53
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	9	0.53
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD11	3	0.53
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	16	0.53
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB3	6	0.52
(3,297)	1:47:A:PHE:HB3	1:48:A:LYS:H	5	0.52
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	13	0.52
(3,256)	1:32:A:VAL:HG22	1:45:A:ILE:HG12	6	0.52
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG23	8	0.52
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	7	0.52
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG2	7	0.52
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG2	13	0.52
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	12	0.52
(3,154)	1:19:A:ARG:HG3	1:19:A:ARG:H	7	0.52
(3,107)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	10	0.52
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	10	0.52
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	10	0.52
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	12	0.52
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	10	0.52
(3,63)	1:104:A:GLU:HG3	1:104:A:GLU:HA	9	0.52
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	7	0.52
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	10	0.52
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	10	0.52
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	13	0.52
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	17	0.52
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB1	1	0.52
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	4	0.52
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG11	2	0.52
(1,2048)	1:10:A:VAL:HG21	1:90:A:GLU:H	20	0.52
(1,1930)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	15	0.52
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	12	0.52
(1,1816)	1:113:A:TRP:H	1:112:A:LYS:HB2	6	0.52
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	4	0.52
(1,1699)	1:7:A:ILE:HD11	1:87:A:LYS:H	20	0.52
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	12	0.52
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	11	0.52
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG13	14	0.52
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	6	0.52
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	17	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	10	0.52
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD11	12	0.52
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	19	0.52
(1,1177)	1:74:A:GLU:HA	1:74:A:GLU:HG2	6	0.52
(1,1132)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	5	0.52
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	6	0.52
(1,1132)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	14	0.52
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	12	0.52
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	14	0.52
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD11	16	0.52
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG21	10	0.52
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	11	0.52
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	16	0.52
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	15	0.52
(1,786)	1:113:A:TRP:H	1:112:A:LYS:HB2	16	0.52
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	15	0.52
(1,525)	1:20:A:ILE:HD11	1:38:A:ASN:H	16	0.52
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	4	0.52
(1,388)	1:65:A:ILE:HG23	1:65:A:ILE:HA	16	0.52
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD2	3	0.52
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG21	3	0.52
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG23	10	0.52
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB1	10	0.52
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	4	0.52
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	14	0.52
(1,85)	1:74:A:GLU:HA	1:74:A:GLU:HG2	2	0.52
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	1	0.52
(1,72)	1:109:A:PRO:HB3	1:97:A:ALA:HB2	14	0.52
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	18	0.52
(1,45)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	5	0.52
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	6	0.52
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD11	15	0.52
(1,21)	1:7:A:ILE:HD12	1:8:A:GLU:H	1	0.52
(3,332)	1:69:A:PHE:HA	1:115:A:SER:HB3	2	0.51
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	10	0.51
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG23	10	0.51
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	12	0.51
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	4	0.51
(3,188)	1:53:A:GLU:HG2	1:53:A:GLU:H	2	0.51
(3,185)	1:47:A:PHE:HB3	1:48:A:LYS:H	5	0.51
(3,169)	1:48:A:LYS:HB3	1:6:A:GLU:H	9	0.51
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	20	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,167)	1:5:A:LYS:HG3	1:6:A:GLU:H	20	0.51
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.51
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	14	0.51
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	20	0.51
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	4	0.51
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	10	0.51
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	19	0.51
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	16	0.51
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	7	0.51
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	1	0.51
(1,1935)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	13	0.51
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	8	0.51
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	9	0.51
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG21	20	0.51
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	1	0.51
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.51
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	14	0.51
(1,1816)	1:113:A:TRP:H	1:112:A:LYS:HB2	11	0.51
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	5	0.51
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	11	0.51
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	8	0.51
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	18	0.51
(1,1541)	1:20:A:ILE:HD12	1:38:A:ASN:H	19	0.51
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	15	0.51
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	20	0.51
(1,1361)	1:35:A:GLN:HA	1:36:A:TYR:HD1	15	0.51
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	19	0.51
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	15	0.51
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD13	7	0.51
(1,1097)	1:10:A:VAL:HG23	1:10:A:VAL:HA	3	0.51
(1,1018)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	12	0.51
(1,927)	1:69:A:PHE:HA	1:115:A:SER:HB2	8	0.51
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	1	0.51
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	4	0.51
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD11	15	0.51
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	18	0.51
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG22	2	0.51
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD11	14	0.51
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	7	0.51
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG21	16	0.51
(1,866)	1:62:A:ARG:H	1:21:A:LEU:HB2	11	0.51
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	7	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD12	18	0.51
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	8	0.51
(1,786)	1:113:A:TRP:H	1:112:A:LYS:HB2	6	0.51
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG22	1	0.51
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	6	0.51
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	9	0.51
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	9	0.51
(1,636)	1:73:A:VAL:HG22	1:74:A:GLU:H	17	0.51
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	5	0.51
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD11	18	0.51
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	19	0.51
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	6	0.51
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG21	17	0.51
(1,388)	1:65:A:ILE:HG21	1:65:A:ILE:HA	12	0.51
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	13	0.51
(1,298)	1:34:A:VAL:HG21	1:24:A:HIS:HE1	6	0.51
(1,253)	1:23:A:TYR:HB2	1:61:A:PHE:HE2	17	0.51
(1,153)	1:61:A:PHE:HD1	1:71:A:THR:HG21	19	0.51
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	1	0.51
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	5	0.51
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	7	0.51
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD12	11	0.51
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD11	15	0.51
(1,94)	1:9:A:ILE:HG21	1:75:A:ALA:HA	15	0.51
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG22	6	0.51
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	13	0.51
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	3	0.51
(1,39)	1:45:A:ILE:HA	1:45:A:ILE:HG12	7	0.51
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD13	18	0.51
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD12	10	0.51
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	19	0.51
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	13	0.5
(3,310)	1:105:A:ARG:H	1:103:A:ASP:HB2	18	0.5
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG23	13	0.5
(3,256)	1:32:A:VAL:HG23	1:45:A:ILE:HG13	7	0.5
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG21	6	0.5
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	8	0.5
(3,218)	1:11:A:ILE:HG22	1:59:A:CYS:HB2	10	0.5
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB3	6	0.5
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	5	0.5
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	3	0.5
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.5
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	9	0.5
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	9	0.5
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	6	0.5
(3,6)	1:9:A:ILE:H	1:9:A:ILE:HG22	1	0.5
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG23	9	0.5
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	6	0.5
(1,2050)	1:73:A:VAL:HG22	1:73:A:VAL:HA	11	0.5
(1,2048)	1:10:A:VAL:HG23	1:90:A:GLU:H	19	0.5
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	7	0.5
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	13	0.5
(1,1936)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	18	0.5
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	15	0.5
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	15	0.5
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD12	3	0.5
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD11	12	0.5
(1,1816)	1:113:A:TRP:H	1:112:A:LYS:HB2	19	0.5
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG23	8	0.5
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG23	19	0.5
(1,1658)	1:73:A:VAL:HG23	1:74:A:GLU:H	1	0.5
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD2	2	0.5
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	13	0.5
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	6	0.5
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	14	0.5
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	17	0.5
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	11	0.5
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	20	0.5
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	16	0.5
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	11	0.5
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	9	0.5
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG13	11	0.5
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	13	0.5
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	19	0.5
(1,1102)	1:98:A:ILE:HD11	1:71:A:THR:HG23	9	0.5
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	5	0.5
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	10	0.5
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	5	0.5
(1,1005)	1:97:A:ALA:HB1	1:109:A:PRO:HB2	18	0.5
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	1	0.5
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	10	0.5
(1,948)	1:10:A:VAL:HG22	1:90:A:GLU:H	12	0.5
(1,919)	1:70:A:PHE:HE2	1:70:A:PHE:HA	11	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	9	0.5
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	17	0.5
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	1	0.5
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	3	0.5
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	5	0.5
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	18	0.5
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	12	0.5
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	14	0.5
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	4	0.5
(1,677)	1:7:A:ILE:HD11	1:87:A:LYS:H	20	0.5
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	12	0.5
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	11	0.5
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	6	0.5
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	5	0.5
(1,336)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	18	0.5
(1,310)	1:39:A:PHE:HD1	1:14:A:THR:HA	18	0.5
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE1	12	0.5
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	7	0.5
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	17	0.5
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG22	1	0.5
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	11	0.5
(1,140)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	10	0.5
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	7	0.5
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB2	9	0.5
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	8	0.5
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD11	7	0.5
(1,106)	1:9:A:ILE:HD12	1:9:A:ILE:HA	3	0.5
(1,106)	1:9:A:ILE:HD11	1:9:A:ILE:HA	13	0.5
(1,94)	1:9:A:ILE:HG23	1:75:A:ALA:HA	5	0.5
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB1	19	0.5
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	11	0.5
(1,51)	1:98:A:ILE:HG22	1:92:A:SER:H	19	0.5
(1,40)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	12	0.5
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	13	0.5
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	9	0.5
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	8	0.5
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	3	0.5
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	1	0.5
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	5	0.5
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG22	13	0.5
(4,43)	1:37:A:LEU:O	1:21:A:LEU:N	15	0.49
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	9	0.49
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	12	0.49
(3,288)	1:6:A:GLU:HG2	1:6:A:GLU:H	2	0.49
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	5	0.49
(3,227)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	19	0.49
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG23	2	0.49
(3,226)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	12	0.49
(3,220)	1:44:A:ILE:HG23	1:8:A:GLU:HG2	1	0.49
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	10	0.49
(3,137)	1:11:A:ILE:H	1:11:A:ILE:HD12	17	0.49
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD11	10	0.49
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	3	0.49
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	8	0.49
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	18	0.49
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB2	17	0.49
(3,15)	1:84:A:LEU:HA	1:85:A:CYS:HB3	4	0.49
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG21	7	0.49
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	10	0.49
(1,2144)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	19	0.49
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	15	0.49
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	15	0.49
(1,2048)	1:10:A:VAL:HG22	1:90:A:GLU:H	5	0.49
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	3	0.49
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	18	0.49
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	10	0.49
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD12	13	0.49
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	14	0.49
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	18	0.49
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	10	0.49
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG22	16	0.49
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG22	12	0.49
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	5	0.49
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	12	0.49
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	19	0.49
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	20	0.49
(1,1389)	1:85:A:CYS:HB2	1:5:A:LYS:H	12	0.49
(1,1238)	1:11:A:ILE:HD13	1:11:A:ILE:HB	17	0.49
(1,1230)	1:9:A:ILE:HD13	1:9:A:ILE:HA	16	0.49
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	1	0.49
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	3	0.49
(1,1132)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	8	0.49
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	15	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:73:A:VAL:HG21	1:91:A:LEU:HB3	13	0.49
(1,1019)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	1	0.49
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	6	0.49
(1,948)	1:10:A:VAL:HG22	1:90:A:GLU:H	8	0.49
(1,911)	1:34:A:VAL:HG21	1:24:A:HIS:HB3	2	0.49
(1,909)	1:10:A:VAL:HG22	1:90:A:GLU:HG2	16	0.49
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG23	15	0.49
(1,889)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	1	0.49
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	1	0.49
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG22	2	0.49
(1,786)	1:113:A:TRP:H	1:112:A:LYS:HB2	11	0.49
(1,786)	1:113:A:TRP:H	1:112:A:LYS:HB2	19	0.49
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	5	0.49
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG23	19	0.49
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	11	0.49
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	8	0.49
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	18	0.49
(1,525)	1:20:A:ILE:HD12	1:38:A:ASN:H	19	0.49
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG13	14	0.49
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	15	0.49
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	20	0.49
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	15	0.49
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	4	0.49
(1,232)	1:104:A:GLU:HA	1:104:A:GLU:HB2	6	0.49
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	6	0.49
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	12	0.49
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD2	11	0.49
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG22	12	0.49
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	6	0.49
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	10	0.49
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	14	0.49
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	18	0.49
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	5	0.49
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	8	0.49
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	19	0.49
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD11	14	0.49
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD11	9	0.49
(1,106)	1:9:A:ILE:HD13	1:9:A:ILE:HA	7	0.49
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	19	0.49
(1,75)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	18	0.49
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB2	14	0.49
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	9	0.49
(1,40)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	17	0.49
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	18	0.49
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	10	0.49
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD11	13	0.49
(1,21)	1:7:A:ILE:HD13	1:8:A:GLU:H	2	0.49
(1,21)	1:7:A:ILE:HD13	1:8:A:GLU:H	5	0.49
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD13	1	0.49
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG21	2	0.49
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	7	0.49
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG23	18	0.49
(4,33)	1:26:A:ARG:O	1:58:A:ASN:N	20	0.48
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	6	0.48
(3,317)	1:47:A:PHE:H	1:8:A:GLU:HG3	7	0.48
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB2	11	0.48
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	5	0.48
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	20	0.48
(3,288)	1:6:A:GLU:HG2	1:6:A:GLU:H	17	0.48
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG13	10	0.48
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	4	0.48
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG21	7	0.48
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	5	0.48
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	20	0.48
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	19	0.48
(3,203)	1:105:A:ARG:H	1:103:A:ASP:HB2	18	0.48
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HG2	6	0.48
(3,192)	1:86:A:GLY:H	1:5:A:LYS:HB3	6	0.48
(3,168)	1:6:A:GLU:HG2	1:6:A:GLU:H	2	0.48
(3,108)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	20	0.48
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	7	0.48
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.48
(3,63)	1:104:A:GLU:HG2	1:104:A:GLU:HA	12	0.48
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	7	0.48
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	16	0.48
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	7	0.48
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	16	0.48
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	14	0.48
(3,34)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	8	0.48
(3,15)	1:84:A:LEU:HA	1:85:A:CYS:HB3	9	0.48
(3,10)	1:37:A:LEU:HA	1:20:A:ILE:HG22	11	0.48
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG23	17	0.48
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	15	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	4	0.48
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	13	0.48
(1,2121)	1:36:A:TYR:HA	1:20:A:ILE:HG22	10	0.48
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	15	0.48
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	9	0.48
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD13	10	0.48
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	5	0.48
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	11	0.48
(1,1935)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	2	0.48
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	9	0.48
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	12	0.48
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	16	0.48
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG23	15	0.48
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG23	20	0.48
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	5	0.48
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	10	0.48
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	15	0.48
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD11	9	0.48
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG12	10	0.48
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	9	0.48
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	6	0.48
(1,1408)	1:10:A:VAL:HG22	1:10:A:VAL:H	12	0.48
(1,1292)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	19	0.48
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD13	7	0.48
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	7	0.48
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	1	0.48
(1,1054)	1:10:A:VAL:HG22	1:42:A:THR:HG22	3	0.48
(1,1052)	1:73:A:VAL:HG22	1:111:A:ASN:HB2	5	0.48
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	5	0.48
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	18	0.48
(1,1037)	1:73:A:VAL:HG23	1:91:A:LEU:HB3	8	0.48
(1,1037)	1:73:A:VAL:HG21	1:91:A:LEU:HB3	20	0.48
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	13	0.48
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	6	0.48
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	13	0.48
(1,906)	1:90:A:GLU:HA	1:10:A:VAL:HG23	13	0.48
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	7	0.48
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	10	0.48
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD12	3	0.48
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD11	12	0.48
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	14	0.48
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	18	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG23	8	0.48
(1,636)	1:73:A:VAL:HG23	1:74:A:GLU:H	1	0.48
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD2	2	0.48
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	5	0.48
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	13	0.48
(1,298)	1:34:A:VAL:HG21	1:24:A:HIS:HE1	10	0.48
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE1	7	0.48
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	4	0.48
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	14	0.48
(1,156)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	8	0.48
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	2	0.48
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	15	0.48
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	7	0.48
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	15	0.48
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	20	0.48
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	1	0.48
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	8	0.48
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD11	4	0.48
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	10	0.48
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD11	12	0.48
(1,106)	1:9:A:ILE:HD13	1:9:A:ILE:HA	15	0.48
(1,94)	1:9:A:ILE:HG23	1:75:A:ALA:HA	9	0.48
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	2	0.48
(1,11)	1:73:A:VAL:HG21	1:98:A:ILE:HD11	13	0.48
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	4	0.48
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG22	9	0.48
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	15	0.48
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	17	0.47
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB3	9	0.47
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	1	0.47
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG23	11	0.47
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG21	15	0.47
(3,246)	1:5:A:LYS:HG3	1:5:A:LYS:HA	3	0.47
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	11	0.47
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG3	1	0.47
(3,225)	1:10:A:VAL:HG22	1:42:A:THR:HA	14	0.47
(3,224)	1:92:A:SER:HB3	1:99:A:TYR:HB3	5	0.47
(3,219)	1:9:A:ILE:HG21	1:76:A:TYR:HB2	1	0.47
(3,219)	1:9:A:ILE:HG23	1:76:A:TYR:HB2	8	0.47
(3,218)	1:11:A:ILE:HG22	1:37:A:LEU:HB2	4	0.47
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	20	0.47
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	9	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	12	0.47
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	4	0.47
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG23	10	0.47
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	9	0.47
(3,107)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	20	0.47
(3,106)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	20	0.47
(3,63)	1:104:A:GLU:HG3	1:104:A:GLU:HA	2	0.47
(3,51)	1:11:A:ILE:HD13	1:75:A:ALA:HA	11	0.47
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	11	0.47
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	11	0.47
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	11	0.47
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	8	0.47
(1,2048)	1:10:A:VAL:HG21	1:90:A:GLU:H	4	0.47
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD11	15	0.47
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	7	0.47
(1,1998)	1:32:A:VAL:HG22	1:32:A:VAL:HA	20	0.47
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	13	0.47
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG23	18	0.47
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	11	0.47
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	11	0.47
(1,1541)	1:20:A:ILE:HD13	1:38:A:ASN:H	6	0.47
(1,1541)	1:20:A:ILE:HD13	1:38:A:ASN:H	9	0.47
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG11	1	0.47
(1,1479)	1:24:A:HIS:H	1:60:A:LEU:HB2	17	0.47
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	1	0.47
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	7	0.47
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	7	0.47
(1,1408)	1:10:A:VAL:HG21	1:10:A:VAL:H	17	0.47
(1,1408)	1:10:A:VAL:HG23	1:10:A:VAL:H	19	0.47
(1,1310)	1:98:A:ILE:HD11	1:71:A:THR:HG22	14	0.47
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	10	0.47
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	11	0.47
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB1	8	0.47
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	12	0.47
(1,1037)	1:73:A:VAL:HG22	1:91:A:LEU:HB3	10	0.47
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG23	19	0.47
(1,948)	1:10:A:VAL:HG21	1:90:A:GLU:H	2	0.47
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	15	0.47
(1,909)	1:10:A:VAL:HG23	1:90:A:GLU:HG2	6	0.47
(1,909)	1:10:A:VAL:HG23	1:90:A:GLU:HG2	14	0.47
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG23	3	0.47
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG21	4	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	4	0.47
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG21	13	0.47
(1,874)	1:45:A:ILE:HG12	1:45:A:ILE:HB	12	0.47
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	10	0.47
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG22	16	0.47
(1,489)	1:30:A:THR:H	1:30:A:THR:HG22	12	0.47
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	12	0.47
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	19	0.47
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	20	0.47
(1,397)	1:85:A:CYS:HB2	1:5:A:LYS:H	12	0.47
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	7	0.47
(1,388)	1:65:A:ILE:HG23	1:65:A:ILE:HA	19	0.47
(1,336)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	14	0.47
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	6	0.47
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG22	5	0.47
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG22	8	0.47
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	12	0.47
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	4	0.47
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	11	0.47
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD11	19	0.47
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	2	0.47
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	18	0.47
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	6	0.47
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	16	0.47
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	8	0.47
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	10	0.47
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	12	0.47
(1,75)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	13	0.47
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG22	11	0.47
(1,53)	1:76:A:TYR:HD1	1:7:A:ILE:HG22	19	0.47
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG21	6	0.47
(1,39)	1:45:A:ILE:HA	1:45:A:ILE:HG12	1	0.47
(1,21)	1:7:A:ILE:HD13	1:8:A:GLU:H	8	0.47
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD13	14	0.47
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	19	0.47
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG22	8	0.47
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.47
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	13	0.46
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	13	0.46
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	4	0.46
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	14	0.46
(3,284)	1:69:A:PHE:HA	1:115:A:SER:HB3	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	8	0.46
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG21	2	0.46
(3,219)	1:9:A:ILE:HG23	1:76:A:TYR:HB2	4	0.46
(3,218)	1:11:A:ILE:HG23	1:37:A:LEU:HB2	15	0.46
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	6	0.46
(3,212)	1:47:A:PHE:H	1:8:A:GLU:HG3	7	0.46
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB2	11	0.46
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	5	0.46
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	17	0.46
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB3	9	0.46
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	20	0.46
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	8	0.46
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	1	0.46
(3,168)	1:6:A:GLU:HG2	1:6:A:GLU:H	17	0.46
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	17	0.46
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	15	0.46
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	5	0.46
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	1	0.46
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	16	0.46
(3,65)	1:6:A:GLU:HG2	1:48:A:LYS:HA	20	0.46
(3,63)	1:104:A:GLU:HG2	1:104:A:GLU:HA	16	0.46
(3,50)	1:10:A:VAL:HG22	1:10:A:VAL:HA	15	0.46
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	3	0.46
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	3	0.46
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	3	0.46
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD12	5	0.46
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	9	0.46
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	9	0.46
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	16	0.46
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	6	0.46
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	14	0.46
(1,1954)	1:90:A:GLU:HA	1:10:A:VAL:HG21	3	0.46
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD13	5	0.46
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	7	0.46
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	6	0.46
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	3	0.46
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD12	19	0.46
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG22	12	0.46
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG22	19	0.46
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	7	0.46
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	4	0.46
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	15	0.46
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	1	0.46
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	1	0.46
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	9	0.46
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	11	0.46
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	17	0.46
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	19	0.46
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	3	0.46
(1,1406)	1:8:A:GLU:HG2	1:8:A:GLU:H	19	0.46
(1,1356)	1:98:A:ILE:HD13	1:71:A:THR:HG23	17	0.46
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB1	11	0.46
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	18	0.46
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	9	0.46
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB3	16	0.46
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	20	0.46
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	4	0.46
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	4	0.46
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	5	0.46
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	20	0.46
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG23	16	0.46
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	1	0.46
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG22	2	0.46
(1,948)	1:10:A:VAL:HG21	1:90:A:GLU:H	1	0.46
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	6	0.46
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	8	0.46
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	3	0.46
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD12	12	0.46
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	17	0.46
(1,892)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	15	0.46
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	8	0.46
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	2	0.46
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	1	0.46
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	9	0.46
(1,854)	1:89:A:TYR:H	1:9:A:ILE:HA	11	0.46
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	12	0.46
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	16	0.46
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG23	15	0.46
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG23	20	0.46
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	5	0.46
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	10	0.46
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	15	0.46
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	11	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD11	9	0.46
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG12	10	0.46
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	9	0.46
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	6	0.46
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	7	0.46
(1,413)	1:10:A:VAL:HG22	1:10:A:VAL:H	12	0.46
(1,388)	1:65:A:ILE:HG23	1:65:A:ILE:HA	8	0.46
(1,336)	1:98:A:ILE:HD12	1:61:A:PHE:HE1	17	0.46
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	13	0.46
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD11	11	0.46
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	9	0.46
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD12	5	0.46
(1,106)	1:9:A:ILE:HD12	1:9:A:ILE:HA	18	0.46
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	14	0.46
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	17	0.46
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	12	0.46
(1,42)	1:7:A:ILE:HD11	1:84:A:LEU:HB3	19	0.46
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD13	20	0.46
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	15	0.46
(1,16)	1:98:A:ILE:HD13	1:94:A:ARG:H	11	0.46
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	3	0.46
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG23	6	0.46
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	15	0.45
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB3	10	0.45
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB3	15	0.45
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	2	0.45
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	17	0.45
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	18	0.45
(3,258)	1:57:A:TRP:HB2	1:75:A:ALA:HB1	6	0.45
(3,257)	1:93:A:ALA:HB3	1:98:A:ILE:HG13	6	0.45
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	13	0.45
(3,220)	1:44:A:ILE:HG21	1:8:A:GLU:HG2	2	0.45
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	11	0.45
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	12	0.45
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	13	0.45
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	10	0.45
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	10	0.45
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	10	0.45
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	20	0.45
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	20	0.45
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	10	0.45
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG21	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	2	0.45
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	15	0.45
(3,1)	1:57:A:TRP:HB2	1:9:A:ILE:HD13	17	0.45
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	2	0.45
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	11	0.45
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD12	18	0.45
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	2	0.45
(1,2147)	1:62:A:ARG:HA	1:70:A:PHE:HA	11	0.45
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	2	0.45
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE2	18	0.45
(1,2037)	1:7:A:ILE:HB	1:7:A:ILE:HD11	3	0.45
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	10	0.45
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD13	2	0.45
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD11	8	0.45
(1,1935)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	17	0.45
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG21	19	0.45
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	11	0.45
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.45
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	13	0.45
(1,1738)	1:94:A:ARG:HB3	1:96:A:ASP:H	15	0.45
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	2	0.45
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	14	0.45
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	8	0.45
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	12	0.45
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG13	2	0.45
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG11	8	0.45
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	11	0.45
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG22	3	0.45
(1,1389)	1:85:A:CYS:HB2	1:5:A:LYS:H	5	0.45
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	4	0.45
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	8	0.45
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD13	1	0.45
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	4	0.45
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	13	0.45
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	5	0.45
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	8	0.45
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	16	0.45
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	10	0.45
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	2	0.45
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	16	0.45
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	4	0.45
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	5	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:73:A:VAL:HG22	1:91:A:LEU:HB3	16	0.45
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	12	0.45
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	14	0.45
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	9	0.45
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	15	0.45
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	13	0.45
(1,896)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	18	0.45
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	9	0.45
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG21	20	0.45
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD12	13	0.45
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	15	0.45
(1,867)	1:14:A:THR:H	1:19:A:ARG:HB3	18	0.45
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	11	0.45
(1,525)	1:20:A:ILE:HD13	1:38:A:ASN:H	6	0.45
(1,525)	1:20:A:ILE:HD13	1:38:A:ASN:H	9	0.45
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG11	1	0.45
(1,469)	1:24:A:HIS:H	1:60:A:LEU:HB2	17	0.45
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	1	0.45
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	3	0.45
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	7	0.45
(1,413)	1:10:A:VAL:HG21	1:10:A:VAL:H	17	0.45
(1,413)	1:10:A:VAL:HG23	1:10:A:VAL:H	19	0.45
(1,388)	1:65:A:ILE:HG21	1:65:A:ILE:HA	9	0.45
(1,378)	1:14:A:THR:HG21	1:14:A:THR:HA	6	0.45
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	1	0.45
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	14	0.45
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	3	0.45
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	5	0.45
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	7	0.45
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	12	0.45
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	13	0.45
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	14	0.45
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	16	0.45
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	18	0.45
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	19	0.45
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	1	0.45
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	16	0.45
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG22	14	0.45
(1,144)	1:95:A:MET:H	1:14:A:THR:HG22	18	0.45
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	19	0.45
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	16	0.45
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	16	0.45
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	5	0.45
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	14	0.45
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	20	0.45
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD13	5	0.45
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	18	0.45
(1,21)	1:7:A:ILE:HD13	1:8:A:GLU:H	19	0.45
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	19	0.45
(1,16)	1:98:A:ILE:HD13	1:94:A:ARG:H	10	0.45
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	10	0.45
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	7	0.44
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	15	0.44
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	5	0.44
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB2	19	0.44
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	4	0.44
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	15	0.44
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	18	0.44
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	3	0.44
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	13	0.44
(3,241)	1:92:A:SER:HA	1:12:A:LYS:HG2	18	0.44
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	8	0.44
(3,228)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	20	0.44
(3,218)	1:11:A:ILE:HG21	1:59:A:CYS:HB2	1	0.44
(3,218)	1:11:A:ILE:HG23	1:37:A:LEU:HB2	3	0.44
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	10	0.44
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	13	0.44
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	17	0.44
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	4	0.44
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	14	0.44
(3,158)	1:93:A:ALA:HB3	1:14:A:THR:HG21	18	0.44
(3,108)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	3	0.44
(3,108)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	12	0.44
(3,107)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	18	0.44
(3,106)	1:10:A:VAL:HG21	1:12:A:LYS:HB2	18	0.44
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	20	0.44
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	2	0.44
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	6	0.44
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	19	0.44
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	19	0.44
(3,35)	1:98:A:ILE:HG21	1:61:A:PHE:HE2	16	0.44
(3,33)	1:76:A:TYR:HD1	1:7:A:ILE:HG22	19	0.44
(3,10)	1:20:A:ILE:HG22	1:21:A:LEU:HA	12	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD13	13	0.44
(1,2250)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	17	0.44
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD12	13	0.44
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	10	0.44
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	6	0.44
(1,2121)	1:36:A:TYR:HA	1:20:A:ILE:HG23	15	0.44
(1,2036)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	12	0.44
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	7	0.44
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	16	0.44
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	4	0.44
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	10	0.44
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD11	15	0.44
(1,1935)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	20	0.44
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	11	0.44
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD11	20	0.44
(1,1820)	1:7:A:ILE:H	1:7:A:ILE:HB	19	0.44
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG22	2	0.44
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	16	0.44
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	2	0.44
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	9	0.44
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	19	0.44
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG12	9	0.44
(1,1517)	1:34:A:VAL:H	1:33:A:GLY:HA2	17	0.44
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	2	0.44
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	13	0.44
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	3	0.44
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	11	0.44
(1,1408)	1:10:A:VAL:HG21	1:10:A:VAL:H	18	0.44
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	4	0.44
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	13	0.44
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB2	13	0.44
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	5	0.44
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	17	0.44
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	5	0.44
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	10	0.44
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	10	0.44
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	3	0.44
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	18	0.44
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	19	0.44
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	7	0.44
(1,895)	1:44:A:ILE:HG21	1:44:A:ILE:HG13	11	0.44
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	19	0.44
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	10	0.44
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD12	19	0.44
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG22	12	0.44
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG22	19	0.44
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	7	0.44
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	4	0.44
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	7	0.44
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	15	0.44
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	1	0.44
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	1	0.44
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	9	0.44
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	12	0.44
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	11	0.44
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	17	0.44
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	19	0.44
(1,411)	1:8:A:GLU:HG2	1:8:A:GLU:H	19	0.44
(1,397)	1:85:A:CYS:HB2	1:5:A:LYS:H	5	0.44
(1,388)	1:65:A:ILE:HG21	1:65:A:ILE:HA	20	0.44
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	1	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	2	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	4	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	8	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	9	0.44
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	11	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	15	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	17	0.44
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	20	0.44
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	1	0.44
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	5	0.44
(1,140)	1:45:A:ILE:HD11	1:9:A:ILE:HD13	13	0.44
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	1	0.44
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB2	14	0.44
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	19	0.44
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	20	0.44
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	3	0.44
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD12	3	0.44
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	8	0.44
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	20	0.44
(1,75)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	2	0.44
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	5	0.44
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD13	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD11	8	0.44
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	10	0.44
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	13	0.44
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	4	0.44
(1,16)	1:98:A:ILE:HD11	1:94:A:ARG:H	12	0.44
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG23	4	0.44
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	4	0.43
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	10	0.43
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	18	0.43
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	10	0.43
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	15	0.43
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	5	0.43
(3,251)	1:99:A:TYR:HA	1:109:A:PRO:HB3	20	0.43
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	4	0.43
(3,219)	1:9:A:ILE:HG22	1:57:A:TRP:HB2	18	0.43
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	15	0.43
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	13	0.43
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	15	0.43
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB3	10	0.43
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB3	15	0.43
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	2	0.43
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	17	0.43
(3,107)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	3	0.43
(3,107)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	12	0.43
(3,106)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	3	0.43
(3,106)	1:10:A:VAL:HG22	1:12:A:LYS:HB2	12	0.43
(3,82)	1:68:A:LYS:HA	1:68:A:LYS:HB3	19	0.43
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	5	0.43
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	6	0.43
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD11	5	0.43
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	2	0.43
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	7	0.43
(3,24)	1:9:A:ILE:H	1:9:A:ILE:HB	15	0.43
(3,16)	1:31:A:ASN:HA	1:26:A:ARG:HB3	8	0.43
(1,2255)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	3	0.43
(1,2250)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	14	0.43
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	8	0.43
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	11	0.43
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	7	0.43
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE2	17	0.43
(1,2024)	1:48:A:LYS:HA	1:6:A:GLU:HA	19	0.43
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	19	0.43
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	1	0.43
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD13	9	0.43
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	18	0.43
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	19	0.43
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.43
(1,1762)	1:102:A:MET:H	1:101:A:LYS:HB2	1	0.43
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	12	0.43
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	8	0.43
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	15	0.43
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	16	0.43
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD12	13	0.43
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	16	0.43
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG12	4	0.43
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG21	8	0.43
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG12	17	0.43
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	6	0.43
(1,1408)	1:10:A:VAL:HG22	1:10:A:VAL:H	9	0.43
(1,1389)	1:85:A:CYS:HB2	1:5:A:LYS:H	1	0.43
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG22	15	0.43
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG23	20	0.43
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD11	5	0.43
(1,1211)	1:32:A:VAL:HG22	1:32:A:VAL:HA	20	0.43
(1,1177)	1:74:A:GLU:HA	1:74:A:GLU:HG2	7	0.43
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	19	0.43
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	9	0.43
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD13	9	0.43
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD11	15	0.43
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	10	0.43
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	11	0.43
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	10	0.43
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	7	0.43
(1,1037)	1:73:A:VAL:HG21	1:91:A:LEU:HB3	7	0.43
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG22	1	0.43
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	15	0.43
(1,948)	1:10:A:VAL:HG21	1:90:A:GLU:H	20	0.43
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	15	0.43
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	5	0.43
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	4	0.43
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	4	0.43
(1,909)	1:10:A:VAL:HG22	1:90:A:GLU:HG2	8	0.43
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	11	0.43
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	9	0.43
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	13	0.43
(1,711)	1:94:A:ARG:HB3	1:96:A:ASP:H	15	0.43
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	2	0.43
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	14	0.43
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	8	0.43
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	9	0.43
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	19	0.43
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG13	2	0.43
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG11	8	0.43
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	11	0.43
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG22	3	0.43
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.43
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD12	14	0.43
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD13	20	0.43
(1,298)	1:34:A:VAL:HG21	1:24:A:HIS:HE1	3	0.43
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	4	0.43
(1,248)	1:36:A:TYR:HD1	1:36:A:TYR:HB2	18	0.43
(1,180)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	6	0.43
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	10	0.43
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	15	0.43
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	18	0.43
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	20	0.43
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	2	0.43
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	3	0.43
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	13	0.43
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	19	0.43
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	16	0.43
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	7	0.43
(1,156)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	10	0.43
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	7	0.43
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG23	2	0.43
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	18	0.43
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD13	8	0.43
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	5	0.43
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	17	0.43
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD11	2	0.43
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	3	0.43
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG21	17	0.43
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	4	0.43
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD11	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:9:A:ILE:HD13	1:7:A:ILE:HG22	1	0.43
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	4	0.43
(1,16)	1:98:A:ILE:HD11	1:94:A:ARG:H	8	0.43
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG22	12	0.43
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG22	17	0.43
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	5	0.42
(3,310)	1:105:A:ARG:H	1:103:A:ASP:HB2	3	0.42
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	11	0.42
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	2	0.42
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	20	0.42
(3,227)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	10	0.42
(3,219)	1:9:A:ILE:HG22	1:57:A:TRP:HB2	5	0.42
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	16	0.42
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	5	0.42
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB2	19	0.42
(3,205)	1:111:A:ASN:H	1:110:A:LEU:HB2	13	0.42
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	4	0.42
(3,199)	1:10:A:VAL:HG21	1:91:A:LEU:H	3	0.42
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	16	0.42
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	18	0.42
(3,167)	1:5:A:LYS:HG2	1:6:A:GLU:H	3	0.42
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG22	3	0.42
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	7	0.42
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	11	0.42
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	6	0.42
(3,50)	1:10:A:VAL:HG22	1:10:A:VAL:HA	10	0.42
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	13	0.42
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	9	0.42
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	11	0.42
(3,1)	1:57:A:TRP:HB2	1:9:A:ILE:HD11	15	0.42
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	19	0.42
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	18	0.42
(1,2229)	1:75:A:ALA:HB2	1:9:A:ILE:HG22	8	0.42
(1,2096)	1:73:A:VAL:HG22	1:72:A:GLU:HA	1	0.42
(1,2072)	1:35:A:GLN:HA	1:36:A:TYR:HD1	10	0.42
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD13	18	0.42
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	4	0.42
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	18	0.42
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	1	0.42
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	5	0.42
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	7	0.42
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD13	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	20	0.42
(1,1930)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	19	0.42
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG21	6	0.42
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	6	0.42
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	12	0.42
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	8	0.42
(1,1505)	1:32:A:VAL:H	1:32:A:VAL:HG12	20	0.42
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG11	13	0.42
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	4	0.42
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	6	0.42
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	16	0.42
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG21	13	0.42
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	13	0.42
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	2	0.42
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	19	0.42
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	18	0.42
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	9	0.42
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	16	0.42
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG21	1	0.42
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	18	0.42
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB1	3	0.42
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	15	0.42
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	8	0.42
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	1	0.42
(1,1173)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	8	0.42
(1,1171)	1:1:A:ALA:HB1	1:83:A:PRO:HA	20	0.42
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	6	0.42
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	8	0.42
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	5	0.42
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	9	0.42
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	7	0.42
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	14	0.42
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	5	0.42
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	15	0.42
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	15	0.42
(1,895)	1:44:A:ILE:HG22	1:44:A:ILE:HG13	20	0.42
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	13	0.42
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	3	0.42
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD11	20	0.42
(1,792)	1:7:A:ILE:H	1:7:A:ILE:HB	19	0.42
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG22	2	0.42
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	15	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	16	0.42
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	16	0.42
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	2	0.42
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG12	9	0.42
(1,503)	1:34:A:VAL:H	1:33:A:GLY:HA2	17	0.42
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	2	0.42
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	3	0.42
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	11	0.42
(1,413)	1:10:A:VAL:HG22	1:10:A:VAL:H	9	0.42
(1,413)	1:10:A:VAL:HG21	1:10:A:VAL:H	18	0.42
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	6	0.42
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	10	0.42
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.42
(1,298)	1:34:A:VAL:HG21	1:24:A:HIS:HE1	16	0.42
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	10	0.42
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	12	0.42
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	15	0.42
(1,186)	1:48:A:LYS:HA	1:6:A:GLU:HA	7	0.42
(1,180)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	10	0.42
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	2	0.42
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	4	0.42
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	7	0.42
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	8	0.42
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	11	0.42
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	14	0.42
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	17	0.42
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	19	0.42
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	10	0.42
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB2	15	0.42
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	16	0.42
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG21	6	0.42
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	8	0.42
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	17	0.42
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	17	0.42
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	10	0.42
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD12	18	0.42
(1,75)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	17	0.42
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	11	0.42
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	16	0.42
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB2	10	0.42
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB3	20	0.42
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD13	9	0.42
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	10	0.42
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	18	0.42
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	19	0.42
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	14	0.42
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	13	0.42
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG22	16	0.42
(1,45)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	11	0.42
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	6	0.42
(1,16)	1:98:A:ILE:HD13	1:94:A:ARG:H	1	0.42
(1,8)	1:10:A:VAL:HG22	1:10:A:VAL:HA	15	0.42
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG21	7	0.42
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB2	12	0.41
(3,289)	1:48:A:LYS:HB3	1:6:A:GLU:H	4	0.41
(3,283)	1:5:A:LYS:HG2	1:5:A:LYS:HA	20	0.41
(3,272)	1:92:A:SER:HB3	1:93:A:ALA:H	17	0.41
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG21	16	0.41
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	12	0.41
(3,241)	1:92:A:SER:HA	1:91:A:LEU:HB3	11	0.41
(3,219)	1:9:A:ILE:HG21	1:76:A:TYR:HB2	13	0.41
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	10	0.41
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	18	0.41
(3,203)	1:105:A:ARG:H	1:103:A:ASP:HB2	3	0.41
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	2	0.41
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	10	0.41
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	15	0.41
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	5	0.41
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	14	0.41
(3,97)	1:56:A:ARG:HB2	1:76:A:TYR:HB3	7	0.41
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	4	0.41
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	6	0.41
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	7	0.41
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	3	0.41
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	5	0.41
(3,44)	1:28:A:GLY:HA2	1:55:A:SER:HB2	19	0.41
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	13	0.41
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	6	0.41
(3,10)	1:37:A:LEU:HA	1:20:A:ILE:HG23	4	0.41
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	4	0.41
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	6	0.41
(1,2029)	1:7:A:ILE:HG12	1:7:A:ILE:HA	19	0.41
(1,1997)	1:32:A:VAL:HA	1:32:A:VAL:HG13	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD12	13	0.41
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG22	13	0.41
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG23	18	0.41
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	3	0.41
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD11	16	0.41
(1,1936)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	8	0.41
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	1	0.41
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG21	15	0.41
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	3	0.41
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	20	0.41
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	11	0.41
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	15	0.41
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	19	0.41
(1,1389)	1:85:A:CYS:HB2	1:5:A:LYS:H	18	0.41
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	2	0.41
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	6	0.41
(1,1293)	1:45:A:ILE:HD11	1:9:A:ILE:HD12	15	0.41
(1,1243)	1:20:A:ILE:HD13	1:20:A:ILE:HB	7	0.41
(1,1230)	1:9:A:ILE:HD13	1:9:A:ILE:HA	1	0.41
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	8	0.41
(1,1177)	1:74:A:GLU:HA	1:74:A:GLU:HG2	14	0.41
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	1	0.41
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	12	0.41
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	18	0.41
(1,1136)	1:7:A:ILE:HB	1:7:A:ILE:HD11	3	0.41
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	17	0.41
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD11	13	0.41
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	16	0.41
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	17	0.41
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	19	0.41
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	15	0.41
(1,948)	1:10:A:VAL:HG23	1:90:A:GLU:H	19	0.41
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	6	0.41
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	1	0.41
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	4	0.41
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	11	0.41
(1,909)	1:10:A:VAL:HG23	1:90:A:GLU:HG2	10	0.41
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	11	0.41
(1,895)	1:44:A:ILE:HG22	1:44:A:ILE:HG13	2	0.41
(1,895)	1:44:A:ILE:HG21	1:44:A:ILE:HG13	7	0.41
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	13	0.41
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG23	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	5	0.41
(1,736)	1:102:A:MET:H	1:101:A:LYS:HB2	1	0.41
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	12	0.41
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	8	0.41
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	12	0.41
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD12	13	0.41
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	8	0.41
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	16	0.41
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG12	4	0.41
(1,492)	1:32:A:VAL:H	1:32:A:VAL:HG12	20	0.41
(1,489)	1:30:A:THR:H	1:30:A:THR:HG21	8	0.41
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG12	17	0.41
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	13	0.41
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	6	0.41
(1,397)	1:85:A:CYS:HB2	1:5:A:LYS:H	1	0.41
(1,388)	1:65:A:ILE:HG22	1:65:A:ILE:HA	2	0.41
(1,293)	1:47:A:PHE:HA	1:47:A:PHE:HD2	8	0.41
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	17	0.41
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	8	0.41
(1,253)	1:23:A:TYR:HB2	1:61:A:PHE:HE2	14	0.41
(1,210)	1:32:A:VAL:HA	1:32:A:VAL:HG13	10	0.41
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	3	0.41
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	5	0.41
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	6	0.41
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	9	0.41
(1,178)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	12	0.41
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	13	0.41
(1,178)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	16	0.41
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	20	0.41
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	15	0.41
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	3	0.41
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB2	6	0.41
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB1	18	0.41
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	5	0.41
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD12	1	0.41
(1,94)	1:9:A:ILE:HG22	1:75:A:ALA:HA	12	0.41
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	19	0.41
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB1	14	0.41
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	7	0.41
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD13	11	0.41
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	20	0.41
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG21	7	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG21	5	0.41
(1,39)	1:45:A:ILE:HA	1:45:A:ILE:HG12	5	0.41
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG23	16	0.41
(1,21)	1:7:A:ILE:HD13	1:8:A:GLU:H	9	0.41
(1,19)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	19	0.41
(1,16)	1:98:A:ILE:HD11	1:94:A:ARG:H	15	0.41
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	16	0.41
(4,43)	1:37:A:LEU:O	1:21:A:LEU:N	10	0.4
(3,315)	1:104:A:GLU:H	1:104:A:GLU:HG2	17	0.4
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	4	0.4
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	10	0.4
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB3	17	0.4
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB2	8	0.4
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	15	0.4
(3,289)	1:48:A:LYS:HB3	1:6:A:GLU:H	16	0.4
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB1	1	0.4
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	12	0.4
(3,257)	1:93:A:ALA:HB2	1:98:A:ILE:HG13	18	0.4
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	12	0.4
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	17	0.4
(3,227)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	11	0.4
(3,220)	1:44:A:ILE:HG21	1:8:A:GLU:HG2	5	0.4
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	14	0.4
(3,192)	1:86:A:GLY:H	1:5:A:LYS:HB3	10	0.4
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	11	0.4
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG23	2	0.4
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG23	12	0.4
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	3	0.4
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	16	0.4
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	17	0.4
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	19	0.4
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	9	0.4
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	4	0.4
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	11	0.4
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD11	2	0.4
(3,51)	1:9:A:ILE:HG13	1:75:A:ALA:HA	8	0.4
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD11	15	0.4
(3,50)	1:10:A:VAL:HG21	1:10:A:VAL:HA	8	0.4
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	18	0.4
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	18	0.4
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	18	0.4
(3,15)	1:84:A:LEU:HA	1:85:A:CYS:HB3	14	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD13	18	0.4
(1,2126)	1:23:A:TYR:HE1	1:36:A:TYR:HA	18	0.4
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE2	14	0.4
(1,2096)	1:73:A:VAL:HG23	1:72:A:GLU:HA	10	0.4
(1,1969)	1:62:A:ARG:HA	1:70:A:PHE:HA	18	0.4
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG22	9	0.4
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	15	0.4
(1,1941)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	13	0.4
(1,1930)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	14	0.4
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	18	0.4
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	3	0.4
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	19	0.4
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG22	17	0.4
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	18	0.4
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	6	0.4
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	9	0.4
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	17	0.4
(1,1560)	1:42:A:THR:H	1:41:A:GLY:HA3	8	0.4
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	9	0.4
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB2	16	0.4
(1,1243)	1:20:A:ILE:HD11	1:20:A:ILE:HB	12	0.4
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	19	0.4
(1,1230)	1:9:A:ILE:HD12	1:9:A:ILE:HA	12	0.4
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	9	0.4
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	4	0.4
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	15	0.4
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD13	6	0.4
(1,1143)	1:98:A:ILE:HG21	1:92:A:SER:H	1	0.4
(1,1132)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	1	0.4
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	16	0.4
(1,1129)	1:45:A:ILE:HA	1:45:A:ILE:HG12	7	0.4
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	16	0.4
(1,1058)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	17	0.4
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	17	0.4
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	2	0.4
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	7	0.4
(1,948)	1:10:A:VAL:HG22	1:90:A:GLU:H	5	0.4
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	10	0.4
(1,930)	1:12:A:LYS:HB3	1:92:A:SER:HB3	12	0.4
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	20	0.4
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	6	0.4
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	7	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	2	0.4
(1,906)	1:90:A:GLU:HA	1:10:A:VAL:HG21	3	0.4
(1,895)	1:44:A:ILE:HG21	1:44:A:ILE:HG13	3	0.4
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	5	0.4
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	8	0.4
(1,895)	1:44:A:ILE:HG22	1:44:A:ILE:HG13	9	0.4
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	7	0.4
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	6	0.4
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	6	0.4
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG11	13	0.4
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	4	0.4
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	6	0.4
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	16	0.4
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG21	13	0.4
(1,453)	1:20:A:ILE:H	1:19:A:ARG:HB3	13	0.4
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	2	0.4
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	19	0.4
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.4
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	20	0.4
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	6	0.4
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	1	0.4
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	4	0.4
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	2	0.4
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG22	7	0.4
(1,75)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	20	0.4
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	3	0.4
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD11	16	0.4
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	5	0.4
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	8	0.4
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG22	15	0.4
(1,48)	1:37:A:LEU:H	1:20:A:ILE:HG22	19	0.4
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	2	0.4
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	11	0.4
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD13	8	0.4
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	10	0.4
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	20	0.4
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD13	5	0.4
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	20	0.4
(1,16)	1:98:A:ILE:HD11	1:94:A:ARG:H	20	0.4
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG23	14	0.4
(3,338)	1:104:A:GLU:HG2	1:104:A:GLU:HA	1	0.39
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	15	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	6	0.39
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	6	0.39
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	4	0.39
(3,256)	1:32:A:VAL:HG22	1:45:A:ILE:HG12	19	0.39
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	20	0.39
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	12	0.39
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	15	0.39
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	12	0.39
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	5	0.39
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB2	12	0.39
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	16	0.39
(3,179)	1:29:A:ASN:H	1:56:A:ARG:HA	2	0.39
(3,169)	1:48:A:LYS:HB3	1:6:A:GLU:H	4	0.39
(3,169)	1:48:A:LYS:HB3	1:6:A:GLU:H	16	0.39
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG22	11	0.39
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	19	0.39
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE2	14	0.39
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	8	0.39
(3,75)	1:30:A:THR:HA	1:30:A:THR:H	9	0.39
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	9	0.39
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	8	0.39
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	8	0.39
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	14	0.39
(3,10)	1:20:A:ILE:HG21	1:21:A:LEU:HA	13	0.39
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	7	0.39
(3,1)	1:76:A:TYR:HB3	1:9:A:ILE:HD13	14	0.39
(1,2274)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	4	0.39
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	14	0.39
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	7	0.39
(1,2224)	1:32:A:VAL:HA	1:32:A:VAL:HG13	10	0.39
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	18	0.39
(1,2111)	1:23:A:TYR:HD2	1:23:A:TYR:HA	2	0.39
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	7	0.39
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	12	0.39
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG22	8	0.39
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.39
(1,1913)	1:9:A:ILE:HD13	1:9:A:ILE:HA	16	0.39
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	7	0.39
(1,1732)	1:95:A:MET:HB3	1:95:A:MET:H	14	0.39
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	20	0.39
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	12	0.39
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	12	0.39
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD13	7	0.39
(1,1541)	1:20:A:ILE:HD11	1:38:A:ASN:H	1	0.39
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG12	20	0.39
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	7	0.39
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	12	0.39
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	14	0.39
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	10	0.39
(1,1356)	1:98:A:ILE:HD11	1:71:A:THR:HG21	18	0.39
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	7	0.39
(1,1293)	1:45:A:ILE:HD11	1:9:A:ILE:HD11	3	0.39
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	13	0.39
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	20	0.39
(1,1168)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	11	0.39
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	18	0.39
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	6	0.39
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	9	0.39
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	11	0.39
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	18	0.39
(1,1110)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	8	0.39
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	19	0.39
(1,1058)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	14	0.39
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	2	0.39
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	11	0.39
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD12	18	0.39
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	18	0.39
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	15	0.39
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG23	1	0.39
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG23	20	0.39
(1,948)	1:10:A:VAL:HG21	1:90:A:GLU:H	4	0.39
(1,939)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	12	0.39
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	20	0.39
(1,895)	1:44:A:ILE:HG21	1:44:A:ILE:HG13	1	0.39
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	6	0.39
(1,895)	1:44:A:ILE:HG22	1:44:A:ILE:HG13	10	0.39
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	1	0.39
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG21	15	0.39
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	17	0.39
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	3	0.39
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	20	0.39
(1,397)	1:85:A:CYS:HB2	1:5:A:LYS:H	18	0.39
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	4	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	6	0.39
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	7	0.39
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	16	0.39
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	17	0.39
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	19	0.39
(1,299)	1:23:A:TYR:HE2	1:45:A:ILE:HD13	7	0.39
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	4	0.39
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	18	0.39
(1,262)	1:93:A:ALA:HB2	1:13:A:ASN:HB2	19	0.39
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE1	20	0.39
(1,229)	1:112:A:LYS:HB3	1:112:A:LYS:HA	6	0.39
(1,229)	1:112:A:LYS:HB3	1:112:A:LYS:HA	11	0.39
(1,229)	1:112:A:LYS:HB3	1:112:A:LYS:HA	16	0.39
(1,229)	1:112:A:LYS:HB3	1:112:A:LYS:HA	19	0.39
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	2	0.39
(1,175)	1:36:A:TYR:HA	1:22:A:GLN:HA	10	0.39
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	8	0.39
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB3	9	0.39
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	18	0.39
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	13	0.39
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	12	0.39
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	6	0.39
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD12	2	0.39
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	15	0.39
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	9	0.39
(1,74)	1:1:A:ALA:HB1	1:83:A:PRO:HA	9	0.39
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	1	0.39
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	6	0.39
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG21	4	0.39
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG21	7	0.39
(1,37)	1:75:A:ALA:HB2	1:9:A:ILE:HG22	4	0.39
(1,23)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	19	0.39
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD11	11	0.39
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	18	0.39
(1,16)	1:98:A:ILE:HD13	1:94:A:ARG:H	5	0.39
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	13	0.39
(1,16)	1:98:A:ILE:HD13	1:94:A:ARG:H	17	0.39
(1,8)	1:10:A:VAL:HG22	1:10:A:VAL:HA	10	0.39
(3,332)	1:69:A:PHE:HA	1:115:A:SER:HB2	17	0.38
(3,327)	1:10:A:VAL:HG22	1:10:A:VAL:HA	15	0.38
(3,325)	1:5:A:LYS:HG2	1:5:A:LYS:HA	20	0.38
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG2	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG2	14	0.38
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	3	0.38
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	13	0.38
(3,294)	1:27:A:SER:HB2	1:28:A:GLY:H	20	0.38
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	10	0.38
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	16	0.38
(3,227)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	15	0.38
(3,219)	1:9:A:ILE:HG23	1:76:A:TYR:HB2	6	0.38
(3,209)	1:104:A:GLU:H	1:104:A:GLU:HG2	17	0.38
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	4	0.38
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	10	0.38
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB3	17	0.38
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB2	8	0.38
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	15	0.38
(3,147)	1:5:A:LYS:HG3	1:6:A:GLU:H	20	0.38
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	1	0.38
(3,134)	1:36:A:TYR:HD1	1:22:A:GLN:HA	5	0.38
(3,134)	1:36:A:TYR:HD1	1:22:A:GLN:HA	12	0.38
(3,119)	1:11:A:ILE:HD12	1:59:A:CYS:HB2	13	0.38
(3,94)	1:87:A:LYS:HB2	1:87:A:LYS:HA	1	0.38
(3,79)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	17	0.38
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	10	0.38
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	12	0.38
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	3	0.38
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	8	0.38
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD13	1	0.38
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD11	17	0.38
(3,34)	1:11:A:ILE:HD13	1:61:A:PHE:HE1	3	0.38
(3,15)	1:85:A:CYS:HB3	1:4:A:CYS:HA	19	0.38
(3,10)	1:20:A:ILE:HG23	1:21:A:LEU:HA	5	0.38
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	6	0.38
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	12	0.38
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	17	0.38
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	12	0.38
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	13	0.38
(1,2111)	1:23:A:TYR:HD2	1:23:A:TYR:HA	3	0.38
(1,2111)	1:23:A:TYR:HD2	1:23:A:TYR:HA	10	0.38
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	19	0.38
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	9	0.38
(1,1955)	1:10:A:VAL:HG22	1:10:A:VAL:HA	15	0.38
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	3	0.38
(1,1927)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1923)	1:23:A:TYR:HE2	1:11:A:ILE:HG21	18	0.38
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	7	0.38
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	8	0.38
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD13	13	0.38
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	2	0.38
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	5	0.38
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	10	0.38
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	2	0.38
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	8	0.38
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	13	0.38
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	1	0.38
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	10	0.38
(1,1620)	1:54:A:ARG:HB3	1:54:A:ARG:H	18	0.38
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	9	0.38
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	12	0.38
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	20	0.38
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	20	0.38
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	5	0.38
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	17	0.38
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	10	0.38
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	4	0.38
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	20	0.38
(1,1242)	1:20:A:ILE:HD12	1:39:A:PHE:H	14	0.38
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG12	14	0.38
(1,1177)	1:74:A:GLU:HA	1:74:A:GLU:HG2	2	0.38
(1,1168)	1:20:A:ILE:HG21	1:36:A:TYR:HB2	20	0.38
(1,1166)	1:47:A:PHE:HD1	1:30:A:THR:HG22	6	0.38
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	3	0.38
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	10	0.38
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	17	0.38
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	7	0.38
(1,1055)	1:42:A:THR:HG22	1:11:A:ILE:H	7	0.38
(1,1055)	1:42:A:THR:HG22	1:11:A:ILE:H	14	0.38
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	11	0.38
(1,1019)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	9	0.38
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	17	0.38
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	2	0.38
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	18	0.38
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	5	0.38
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	14	0.38
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG21	11	0.38
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG21	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	7	0.38
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG22	17	0.38
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	18	0.38
(1,705)	1:95:A:MET:HB3	1:95:A:MET:H	14	0.38
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	6	0.38
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	9	0.38
(1,542)	1:42:A:THR:H	1:41:A:GLY:HA3	8	0.38
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG12	20	0.38
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	9	0.38
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	1	0.38
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	2	0.38
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	3	0.38
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	5	0.38
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	8	0.38
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	9	0.38
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	11	0.38
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	13	0.38
(1,314)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	14	0.38
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	18	0.38
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	2	0.38
(1,290)	1:20:A:ILE:HD13	1:20:A:ILE:HB	2	0.38
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	20	0.38
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD11	5	0.38
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	16	0.38
(1,159)	1:111:A:ASN:H	1:97:A:ALA:HB1	11	0.38
(1,156)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	4	0.38
(1,140)	1:45:A:ILE:HD13	1:9:A:ILE:HD11	17	0.38
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	6	0.38
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	9	0.38
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD13	17	0.38
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	4	0.38
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	6	0.38
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	17	0.38
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	2	0.38
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	4	0.38
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	12	0.38
(1,53)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	3	0.38
(1,53)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	4	0.38
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	3	0.38
(1,48)	1:37:A:LEU:H	1:20:A:ILE:HG22	8	0.38
(1,47)	1:20:A:ILE:HG23	1:21:A:LEU:H	20	0.38
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	6	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD11	19	0.38
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	3	0.38
(1,16)	1:98:A:ILE:HD11	1:94:A:ARG:H	7	0.38
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	9	0.38
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG21	13	0.38
(3,338)	1:104:A:GLU:HG3	1:104:A:GLU:HA	9	0.37
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	9	0.37
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	19	0.37
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	10	0.37
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	9	0.37
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	20	0.37
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	6	0.37
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	19	0.37
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	6	0.37
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	8	0.37
(3,251)	1:99:A:TYR:HA	1:109:A:PRO:HB3	2	0.37
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	9	0.37
(3,219)	1:9:A:ILE:HG21	1:57:A:TRP:HB2	19	0.37
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	13	0.37
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	15	0.37
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	6	0.37
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	6	0.37
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	8	0.37
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	8	0.37
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	13	0.37
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	1	0.37
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	5	0.37
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	15	0.37
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	16	0.37
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	17	0.37
(3,106)	1:10:A:VAL:HG23	1:12:A:LYS:HB2	4	0.37
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	14	0.37
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	16	0.37
(3,68)	1:1:A:ALA:HB3	1:84:A:LEU:HA	7	0.37
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	8	0.37
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD12	14	0.37
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	18	0.37
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	20	0.37
(3,34)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	10	0.37
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	14	0.37
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	3	0.37
(1,1956)	1:10:A:VAL:HG23	1:42:A:THR:HB	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG23	6	0.37
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	10	0.37
(1,1927)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	8	0.37
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD12	5	0.37
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD11	1	0.37
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD12	2	0.37
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	9	0.37
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	7	0.37
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG23	1	0.37
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	3	0.37
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	2	0.37
(1,1408)	1:10:A:VAL:HG22	1:10:A:VAL:H	5	0.37
(1,1408)	1:10:A:VAL:HG23	1:10:A:VAL:H	11	0.37
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG23	4	0.37
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG21	16	0.37
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	12	0.37
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB2	2	0.37
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB1	10	0.37
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	4	0.37
(1,1243)	1:20:A:ILE:HD12	1:20:A:ILE:HB	3	0.37
(1,1243)	1:20:A:ILE:HD13	1:20:A:ILE:HB	6	0.37
(1,1243)	1:20:A:ILE:HD11	1:20:A:ILE:HB	9	0.37
(1,1243)	1:20:A:ILE:HD13	1:20:A:ILE:HB	16	0.37
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	16	0.37
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	1	0.37
(1,1172)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	18	0.37
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	13	0.37
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	20	0.37
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD11	14	0.37
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	3	0.37
(1,1137)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	5	0.37
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	9	0.37
(1,1102)	1:98:A:ILE:HD13	1:71:A:THR:HG21	2	0.37
(1,1097)	1:10:A:VAL:HG23	1:10:A:VAL:HA	7	0.37
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	1	0.37
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	5	0.37
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG22	13	0.37
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	8	0.37
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD12	13	0.37
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	1	0.37
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	2	0.37
(1,1055)	1:42:A:THR:HG22	1:11:A:ILE:H	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	13	0.37
(1,1055)	1:42:A:THR:HG22	1:11:A:ILE:H	15	0.37
(1,1055)	1:42:A:THR:HG22	1:11:A:ILE:H	19	0.37
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	7	0.37
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	18	0.37
(1,1037)	1:73:A:VAL:HG23	1:91:A:LEU:HB3	4	0.37
(1,1005)	1:97:A:ALA:HB1	1:109:A:PRO:HB2	14	0.37
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE2	18	0.37
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD13	18	0.37
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD12	13	0.37
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD13	16	0.37
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG22	6	0.37
(1,895)	1:44:A:ILE:HG23	1:44:A:ILE:HG13	4	0.37
(1,895)	1:44:A:ILE:HG22	1:44:A:ILE:HG13	12	0.37
(1,895)	1:44:A:ILE:HG22	1:44:A:ILE:HG13	18	0.37
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	20	0.37
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	12	0.37
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	1	0.37
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	2	0.37
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	10	0.37
(1,596)	1:54:A:ARG:HB3	1:54:A:ARG:H	18	0.37
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	12	0.37
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	9	0.37
(1,525)	1:20:A:ILE:HD11	1:38:A:ASN:H	1	0.37
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	7	0.37
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	12	0.37
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	14	0.37
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	10	0.37
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	12	0.37
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	20	0.37
(1,306)	1:30:A:THR:HB	1:47:A:PHE:HE1	4	0.37
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	7	0.37
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD11	11	0.37
(1,262)	1:93:A:ALA:HB2	1:13:A:ASN:HB2	8	0.37
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	14	0.37
(1,157)	1:73:A:VAL:HG21	1:61:A:PHE:HD1	8	0.37
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	10	0.37
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	20	0.37
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	6	0.37
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	17	0.37
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	16	0.37
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD11	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	14	0.37
(1,111)	1:11:A:ILE:H	1:11:A:ILE:HG13	12	0.37
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG23	16	0.37
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	1	0.37
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	18	0.37
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	19	0.37
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	2	0.37
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	20	0.37
(1,56)	1:94:A:ARG:H	1:93:A:ALA:HB2	18	0.37
(1,53)	1:76:A:TYR:HD1	1:7:A:ILE:HG21	6	0.37
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	5	0.37
(1,45)	1:9:A:ILE:HD13	1:7:A:ILE:HG21	16	0.37
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	11	0.37
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	8	0.37
(1,21)	1:7:A:ILE:HD12	1:8:A:GLU:H	6	0.37
(1,21)	1:7:A:ILE:HD13	1:8:A:GLU:H	11	0.37
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD12	20	0.37
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD13	13	0.37
(1,8)	1:10:A:VAL:HG21	1:10:A:VAL:HA	8	0.37
(4,13)	1:90:A:GLU:H	1:101:A:LYS:O	12	0.36
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	17	0.36
(3,326)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	1	0.36
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	7	0.36
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	10	0.36
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	14	0.36
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG3	8	0.36
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB2	6	0.36
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	5	0.36
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	15	0.36
(3,255)	1:12:A:LYS:HB3	1:14:A:THR:HG22	3	0.36
(3,227)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	9	0.36
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	3	0.36
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG2	5	0.36
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	3	0.36
(3,178)	1:27:A:SER:HB2	1:28:A:GLY:H	20	0.36
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	13	0.36
(3,160)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	19	0.36
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	2	0.36
(3,118)	1:90:A:GLU:HB2	1:10:A:VAL:HG12	3	0.36
(3,108)	1:9:A:ILE:HG23	1:88:A:ARG:HB3	18	0.36
(3,97)	1:56:A:ARG:HB2	1:76:A:TYR:HB3	3	0.36
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	16	0.36
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	1	0.36
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	14	0.36
(3,65)	1:6:A:GLU:HG2	1:48:A:LYS:HA	14	0.36
(3,51)	1:18:A:SER:HB3	1:20:A:ILE:HD11	4	0.36
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	2	0.36
(3,40)	1:15:A:LEU:HA	1:94:A:ARG:HA	1	0.36
(3,39)	1:15:A:LEU:HA	1:94:A:ARG:HA	1	0.36
(3,33)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	4	0.36
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB3	10	0.36
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD13	10	0.36
(3,1)	1:76:A:TYR:HB3	1:9:A:ILE:HD12	4	0.36
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	14	0.36
(1,2255)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	4	0.36
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	4	0.36
(1,2228)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	8	0.36
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	17	0.36
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	1	0.36
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	5	0.36
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	17	0.36
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG23	4	0.36
(1,1935)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	14	0.36
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	7	0.36
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	10	0.36
(1,1927)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	19	0.36
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	18	0.36
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	1	0.36
(1,1802)	1:56:A:ARG:H	1:56:A:ARG:HB3	2	0.36
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	15	0.36
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	14	0.36
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD2	9	0.36
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG21	2	0.36
(1,1560)	1:42:A:THR:H	1:41:A:GLY:HA3	17	0.36
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	15	0.36
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	1	0.36
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG13	2	0.36
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	5	0.36
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	8	0.36
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	2	0.36
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD2	15	0.36
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	14	0.36
(1,1310)	1:98:A:ILE:HD11	1:71:A:THR:HG23	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG21	3	0.36
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG23	10	0.36
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	13	0.36
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	8	0.36
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	7	0.36
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG11	2	0.36
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD13	2	0.36
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	7	0.36
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	11	0.36
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	9	0.36
(1,1143)	1:98:A:ILE:HG22	1:92:A:SER:H	19	0.36
(1,1129)	1:45:A:ILE:HA	1:45:A:ILE:HG12	1	0.36
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD13	18	0.36
(1,1097)	1:10:A:VAL:HG23	1:10:A:VAL:HA	4	0.36
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG23	18	0.36
(1,1061)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	3	0.36
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	19	0.36
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG21	8	0.36
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	4	0.36
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG22	16	0.36
(1,982)	1:73:A:VAL:HG22	1:72:A:GLU:HA	1	0.36
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	17	0.36
(1,909)	1:10:A:VAL:HG23	1:90:A:GLU:HG2	11	0.36
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	4	0.36
(1,896)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	8	0.36
(1,892)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	19	0.36
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG21	6	0.36
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	8	0.36
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD13	13	0.36
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	2	0.36
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	5	0.36
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	10	0.36
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	2	0.36
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	8	0.36
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	13	0.36
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	12	0.36
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	20	0.36
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	20	0.36
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	5	0.36
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	17	0.36
(1,330)	1:19:A:ARG:HB2	1:15:A:LEU:HD12	5	0.36
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD11	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:20:A:ILE:HD12	1:20:A:ILE:HB	20	0.36
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	1	0.36
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	12	0.36
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	16	0.36
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	3	0.36
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB3	5	0.36
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	2	0.36
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	3	0.36
(1,191)	1:14:A:THR:HB	1:14:A:THR:HA	13	0.36
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	4	0.36
(1,175)	1:36:A:TYR:HA	1:22:A:GLN:HA	15	0.36
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	7	0.36
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	15	0.36
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	16	0.36
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	15	0.36
(1,117)	1:20:A:ILE:HD13	1:39:A:PHE:H	11	0.36
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD13	16	0.36
(1,74)	1:1:A:ALA:HB2	1:83:A:PRO:HA	16	0.36
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	5	0.36
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	8	0.36
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	7	0.36
(1,51)	1:98:A:ILE:HG22	1:92:A:SER:H	14	0.36
(1,42)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	15	0.36
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD12	2	0.36
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	4	0.36
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	14	0.36
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	8	0.36
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	9	0.36
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	2	0.36
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	18	0.36
(3,327)	1:10:A:VAL:HG22	1:10:A:VAL:HA	10	0.35
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	3	0.35
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	8	0.35
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	4	0.35
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	11	0.35
(3,289)	1:48:A:LYS:HB3	1:6:A:GLU:H	2	0.35
(3,251)	1:99:A:TYR:HA	1:110:A:LEU:HB2	1	0.35
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	14	0.35
(3,228)	1:7:A:ILE:HG23	1:84:A:LEU:HB3	14	0.35
(3,227)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	2	0.35
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	9	0.35
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	10	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	9	0.35
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG2	14	0.35
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	20	0.35
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	6	0.35
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	19	0.35
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG23	20	0.35
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	6	0.35
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	19	0.35
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	11	0.35
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	3	0.35
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	9	0.35
(3,33)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	3	0.35
(3,24)	1:9:A:ILE:H	1:9:A:ILE:HB	7	0.35
(3,24)	1:9:A:ILE:H	1:9:A:ILE:HB	10	0.35
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	12	0.35
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	8	0.35
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD12	1	0.35
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD12	3	0.35
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	13	0.35
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	9	0.35
(1,2134)	1:15:A:LEU:H	1:95:A:MET:HA	18	0.35
(1,2096)	1:73:A:VAL:HG21	1:72:A:GLU:HA	8	0.35
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	1	0.35
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	9	0.35
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	13	0.35
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	15	0.35
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD13	5	0.35
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD13	14	0.35
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	2	0.35
(1,1955)	1:10:A:VAL:HG22	1:10:A:VAL:HA	10	0.35
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG22	12	0.35
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG22	17	0.35
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG22	2	0.35
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD11	13	0.35
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD12	17	0.35
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	3	0.35
(1,1850)	1:71:A:THR:H	1:70:A:PHE:HE2	18	0.35
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD11	2	0.35
(1,1785)	1:115:A:SER:H	1:114:A:ARG:HA	10	0.35
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG21	3	0.35
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	12	0.35
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	19	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1699)	1:7:A:ILE:HD13	1:87:A:LYS:H	17	0.35
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	15	0.35
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG11	7	0.35
(1,1501)	1:29:A:ASN:HB2	1:30:A:THR:H	4	0.35
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	1	0.35
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	11	0.35
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD11	14	0.35
(1,1230)	1:9:A:ILE:HD12	1:9:A:ILE:HA	3	0.35
(1,1230)	1:9:A:ILE:HD11	1:9:A:ILE:HA	13	0.35
(1,1172)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	13	0.35
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG21	6	0.35
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG22	9	0.35
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	15	0.35
(1,1072)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	4	0.35
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	6	0.35
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	10	0.35
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	6	0.35
(1,1037)	1:73:A:VAL:HG22	1:91:A:LEU:HB3	15	0.35
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE2	17	0.35
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	2	0.35
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	18	0.35
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	3	0.35
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	2	0.35
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	19	0.35
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD11	1	0.35
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD12	2	0.35
(1,847)	1:7:A:ILE:H	1:48:A:LYS:HA	7	0.35
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	9	0.35
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD2	9	0.35
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG21	2	0.35
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	7	0.35
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	1	0.35
(1,489)	1:30:A:THR:H	1:30:A:THR:HG23	1	0.35
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	3	0.35
(1,413)	1:10:A:VAL:HG22	1:10:A:VAL:H	5	0.35
(1,413)	1:10:A:VAL:HG23	1:10:A:VAL:H	11	0.35
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	2	0.35
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	10	0.35
(1,314)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	15	0.35
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	3	0.35
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB1	13	0.35
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	12	0.35
(1,144)	1:95:A:MET:H	1:14:A:THR:HG23	6	0.35
(1,144)	1:95:A:MET:H	1:14:A:THR:HG23	17	0.35
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG22	11	0.35
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	1	0.35
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB1	17	0.35
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	11	0.35
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	4	0.35
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	16	0.35
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	3	0.35
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	6	0.35
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	7	0.35
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	10	0.35
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	18	0.35
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	5	0.35
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	6	0.35
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	16	0.35
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD11	14	0.35
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	20	0.35
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	2	0.35
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD13	10	0.35
(1,16)	1:98:A:ILE:HD11	1:94:A:ARG:H	6	0.35
(4,3)	1:47:A:PHE:H	1:7:A:ILE:O	19	0.34
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	15	0.34
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	16	0.34
(3,284)	1:69:A:PHE:HA	1:115:A:SER:HB2	17	0.34
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	3	0.34
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	19	0.34
(3,251)	1:99:A:TYR:HA	1:110:A:LEU:HB2	6	0.34
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	8	0.34
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	17	0.34
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	4	0.34
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	14	0.34
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	4	0.34
(3,227)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	1	0.34
(3,227)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	14	0.34
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	7	0.34
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	10	0.34
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	19	0.34
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	8	0.34
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	19	0.34
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB2	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,205)	1:111:A:ASN:H	1:110:A:LEU:HB2	18	0.34
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	18	0.34
(3,192)	1:86:A:GLY:H	1:5:A:LYS:HB3	14	0.34
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	11	0.34
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	6	0.34
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	8	0.34
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	1	0.34
(3,108)	1:9:A:ILE:HG23	1:88:A:ARG:HB3	5	0.34
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	1	0.34
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	12	0.34
(3,42)	1:47:A:PHE:HB2	1:47:A:PHE:HA	19	0.34
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	6	0.34
(3,34)	1:11:A:ILE:HD13	1:61:A:PHE:HE1	1	0.34
(3,33)	1:76:A:TYR:HD1	1:7:A:ILE:HG21	6	0.34
(3,10)	1:20:A:ILE:HG22	1:21:A:LEU:HA	2	0.34
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD13	20	0.34
(1,2237)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	15	0.34
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	9	0.34
(1,2111)	1:23:A:TYR:HD2	1:23:A:TYR:HA	11	0.34
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	12	0.34
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	7	0.34
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	12	0.34
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	19	0.34
(1,2074)	1:113:A:TRP:HA	1:71:A:THR:HG21	6	0.34
(1,2072)	1:35:A:GLN:HA	1:36:A:TYR:HD1	15	0.34
(1,2063)	1:73:A:VAL:HG22	1:73:A:VAL:HA	11	0.34
(1,2039)	1:7:A:ILE:HD11	1:7:A:ILE:HA	19	0.34
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD13	2	0.34
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD11	8	0.34
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG21	7	0.34
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	6	0.34
(1,1927)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	2	0.34
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	4	0.34
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	11	0.34
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	18	0.34
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	19	0.34
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG22	7	0.34
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	10	0.34
(1,1732)	1:95:A:MET:HB3	1:95:A:MET:H	17	0.34
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	1	0.34
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	13	0.34
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	17	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	13	0.34
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG23	2	0.34
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	8	0.34
(1,1547)	1:39:A:PHE:HD1	1:39:A:PHE:H	13	0.34
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	20	0.34
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	3	0.34
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG22	1	0.34
(1,1293)	1:45:A:ILE:HD12	1:9:A:ILE:HD13	10	0.34
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	19	0.34
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB2	9	0.34
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	20	0.34
(1,1243)	1:20:A:ILE:HD13	1:20:A:ILE:HB	15	0.34
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	2	0.34
(1,1242)	1:20:A:ILE:HD12	1:39:A:PHE:H	18	0.34
(1,1230)	1:9:A:ILE:HD13	1:9:A:ILE:HA	7	0.34
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	19	0.34
(1,1166)	1:47:A:PHE:HD1	1:30:A:THR:HG22	11	0.34
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	12	0.34
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD11	13	0.34
(1,1156)	1:15:A:LEU:HB3	1:15:A:LEU:HD12	14	0.34
(1,1145)	1:76:A:TYR:HD1	1:7:A:ILE:HG22	19	0.34
(1,1132)	1:98:A:ILE:HD12	1:61:A:PHE:HB2	12	0.34
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	13	0.34
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	19	0.34
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG22	8	0.34
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.34
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	8	0.34
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	18	0.34
(1,982)	1:73:A:VAL:HG23	1:72:A:GLU:HA	10	0.34
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	7	0.34
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	12	0.34
(1,938)	1:7:A:ILE:HG12	1:7:A:ILE:HA	19	0.34
(1,919)	1:70:A:PHE:HE2	1:70:A:PHE:HA	18	0.34
(1,909)	1:10:A:VAL:HG21	1:90:A:GLU:HG2	20	0.34
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	16	0.34
(1,892)	1:98:A:ILE:HG21	1:61:A:PHE:HE1	14	0.34
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	10	0.34
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	14	0.34
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	18	0.34
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	7	0.34
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	18	0.34
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:56:A:ARG:H	1:56:A:ARG:HB3	2	0.34
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	15	0.34
(1,759)	1:115:A:SER:H	1:114:A:ARG:HA	10	0.34
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	14	0.34
(1,542)	1:42:A:THR:H	1:41:A:GLY:HA3	17	0.34
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	15	0.34
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG11	7	0.34
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG13	2	0.34
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	5	0.34
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	8	0.34
(1,453)	1:20:A:ILE:H	1:19:A:ARG:HB3	2	0.34
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD2	15	0.34
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	14	0.34
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	20	0.34
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD13	6	0.34
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	7	0.34
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	11	0.34
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	9	0.34
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	13	0.34
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	16	0.34
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	11	0.34
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	9	0.34
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	18	0.34
(1,242)	1:39:A:PHE:HD2	1:17:A:PRO:HA	19	0.34
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	1	0.34
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG23	8	0.34
(1,153)	1:61:A:PHE:HD1	1:71:A:THR:HG22	9	0.34
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	3	0.34
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	4	0.34
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	5	0.34
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG23	7	0.34
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG22	10	0.34
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	20	0.34
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD12	20	0.34
(1,72)	1:109:A:PRO:HB3	1:97:A:ALA:HB3	17	0.34
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	9	0.34
(1,69)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	15	0.34
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	10	0.34
(1,54)	1:7:A:ILE:HG21	1:8:A:GLU:H	19	0.34
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG22	7	0.34
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	12	0.34
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:7:A:ILE:HD12	1:8:A:GLU:H	18	0.34
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	7	0.34
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD13	11	0.34
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	15	0.34
(1,11)	1:73:A:VAL:HG22	1:98:A:ILE:HD12	15	0.34
(4,13)	1:90:A:GLU:H	1:101:A:LYS:O	14	0.33
(3,327)	1:10:A:VAL:HG21	1:10:A:VAL:HA	8	0.33
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	8	0.33
(3,319)	1:19:A:ARG:HG3	1:95:A:MET:H	8	0.33
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	16	0.33
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	4	0.33
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	6	0.33
(3,315)	1:104:A:GLU:H	1:104:A:GLU:HG2	7	0.33
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG3	4	0.33
(3,294)	1:27:A:SER:HB2	1:28:A:GLY:H	13	0.33
(3,287)	1:4:A:CYS:HB3	1:5:A:LYS:H	10	0.33
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	9	0.33
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	14	0.33
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	5	0.33
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	14	0.33
(3,227)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	3	0.33
(3,227)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	17	0.33
(3,218)	1:11:A:ILE:HG21	1:37:A:LEU:HB2	19	0.33
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	14	0.33
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB3	8	0.33
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG3	8	0.33
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	14	0.33
(3,192)	1:86:A:GLY:H	1:5:A:LYS:HB3	18	0.33
(3,179)	1:29:A:ASN:H	1:56:A:ARG:HA	18	0.33
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	4	0.33
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	11	0.33
(3,169)	1:48:A:LYS:HB3	1:6:A:GLU:H	2	0.33
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	12	0.33
(3,148)	1:111:A:ASN:H	1:110:A:LEU:HB2	13	0.33
(3,119)	1:90:A:GLU:HB2	1:10:A:VAL:HG12	3	0.33
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	12	0.33
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG22	13	0.33
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	16	0.33
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD12	9	0.33
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	1	0.33
(3,50)	1:10:A:VAL:HG22	1:10:A:VAL:HA	14	0.33
(3,44)	1:28:A:GLY:HA2	1:55:A:SER:HB2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	4	0.33
(3,10)	1:20:A:ILE:HG22	1:21:A:LEU:HA	3	0.33
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB1	11	0.33
(1,2255)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	11	0.33
(1,2255)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	16	0.33
(1,2250)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	18	0.33
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	1	0.33
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	14	0.33
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	8	0.33
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	8	0.33
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	11	0.33
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	16	0.33
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	18	0.33
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	20	0.33
(1,2048)	1:10:A:VAL:HG21	1:90:A:GLU:H	18	0.33
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	4	0.33
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD11	15	0.33
(1,2001)	1:39:A:PHE:HD2	1:17:A:PRO:HA	16	0.33
(1,1955)	1:10:A:VAL:HG21	1:10:A:VAL:HA	8	0.33
(1,1947)	1:111:A:ASN:HB2	1:71:A:THR:HG21	12	0.33
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	11	0.33
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG22	16	0.33
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	5	0.33
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	14	0.33
(1,1883)	1:113:A:TRP:HB3	1:114:A:ARG:H	9	0.33
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.33
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	4	0.33
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	5	0.33
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	6	0.33
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG23	19	0.33
(1,1747)	1:98:A:ILE:H	1:98:A:ILE:HG23	14	0.33
(1,1732)	1:95:A:MET:HB3	1:95:A:MET:H	2	0.33
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	16	0.33
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	2	0.33
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	14	0.33
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	11	0.33
(1,1541)	1:20:A:ILE:HD12	1:38:A:ASN:H	5	0.33
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG12	11	0.33
(1,1497)	1:29:A:ASN:H	1:29:A:ASN:HB2	6	0.33
(1,1479)	1:24:A:HIS:H	1:60:A:LEU:HB2	18	0.33
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD2	16	0.33
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	9	0.33
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	2	0.33
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	6	0.33
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	7	0.33
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	10	0.33
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	11	0.33
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	15	0.33
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	20	0.33
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	1	0.33
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG22	12	0.33
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	5	0.33
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	7	0.33
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	8	0.33
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	15	0.33
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	19	0.33
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD11	19	0.33
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	1	0.33
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	8	0.33
(1,1230)	1:9:A:ILE:HD13	1:9:A:ILE:HA	15	0.33
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD13	5	0.33
(1,1134)	1:7:A:ILE:HD11	1:84:A:LEU:HB3	19	0.33
(1,1132)	1:98:A:ILE:HD13	1:61:A:PHE:HB2	17	0.33
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	3	0.33
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG23	6	0.33
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	3	0.33
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	14	0.33
(1,1027)	1:84:A:LEU:HB3	1:7:A:ILE:HG12	11	0.33
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	12	0.33
(1,995)	1:23:A:TYR:HE1	1:36:A:TYR:HA	18	0.33
(1,963)	1:80:A:LEU:HA	1:80:A:LEU:HB2	11	0.33
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	9	0.33
(1,889)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	20	0.33
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	15	0.33
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD12	5	0.33
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD12	17	0.33
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	3	0.33
(1,817)	1:71:A:THR:H	1:70:A:PHE:HE2	18	0.33
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD11	2	0.33
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG21	3	0.33
(1,705)	1:95:A:MET:HB3	1:95:A:MET:H	17	0.33
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	12	0.33
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:7:A:ILE:HD13	1:87:A:LYS:H	17	0.33
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	13	0.33
(1,622)	1:71:A:THR:H	1:71:A:THR:HG23	2	0.33
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	8	0.33
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	15	0.33
(1,488)	1:29:A:ASN:HB2	1:30:A:THR:H	4	0.33
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	1	0.33
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	1	0.33
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	2	0.33
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	3	0.33
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	10	0.33
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	12	0.33
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	14	0.33
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	15	0.33
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	16	0.33
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	17	0.33
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	19	0.33
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	20	0.33
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	14	0.33
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	6	0.33
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	14	0.33
(1,273)	1:73:A:VAL:HG22	1:73:A:VAL:HA	17	0.33
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	10	0.33
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	13	0.33
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	14	0.33
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	15	0.33
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	19	0.33
(1,262)	1:93:A:ALA:HB3	1:13:A:ASN:HB2	15	0.33
(1,256)	1:68:A:LYS:HA	1:68:A:LYS:HB3	19	0.33
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	18	0.33
(1,157)	1:73:A:VAL:HG21	1:61:A:PHE:HD1	5	0.33
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	6	0.33
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG23	13	0.33
(1,144)	1:95:A:MET:H	1:14:A:THR:HG22	2	0.33
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	1	0.33
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	9	0.33
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	16	0.33
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG21	19	0.33
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	1	0.33
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD11	15	0.33
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	2	0.33
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB2	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	18	0.33
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	12	0.33
(1,51)	1:98:A:ILE:HG22	1:92:A:SER:H	15	0.33
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	8	0.33
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD12	4	0.33
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	20	0.33
(1,19)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	10	0.33
(1,11)	1:73:A:VAL:HG21	1:98:A:ILE:HD12	12	0.33
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	2	0.33
(3,338)	1:104:A:GLU:HG3	1:104:A:GLU:HA	2	0.32
(3,338)	1:104:A:GLU:HG2	1:104:A:GLU:HA	12	0.32
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	11	0.32
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG3	5	0.32
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB2	2	0.32
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	19	0.32
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	15	0.32
(3,228)	1:7:A:ILE:HG22	1:84:A:LEU:HB3	18	0.32
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	3	0.32
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB2	15	0.32
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	12	0.32
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	16	0.32
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	19	0.32
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	17	0.32
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG22	9	0.32
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	15	0.32
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	15	0.32
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	1	0.32
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	15	0.32
(3,65)	1:6:A:GLU:HG2	1:48:A:LYS:HA	9	0.32
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	15	0.32
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD11	6	0.32
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	5	0.32
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	16	0.32
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD13	8	0.32
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD13	16	0.32
(3,1)	1:57:A:TRP:HB2	1:9:A:ILE:HD11	1	0.32
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	17	0.32
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	3	0.32
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	5	0.32
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	8	0.32
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	4	0.32
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	2	0.32
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	4	0.32
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	5	0.32
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	10	0.32
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	17	0.32
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	5	0.32
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	1	0.32
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD13	9	0.32
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	10	0.32
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	17	0.32
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG23	14	0.32
(1,1935)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	4	0.32
(1,1927)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	17	0.32
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG22	14	0.32
(1,1920)	1:11:A:ILE:H	1:11:A:ILE:HG21	17	0.32
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD11	16	0.32
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	14	0.32
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	6	0.32
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	13	0.32
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG22	2	0.32
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	7	0.32
(1,1738)	1:94:A:ARG:HB3	1:96:A:ASP:H	12	0.32
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	18	0.32
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	1	0.32
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	6	0.32
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	7	0.32
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	15	0.32
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	16	0.32
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	18	0.32
(1,1658)	1:73:A:VAL:HG21	1:74:A:GLU:H	11	0.32
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	5	0.32
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	10	0.32
(1,1576)	1:46:A:LYS:HB3	1:46:A:LYS:H	2	0.32
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD13	1	0.32
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD12	5	0.32
(1,1501)	1:29:A:ASN:HB2	1:30:A:THR:H	13	0.32
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD1	15	0.32
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD2	19	0.32
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB1	6	0.32
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB3	17	0.32
(1,1408)	1:10:A:VAL:HG22	1:10:A:VAL:H	16	0.32
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	3	0.32
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	4	0.32
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	5	0.32
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	8	0.32
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	9	0.32
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	12	0.32
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	13	0.32
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	16	0.32
(1,1343)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	17	0.32
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	18	0.32
(1,1247)	1:20:A:ILE:HA	1:20:A:ILE:HD11	13	0.32
(1,1243)	1:20:A:ILE:HD13	1:20:A:ILE:HB	5	0.32
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	6	0.32
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	2	0.32
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	12	0.32
(1,1172)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	2	0.32
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	17	0.32
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD12	12	0.32
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD13	2	0.32
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD11	8	0.32
(1,1105)	1:98:A:ILE:HD13	1:94:A:ARG:H	11	0.32
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	10	0.32
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	2	0.32
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	4	0.32
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	5	0.32
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	6	0.32
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	10	0.32
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	15	0.32
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	20	0.32
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE2	14	0.32
(1,979)	1:90:A:GLU:HA	1:90:A:GLU:HG2	3	0.32
(1,909)	1:10:A:VAL:HG22	1:90:A:GLU:HG2	9	0.32
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	3	0.32
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	19	0.32
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD11	13	0.32
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	19	0.32
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG22	7	0.32
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	5	0.32
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	10	0.32
(1,722)	1:98:A:ILE:H	1:98:A:ILE:HG23	14	0.32
(1,705)	1:95:A:MET:HB3	1:95:A:MET:H	2	0.32
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	13	0.32
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	17	0.32
(1,531)	1:39:A:PHE:HD1	1:39:A:PHE:H	13	0.32
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	20	0.32
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD2	16	0.32
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD11	11	0.32
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	4	0.32
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	5	0.32
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	6	0.32
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	8	0.32
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	9	0.32
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	13	0.32
(1,303)	1:47:A:PHE:HE1	1:47:A:PHE:HD1	18	0.32
(1,286)	1:45:A:ILE:HG22	1:9:A:ILE:HG12	15	0.32
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	19	0.32
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	4	0.32
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	17	0.32
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD12	20	0.32
(1,264)	1:42:A:THR:HG23	1:12:A:LYS:HG2	1	0.32
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD2	8	0.32
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	3	0.32
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	17	0.32
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	10	0.32
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	9	0.32
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	12	0.32
(1,144)	1:95:A:MET:H	1:14:A:THR:HG21	14	0.32
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG23	15	0.32
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	8	0.32
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	10	0.32
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	20	0.32
(1,139)	1:25:A:CYS:HB3	1:45:A:ILE:HD12	12	0.32
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	2	0.32
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	10	0.32
(1,117)	1:20:A:ILE:HD13	1:39:A:PHE:H	16	0.32
(1,115)	1:38:A:ASN:HB2	1:20:A:ILE:HD12	8	0.32
(1,106)	1:9:A:ILE:HD12	1:9:A:ILE:HA	10	0.32
(1,75)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	14	0.32
(1,74)	1:1:A:ALA:HB1	1:83:A:PRO:HA	17	0.32
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	11	0.32
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	19	0.32
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	16	0.32
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	9	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:98:A:ILE:HG22	1:92:A:SER:H	8	0.32
(1,51)	1:98:A:ILE:HG21	1:92:A:SER:H	16	0.32
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	18	0.32
(1,47)	1:20:A:ILE:HG21	1:21:A:LEU:H	17	0.32
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	9	0.32
(1,31)	1:9:A:ILE:HG12	1:45:A:ILE:HD13	1	0.32
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	13	0.32
(1,19)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	11	0.32
(1,11)	1:73:A:VAL:HG23	1:98:A:ILE:HD13	18	0.32
(3,338)	1:104:A:GLU:HG2	1:104:A:GLU:HA	16	0.31
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	20	0.31
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	8	0.31
(3,310)	1:105:A:ARG:H	1:103:A:ASP:HB2	20	0.31
(3,296)	1:45:A:ILE:HG12	1:46:A:LYS:H	8	0.31
(3,287)	1:4:A:CYS:HB2	1:5:A:LYS:H	4	0.31
(3,257)	1:93:A:ALA:HB3	1:98:A:ILE:HG13	2	0.31
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	9	0.31
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG22	20	0.31
(3,227)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	5	0.31
(3,226)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	1	0.31
(3,216)	1:19:A:ARG:HG3	1:95:A:MET:H	8	0.31
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	15	0.31
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	16	0.31
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	1	0.31
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	6	0.31
(3,209)	1:104:A:GLU:H	1:104:A:GLU:HG2	7	0.31
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG3	4	0.31
(3,178)	1:27:A:SER:HB2	1:28:A:GLY:H	13	0.31
(3,165)	1:4:A:CYS:HB3	1:5:A:LYS:H	10	0.31
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	1	0.31
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	19	0.31
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	8	0.31
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	9	0.31
(3,97)	1:56:A:ARG:HB2	1:76:A:TYR:HB3	6	0.31
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG22	8	0.31
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.31
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	9	0.31
(3,75)	1:76:A:TYR:HA	1:76:A:TYR:HD1	20	0.31
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	16	0.31
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	15	0.31
(3,14)	1:50:A:ASP:HA	1:50:A:ASP:HB3	1	0.31
(3,14)	1:50:A:ASP:HA	1:50:A:ASP:HB3	19	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	2	0.31
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	13	0.31
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	16	0.31
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	19	0.31
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	6	0.31
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	11	0.31
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	17	0.31
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	18	0.31
(1,2123)	1:36:A:TYR:HA	1:22:A:GLN:HA	10	0.31
(1,2096)	1:73:A:VAL:HG23	1:72:A:GLU:HA	15	0.31
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	6	0.31
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	20	0.31
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	18	0.31
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	19	0.31
(1,1998)	1:32:A:VAL:HG22	1:32:A:VAL:HA	10	0.31
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD12	17	0.31
(1,1958)	1:11:A:ILE:H	1:10:A:VAL:HG23	3	0.31
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	6	0.31
(1,1916)	1:9:A:ILE:HD12	1:9:A:ILE:HG23	11	0.31
(1,1913)	1:9:A:ILE:HD13	1:9:A:ILE:HA	1	0.31
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	5	0.31
(1,1850)	1:71:A:THR:H	1:70:A:PHE:HE1	17	0.31
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD12	12	0.31
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	8	0.31
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG22	13	0.31
(1,1796)	1:32:A:VAL:H	1:26:A:ARG:HA	18	0.31
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	6	0.31
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	18	0.31
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	4	0.31
(1,1732)	1:95:A:MET:HB3	1:95:A:MET:H	18	0.31
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	10	0.31
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG21	4	0.31
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG22	19	0.31
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD12	5	0.31
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	14	0.31
(1,1343)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	19	0.31
(1,1333)	1:23:A:TYR:HD2	1:23:A:TYR:HA	2	0.31
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG22	5	0.31
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG22	8	0.31
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	3	0.31
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	20	0.31
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	9	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:9:A:ILE:HD12	1:9:A:ILE:HA	18	0.31
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	14	0.31
(1,1166)	1:47:A:PHE:HD2	1:30:A:THR:HG21	5	0.31
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	14	0.31
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	20	0.31
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	4	0.31
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD11	15	0.31
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	10	0.31
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	13	0.31
(1,1105)	1:98:A:ILE:HD13	1:94:A:ARG:H	10	0.31
(1,1105)	1:98:A:ILE:HD11	1:94:A:ARG:H	12	0.31
(1,1097)	1:10:A:VAL:HG22	1:10:A:VAL:HA	15	0.31
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG23	4	0.31
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG22	12	0.31
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	14	0.31
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB2	11	0.31
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	13	0.31
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG23	15	0.31
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	9	0.31
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	13	0.31
(1,963)	1:80:A:LEU:HA	1:80:A:LEU:HB2	8	0.31
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD13	14	0.31
(1,909)	1:10:A:VAL:HG23	1:90:A:GLU:HG2	15	0.31
(1,907)	1:10:A:VAL:HG23	1:42:A:THR:HB	3	0.31
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	1	0.31
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG21	17	0.31
(1,889)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	8	0.31
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	10	0.31
(1,889)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	19	0.31
(1,883)	1:23:A:TYR:HE2	1:11:A:ILE:HG21	18	0.31
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	14	0.31
(1,850)	1:113:A:TRP:HB3	1:114:A:ARG:H	9	0.31
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	14	0.31
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	7	0.31
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	6	0.31
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	4	0.31
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	6	0.31
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG23	19	0.31
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	16	0.31
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	2	0.31
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	16	0.31
(1,634)	1:74:A:GLU:HB2	1:74:A:GLU:H	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	14	0.31
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	11	0.31
(1,525)	1:20:A:ILE:HD12	1:38:A:ASN:H	5	0.31
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG12	11	0.31
(1,484)	1:29:A:ASN:H	1:29:A:ASN:HB2	6	0.31
(1,469)	1:24:A:HIS:H	1:60:A:LEU:HB2	18	0.31
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD1	15	0.31
(1,413)	1:10:A:VAL:HG22	1:10:A:VAL:H	16	0.31
(1,286)	1:45:A:ILE:HG22	1:9:A:ILE:HG12	17	0.31
(1,273)	1:73:A:VAL:HG22	1:73:A:VAL:HA	8	0.31
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	17	0.31
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	18	0.31
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	20	0.31
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD11	1	0.31
(1,262)	1:93:A:ALA:HB3	1:13:A:ASN:HB2	5	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	1	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	2	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	3	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	4	0.31
(1,177)	1:23:A:TYR:HD1	1:23:A:TYR:HE1	5	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	6	0.31
(1,177)	1:23:A:TYR:HD1	1:23:A:TYR:HE1	8	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	9	0.31
(1,177)	1:23:A:TYR:HD1	1:23:A:TYR:HE1	11	0.31
(1,177)	1:23:A:TYR:HD1	1:23:A:TYR:HE1	12	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	13	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	14	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	15	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	16	0.31
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	19	0.31
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD2	9	0.31
(1,156)	1:73:A:VAL:HG23	1:61:A:PHE:HE2	11	0.31
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG22	2	0.31
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG23	13	0.31
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	2	0.31
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD11	3	0.31
(1,117)	1:20:A:ILE:HD13	1:39:A:PHE:H	7	0.31
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD12	6	0.31
(1,74)	1:1:A:ALA:HB3	1:83:A:PRO:HA	8	0.31
(1,74)	1:1:A:ALA:HB1	1:83:A:PRO:HA	13	0.31
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	6	0.31
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	14	0.31
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB1	6	0.31
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG22	14	0.31
(1,43)	1:7:A:ILE:HD12	1:7:A:ILE:HG21	3	0.31
(1,30)	1:45:A:ILE:HD13	1:45:A:ILE:HB	5	0.31
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD12	17	0.31
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	16	0.31
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	12	0.31
(4,10)	1:95:A:MET:H	1:14:A:THR:O	6	0.3
(4,10)	1:95:A:MET:H	1:14:A:THR:O	12	0.3
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	4	0.3
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	10	0.3
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	14	0.3
(3,310)	1:105:A:ARG:H	1:103:A:ASP:HB2	7	0.3
(3,303)	1:88:A:ARG:HB3	1:88:A:ARG:H	11	0.3
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	2	0.3
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	17	0.3
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	18	0.3
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	11	0.3
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	4	0.3
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG3	5	0.3
(3,206)	1:7:A:ILE:H	1:6:A:GLU:HB2	2	0.3
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	11	0.3
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	19	0.3
(3,161)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	10	0.3
(3,147)	1:5:A:LYS:HG2	1:6:A:GLU:H	3	0.3
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	3	0.3
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	19	0.3
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	8	0.3
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD12	7	0.3
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	7	0.3
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	16	0.3
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	12	0.3
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	16	0.3
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	5	0.3
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	9	0.3
(3,14)	1:50:A:ASP:HA	1:50:A:ASP:HB3	5	0.3
(3,14)	1:50:A:ASP:HA	1:50:A:ASP:HB3	12	0.3
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG21	4	0.3
(1,2257)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	5	0.3
(1,2255)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	10	0.3
(1,2236)	1:73:A:VAL:HG22	1:61:A:PHE:HD2	3	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	10	0.3
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB2	15	0.3
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	20	0.3
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	19	0.3
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	3	0.3
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	6	0.3
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	7	0.3
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	18	0.3
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	14	0.3
(1,2051)	1:101:A:LYS:HB2	1:107:A:PRO:HA	20	0.3
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	10	0.3
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	7	0.3
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD13	11	0.3
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD11	16	0.3
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	20	0.3
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	6	0.3
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE1	17	0.3
(1,1928)	1:98:A:ILE:HG21	1:98:A:ILE:HA	2	0.3
(1,1913)	1:9:A:ILE:HD12	1:9:A:ILE:HA	12	0.3
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	1	0.3
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	12	0.3
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	13	0.3
(1,1765)	1:104:A:GLU:H	1:104:A:GLU:HB2	2	0.3
(1,1731)	1:94:A:ARG:HB3	1:95:A:MET:H	15	0.3
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	4	0.3
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG22	8	0.3
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG22	18	0.3
(1,1541)	1:20:A:ILE:HD12	1:38:A:ASN:H	8	0.3
(1,1524)	1:36:A:TYR:H	1:36:A:TYR:HD1	15	0.3
(1,1464)	1:22:A:GLN:HG3	1:22:A:GLN:H	18	0.3
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	4	0.3
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	20	0.3
(1,1408)	1:10:A:VAL:HG23	1:10:A:VAL:H	6	0.3
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	20	0.3
(1,1333)	1:23:A:TYR:HD2	1:23:A:TYR:HA	3	0.3
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	19	0.3
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG22	18	0.3
(1,1243)	1:20:A:ILE:HD12	1:20:A:ILE:HB	19	0.3
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	12	0.3
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	16	0.3
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	1	0.3
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD13	9	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	10	0.3
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	18	0.3
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG22	16	0.3
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	18	0.3
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	4	0.3
(1,1105)	1:98:A:ILE:HD11	1:94:A:ARG:H	8	0.3
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG22	17	0.3
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	7	0.3
(1,1071)	1:44:A:ILE:HD12	1:44:A:ILE:HG12	16	0.3
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	17	0.3
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	9	0.3
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	13	0.3
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	1	0.3
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	12	0.3
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	15	0.3
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	19	0.3
(1,963)	1:80:A:LEU:HA	1:80:A:LEU:HB2	10	0.3
(1,940)	1:7:A:ILE:HD11	1:7:A:ILE:HA	19	0.3
(1,913)	1:15:A:LEU:HD12	1:19:A:ARG:HB3	14	0.3
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG22	14	0.3
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	3	0.3
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	11	0.3
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	5	0.3
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD12	12	0.3
(1,798)	1:9:A:ILE:H	1:9:A:ILE:HG12	18	0.3
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	13	0.3
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG22	2	0.3
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	7	0.3
(1,712)	1:96:A:ASP:H	1:95:A:MET:HB3	17	0.3
(1,711)	1:94:A:ARG:HB3	1:96:A:ASP:H	12	0.3
(1,705)	1:95:A:MET:HB3	1:95:A:MET:H	18	0.3
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	18	0.3
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	1	0.3
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	6	0.3
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	7	0.3
(1,668)	1:85:A:CYS:H	1:84:A:LEU:HA	16	0.3
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	15	0.3
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	18	0.3
(1,636)	1:73:A:VAL:HG21	1:74:A:GLU:H	11	0.3
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	5	0.3
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	10	0.3
(1,557)	1:46:A:LYS:HB3	1:46:A:LYS:H	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,488)	1:29:A:ASN:HB2	1:30:A:THR:H	13	0.3
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD2	19	0.3
(1,427)	1:14:A:THR:H	1:93:A:ALA:HB1	6	0.3
(1,427)	1:14:A:THR:H	1:93:A:ALA:HB3	17	0.3
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	14	0.3
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	8	0.3
(1,303)	1:47:A:PHE:HE2	1:47:A:PHE:HD2	11	0.3
(1,286)	1:45:A:ILE:HG22	1:9:A:ILE:HG12	2	0.3
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	10	0.3
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	6	0.3
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	7	0.3
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	10	0.3
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	17	0.3
(1,177)	1:23:A:TYR:HD1	1:23:A:TYR:HE1	20	0.3
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	12	0.3
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE2	3	0.3
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG22	8	0.3
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG23	20	0.3
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	19	0.3
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	4	0.3
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	7	0.3
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	9	0.3
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	20	0.3
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	10	0.3
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	4	0.3
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	2	0.3
(1,106)	1:9:A:ILE:HD11	1:9:A:ILE:HA	5	0.3
(1,74)	1:1:A:ALA:HB2	1:83:A:PRO:HA	1	0.3
(1,65)	1:34:A:VAL:HG22	1:34:A:VAL:HA	16	0.3
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	6	0.3
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	13	0.3
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	10	0.3
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG22	2	0.3
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG23	11	0.3
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	9	0.3
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	10	0.3
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	6	0.3
(1,30)	1:45:A:ILE:HD11	1:45:A:ILE:HB	7	0.3
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	1	0.3
(1,8)	1:10:A:VAL:HG22	1:10:A:VAL:HA	14	0.3
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	2	0.29
(3,317)	1:47:A:PHE:H	1:8:A:GLU:HG3	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,303)	1:88:A:ARG:HB3	1:88:A:ARG:H	14	0.29
(3,289)	1:48:A:LYS:HB3	1:6:A:GLU:H	6	0.29
(3,265)	1:31:A:ASN:HA	1:26:A:ARG:HB3	8	0.29
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	1	0.29
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	6	0.29
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	18	0.29
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	20	0.29
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	9	0.29
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	8	0.29
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	7	0.29
(3,203)	1:105:A:ARG:H	1:103:A:ASP:HB2	20	0.29
(3,195)	1:88:A:ARG:HB3	1:88:A:ARG:H	11	0.29
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	13	0.29
(3,192)	1:86:A:GLY:H	1:5:A:LYS:HB3	7	0.29
(3,182)	1:45:A:ILE:HG12	1:46:A:LYS:H	8	0.29
(3,165)	1:4:A:CYS:HB2	1:5:A:LYS:H	4	0.29
(3,161)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	4	0.29
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG22	7	0.29
(3,134)	1:36:A:TYR:HD2	1:37:A:LEU:HA	4	0.29
(3,125)	1:73:A:VAL:HG13	1:73:A:VAL:HG23	18	0.29
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB2	11	0.29
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	11	0.29
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG23	6	0.29
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	10	0.29
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	5	0.29
(3,79)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	15	0.29
(3,76)	1:33:A:GLY:HA3	1:24:A:HIS:HD1	13	0.29
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	14	0.29
(3,62)	1:56:A:ARG:HB3	1:55:A:SER:HB3	6	0.29
(3,48)	1:45:A:ILE:HA	1:45:A:ILE:HG13	1	0.29
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	1	0.29
(3,14)	1:50:A:ASP:HA	1:50:A:ASP:HB3	13	0.29
(3,14)	1:111:A:ASN:HA	1:111:A:ASN:HB2	16	0.29
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	12	0.29
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	12	0.29
(1,2203)	1:103:A:ASP:HA	1:103:A:ASP:HB2	13	0.29
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	12	0.29
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	14	0.29
(1,2096)	1:73:A:VAL:HG22	1:72:A:GLU:HA	13	0.29
(1,2096)	1:73:A:VAL:HG22	1:72:A:GLU:HA	20	0.29
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	10	0.29
(1,2051)	1:101:A:LYS:HB2	1:107:A:PRO:HA	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	3	0.29
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	3	0.29
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	2	0.29
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	6	0.29
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG21	2	0.29
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG22	1	0.29
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	5	0.29
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	9	0.29
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD12	18	0.29
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	13	0.29
(1,1828)	1:9:A:ILE:H	1:9:A:ILE:HG12	18	0.29
(1,1787)	1:115:A:SER:H	1:114:A:ARG:HB3	19	0.29
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	17	0.29
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG23	20	0.29
(1,1731)	1:94:A:ARG:HB3	1:95:A:MET:H	4	0.29
(1,1721)	1:57:A:TRP:H	1:76:A:TYR:H	16	0.29
(1,1698)	1:86:A:GLY:H	1:85:A:CYS:HB2	14	0.29
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	16	0.29
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	9	0.29
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG21	11	0.29
(1,1596)	1:49:A:ASP:HB3	1:49:A:ASP:H	8	0.29
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD11	2	0.29
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	17	0.29
(1,1524)	1:36:A:TYR:H	1:36:A:TYR:HD1	10	0.29
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG23	5	0.29
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	2	0.29
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	6	0.29
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	7	0.29
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	10	0.29
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	11	0.29
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	15	0.29
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	20	0.29
(1,1333)	1:23:A:TYR:HD2	1:23:A:TYR:HA	10	0.29
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG22	14	0.29
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	1	0.29
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB2	14	0.29
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	3	0.29
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	5	0.29
(1,1172)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	17	0.29
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	7	0.29
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	19	0.29
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	14	0.29
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	13	0.29
(1,1129)	1:45:A:ILE:HA	1:45:A:ILE:HG12	5	0.29
(1,1107)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	19	0.29
(1,1105)	1:98:A:ILE:HD13	1:94:A:ARG:H	1	0.29
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG21	7	0.29
(1,1071)	1:44:A:ILE:HD12	1:44:A:ILE:HG12	13	0.29
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	14	0.29
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	18	0.29
(1,1071)	1:44:A:ILE:HD12	1:44:A:ILE:HG12	19	0.29
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG23	17	0.29
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	13	0.29
(1,982)	1:73:A:VAL:HG21	1:72:A:GLU:HA	8	0.29
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	7	0.29
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	8	0.29
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	16	0.29
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	18	0.29
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	20	0.29
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	19	0.29
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG22	2	0.29
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG21	7	0.29
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	4	0.29
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	18	0.29
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	14	0.29
(1,817)	1:71:A:THR:H	1:70:A:PHE:HE1	17	0.29
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	8	0.29
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG22	13	0.29
(1,769)	1:32:A:VAL:H	1:26:A:ARG:HA	18	0.29
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	12	0.29
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	6	0.29
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	18	0.29
(1,739)	1:104:A:GLU:H	1:104:A:GLU:HB2	2	0.29
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	4	0.29
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	10	0.29
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG21	4	0.29
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG22	19	0.29
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD12	5	0.29
(1,336)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	15	0.29
(1,319)	1:90:A:GLU:HA	1:10:A:VAL:H	11	0.29
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	3	0.29
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	12	0.29
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:45:A:ILE:HG21	1:9:A:ILE:HG12	9	0.29
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	3	0.29
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	7	0.29
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	8	0.29
(1,244)	1:70:A:PHE:HD1	1:70:A:PHE:HB3	13	0.29
(1,198)	1:92:A:SER:HA	1:92:A:SER:HB3	12	0.29
(1,198)	1:92:A:SER:HA	1:92:A:SER:HB3	17	0.29
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	4	0.29
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	14	0.29
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	9	0.29
(1,157)	1:73:A:VAL:HG21	1:61:A:PHE:HD1	4	0.29
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	5	0.29
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	7	0.29
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	19	0.29
(1,124)	1:45:A:ILE:HG21	1:45:A:ILE:HD13	12	0.29
(1,124)	1:45:A:ILE:HG23	1:45:A:ILE:HD11	18	0.29
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	19	0.29
(1,94)	1:9:A:ILE:HG22	1:75:A:ALA:HA	3	0.29
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	14	0.29
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG21	15	0.29
(1,65)	1:34:A:VAL:HG23	1:34:A:VAL:HA	1	0.29
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	13	0.29
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG21	13	0.29
(1,45)	1:9:A:ILE:HD12	1:7:A:ILE:HG22	14	0.29
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	15	0.29
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	3	0.29
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD11	17	0.29
(1,15)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	18	0.29
(1,14)	1:98:A:ILE:HD12	1:71:A:THR:HG22	6	0.29
(1,2)	1:30:A:THR:HA	1:30:A:THR:HG22	18	0.29
(3,319)	1:19:A:ARG:HG3	1:95:A:MET:H	5	0.28
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	8	0.28
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	9	0.28
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	12	0.28
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	17	0.28
(3,297)	1:47:A:PHE:HB3	1:48:A:LYS:H	7	0.28
(3,297)	1:47:A:PHE:HB3	1:48:A:LYS:H	11	0.28
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	8	0.28
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	18	0.28
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	20	0.28
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	1	0.28
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,228)	1:7:A:ILE:HG22	1:84:A:LEU:HB3	7	0.28
(3,227)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	6	0.28
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	8	0.28
(3,218)	1:11:A:ILE:HG23	1:37:A:LEU:HB2	5	0.28
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	4	0.28
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	1	0.28
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	10	0.28
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	14	0.28
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	4	0.28
(3,203)	1:105:A:ARG:H	1:103:A:ASP:HB2	7	0.28
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	4	0.28
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	5	0.28
(3,134)	1:36:A:TYR:HD1	1:22:A:GLN:HA	3	0.28
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG23	4	0.28
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	11	0.28
(3,75)	1:76:A:TYR:HA	1:76:A:TYR:HD2	7	0.28
(3,73)	1:45:A:ILE:HB	1:9:A:ILE:HD11	17	0.28
(3,65)	1:6:A:GLU:HG2	1:48:A:LYS:HA	13	0.28
(3,64)	1:6:A:GLU:HG3	1:48:A:LYS:HA	7	0.28
(3,50)	1:10:A:VAL:HG21	1:10:A:VAL:HA	5	0.28
(3,50)	1:10:A:VAL:HG21	1:10:A:VAL:HA	16	0.28
(3,48)	1:45:A:ILE:HA	1:45:A:ILE:HG13	5	0.28
(3,48)	1:45:A:ILE:HA	1:45:A:ILE:HG13	7	0.28
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	13	0.28
(3,4)	1:45:A:ILE:HG13	1:45:A:ILE:HB	12	0.28
(1,2250)	1:11:A:ILE:HD12	1:61:A:PHE:HE1	19	0.28
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	9	0.28
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	1	0.28
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	6	0.28
(1,2237)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	8	0.28
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	8	0.28
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB3	9	0.28
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	2	0.28
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	12	0.28
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	14	0.28
(1,2123)	1:36:A:TYR:HA	1:22:A:GLN:HA	15	0.28
(1,2111)	1:23:A:TYR:HD2	1:23:A:TYR:HA	15	0.28
(1,2096)	1:73:A:VAL:HG22	1:72:A:GLU:HA	7	0.28
(1,1948)	1:61:A:PHE:HD1	1:71:A:THR:HG21	19	0.28
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	3	0.28
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	9	0.28
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.28
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	4	0.28
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	5	0.28
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	19	0.28
(1,1631)	1:58:A:ASN:HB3	1:59:A:CYS:H	5	0.28
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	20	0.28
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG22	3	0.28
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG23	18	0.28
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD1	1	0.28
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD2	5	0.28
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	1	0.28
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	3	0.28
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	4	0.28
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	5	0.28
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	8	0.28
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	9	0.28
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	12	0.28
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	13	0.28
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	16	0.28
(1,1362)	1:70:A:PHE:HE2	1:70:A:PHE:HD2	17	0.28
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	18	0.28
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	5	0.28
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	17	0.28
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	18	0.28
(1,1293)	1:45:A:ILE:HD11	1:9:A:ILE:HD13	13	0.28
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	19	0.28
(1,1247)	1:20:A:ILE:HA	1:20:A:ILE:HD13	18	0.28
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	17	0.28
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG21	5	0.28
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	17	0.28
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	3	0.28
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	18	0.28
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	3	0.28
(1,1172)	1:20:A:ILE:HG21	1:20:A:ILE:HG13	20	0.28
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	19	0.28
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB1	14	0.28
(1,1163)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	8	0.28
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	11	0.28
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	16	0.28
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	3	0.28
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD13	11	0.28
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD11	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG21	5	0.28
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG22	15	0.28
(1,1137)	1:9:A:ILE:HD13	1:7:A:ILE:HG22	1	0.28
(1,1137)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	11	0.28
(1,1110)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	19	0.28
(1,1105)	1:98:A:ILE:HD11	1:94:A:ARG:H	15	0.28
(1,1097)	1:10:A:VAL:HG22	1:10:A:VAL:HA	10	0.28
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	11	0.28
(1,1061)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	4	0.28
(1,1058)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	18	0.28
(1,1022)	1:73:A:VAL:HG22	1:91:A:LEU:HB2	6	0.28
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	5	0.28
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	10	0.28
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	11	0.28
(1,965)	1:113:A:TRP:HA	1:71:A:THR:HG21	6	0.28
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	11	0.28
(1,900)	1:111:A:ASN:HB2	1:71:A:THR:HG21	12	0.28
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	11	0.28
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG21	6	0.28
(1,889)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	2	0.28
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	5	0.28
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	1	0.28
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	13	0.28
(1,734)	1:102:A:MET:H	1:102:A:MET:HG2	10	0.28
(1,704)	1:94:A:ARG:HB3	1:95:A:MET:H	15	0.28
(1,678)	1:87:A:LYS:HB3	1:88:A:ARG:H	11	0.28
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	16	0.28
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	4	0.28
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG22	8	0.28
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG22	18	0.28
(1,576)	1:49:A:ASP:HB3	1:49:A:ASP:H	8	0.28
(1,525)	1:20:A:ILE:HD12	1:38:A:ASN:H	8	0.28
(1,510)	1:36:A:TYR:H	1:36:A:TYR:HD1	15	0.28
(1,460)	1:22:A:GLN:HG3	1:22:A:GLN:H	18	0.28
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	4	0.28
(1,413)	1:10:A:VAL:HG23	1:10:A:VAL:H	6	0.28
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	20	0.28
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	14	0.28
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	2	0.28
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	1	0.28
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	2	0.28
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	15	0.28
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	3	0.28
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD11	14	0.28
(1,240)	1:24:A:HIS:HD1	1:24:A:HIS:HA	18	0.28
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	1	0.28
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	5	0.28
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	10	0.28
(1,177)	1:23:A:TYR:HD2	1:23:A:TYR:HE2	18	0.28
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	8	0.28
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	9	0.28
(1,157)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	19	0.28
(1,156)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	2	0.28
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG23	12	0.28
(1,145)	1:42:A:THR:HG21	1:12:A:LYS:HA	11	0.28
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	2	0.28
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	11	0.28
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	6	0.28
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	17	0.28
(1,75)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	4	0.28
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	9	0.28
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	10	0.28
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	4	0.28
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	14	0.28
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG22	3	0.28
(1,40)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	18	0.28
(1,30)	1:45:A:ILE:HD11	1:45:A:ILE:HB	1	0.28
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD11	20	0.28
(1,22)	1:9:A:ILE:HD12	1:9:A:ILE:HG23	11	0.28
(1,17)	1:99:A:TYR:H	1:98:A:ILE:HD12	16	0.28
(1,16)	1:98:A:ILE:HD12	1:94:A:ARG:H	14	0.28
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	16	0.27
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	17	0.27
(3,317)	1:47:A:PHE:H	1:8:A:GLU:HG3	2	0.27
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG2	7	0.27
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG2	1	0.27
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG3	16	0.27
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB2	2	0.27
(3,289)	1:48:A:LYS:HB3	1:6:A:GLU:H	12	0.27
(3,272)	1:92:A:SER:HB3	1:93:A:ALA:H	18	0.27
(3,257)	1:93:A:ALA:HB3	1:98:A:ILE:HG13	9	0.27
(3,245)	1:5:A:LYS:HA	1:5:A:LYS:HB3	3	0.27
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	15	0.27
(3,218)	1:11:A:ILE:HG22	1:37:A:LEU:HB2	11	0.27
(3,212)	1:47:A:PHE:H	1:8:A:GLU:HG3	13	0.27
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	19	0.27
(3,195)	1:88:A:ARG:HB3	1:88:A:ARG:H	14	0.27
(3,185)	1:47:A:PHE:HB3	1:48:A:LYS:H	7	0.27
(3,185)	1:47:A:PHE:HB3	1:48:A:LYS:H	11	0.27
(3,179)	1:55:A:SER:HB2	1:29:A:ASN:H	3	0.27
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	8	0.27
(3,169)	1:48:A:LYS:HB3	1:6:A:GLU:H	6	0.27
(3,161)	1:7:A:ILE:HG22	1:84:A:LEU:HB3	9	0.27
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG23	11	0.27
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG22	1	0.27
(3,156)	1:10:A:VAL:HG21	1:91:A:LEU:H	3	0.27
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG22	17	0.27
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	6	0.27
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	7	0.27
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	3	0.27
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD13	3	0.27
(3,50)	1:10:A:VAL:HG22	1:10:A:VAL:HA	6	0.27
(3,49)	1:98:A:ILE:HG21	1:98:A:ILE:HA	2	0.27
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	13	0.27
(3,16)	1:26:A:ARG:HB2	1:31:A:ASN:HA	14	0.27
(3,10)	1:20:A:ILE:HG22	1:21:A:LEU:HA	1	0.27
(1,2274)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	17	0.27
(1,2274)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	20	0.27
(1,2255)	1:73:A:VAL:HG22	1:59:A:CYS:HB3	1	0.27
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	14	0.27
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	16	0.27
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	12	0.27
(1,2103)	1:90:A:GLU:HG3	1:91:A:LEU:HA	3	0.27
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	6	0.27
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	13	0.27
(1,1982)	1:47:A:PHE:HD1	1:30:A:THR:HB	9	0.27
(1,1962)	1:34:A:VAL:HG22	1:34:A:VAL:HA	16	0.27
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	20	0.27
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD11	12	0.27
(1,1930)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	8	0.27
(1,1928)	1:98:A:ILE:HG22	1:98:A:ILE:HA	19	0.27
(1,1927)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	15	0.27
(1,1832)	1:90:A:GLU:H	1:89:A:TYR:HB3	7	0.27
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG22	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG22	16	0.27
(1,1762)	1:102:A:MET:H	1:101:A:LYS:HB2	14	0.27
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	11	0.27
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	10	0.27
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	2	0.27
(1,1501)	1:29:A:ASN:HB2	1:30:A:THR:H	16	0.27
(1,1474)	1:23:A:TYR:H	1:34:A:VAL:HG13	5	0.27
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	13	0.27
(1,1425)	1:13:A:ASN:HB3	1:13:A:ASN:H	4	0.27
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	5	0.27
(1,1408)	1:10:A:VAL:HG21	1:10:A:VAL:H	20	0.27
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	14	0.27
(1,1362)	1:70:A:PHE:HE1	1:70:A:PHE:HD1	19	0.27
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	3	0.27
(1,1300)	1:33:A:GLY:H	1:34:A:VAL:HG23	2	0.27
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	10	0.27
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD12	18	0.27
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	5	0.27
(1,1211)	1:32:A:VAL:HG22	1:32:A:VAL:HA	10	0.27
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG21	17	0.27
(1,1160)	1:34:A:VAL:HG21	1:34:A:VAL:HA	2	0.27
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG21	7	0.27
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	16	0.27
(1,1102)	1:98:A:ILE:HD11	1:71:A:THR:HG21	13	0.27
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG23	14	0.27
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	17	0.27
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	9	0.27
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	8	0.27
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	11	0.27
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	17	0.27
(1,999)	1:15:A:LEU:H	1:95:A:MET:HA	18	0.27
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	2	0.27
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	4	0.27
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	6	0.27
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	17	0.27
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	5	0.27
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD12	17	0.27
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	17	0.27
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG21	9	0.27
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	15	0.27
(1,898)	1:94:A:ARG:HA	1:15:A:LEU:HD12	13	0.27
(1,889)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	11	0.27
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD11	16	0.27
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD12	18	0.27
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	13	0.27
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	18	0.27
(1,761)	1:115:A:SER:H	1:114:A:ARG:HB3	19	0.27
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	17	0.27
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	4	0.27
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG23	20	0.27
(1,704)	1:94:A:ARG:HB3	1:95:A:MET:H	4	0.27
(1,695)	1:57:A:TRP:H	1:76:A:TYR:H	16	0.27
(1,676)	1:86:A:GLY:H	1:85:A:CYS:HB2	14	0.27
(1,668)	1:85:A:CYS:H	1:84:A:LEU:HA	7	0.27
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	9	0.27
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG21	11	0.27
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD11	2	0.27
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	17	0.27
(1,510)	1:36:A:TYR:H	1:36:A:TYR:HD1	10	0.27
(1,489)	1:30:A:THR:H	1:30:A:THR:HG23	5	0.27
(1,319)	1:90:A:GLU:HA	1:10:A:VAL:H	3	0.27
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	17	0.27
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	3	0.27
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	1	0.27
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	15	0.27
(1,293)	1:47:A:PHE:HA	1:47:A:PHE:HD2	5	0.27
(1,273)	1:73:A:VAL:HG22	1:73:A:VAL:HA	4	0.27
(1,250)	1:61:A:PHE:HB3	1:61:A:PHE:HD2	3	0.27
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	16	0.27
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	20	0.27
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	16	0.27
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD1	5	0.27
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	13	0.27
(1,156)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	5	0.27
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	20	0.27
(1,143)	1:95:A:MET:HG3	1:14:A:THR:HG22	18	0.27
(1,133)	1:92:A:SER:HA	1:93:A:ALA:HB3	12	0.27
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	8	0.27
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	3	0.27
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	15	0.27
(1,85)	1:74:A:GLU:HA	1:74:A:GLU:HG2	5	0.27
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	5	0.27
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	5	0.27
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB2	15	0.27
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	12	0.27
(1,51)	1:98:A:ILE:HG21	1:92:A:SER:H	17	0.27
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG23	10	0.27
(1,42)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	14	0.27
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	5	0.27
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD11	17	0.27
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	1	0.27
(1,19)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	9	0.27
(1,11)	1:73:A:VAL:HG22	1:98:A:ILE:HD12	6	0.27
(4,42)	1:10:A:VAL:O	1:91:A:LEU:N	3	0.26
(4,33)	1:26:A:ARG:O	1:58:A:ASN:N	4	0.26
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	7	0.26
(3,332)	1:69:A:PHE:HA	1:115:A:SER:HB3	10	0.26
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	1	0.26
(3,327)	1:10:A:VAL:HG22	1:10:A:VAL:HA	14	0.26
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	14	0.26
(3,319)	1:19:A:ARG:HG3	1:95:A:MET:H	1	0.26
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG3	15	0.26
(3,310)	1:105:A:ARG:H	1:103:A:ASP:HB2	10	0.26
(3,297)	1:47:A:PHE:HB3	1:48:A:LYS:H	18	0.26
(3,287)	1:4:A:CYS:HB2	1:5:A:LYS:H	9	0.26
(3,216)	1:19:A:ARG:HG3	1:95:A:MET:H	5	0.26
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	9	0.26
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	13	0.26
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	9	0.26
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	12	0.26
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	17	0.26
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	5	0.26
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	16	0.26
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	18	0.26
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG23	2	0.26
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	9	0.26
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	1	0.26
(3,134)	1:36:A:TYR:HD1	1:22:A:GLN:HA	20	0.26
(3,92)	1:52:A:THR:HB	1:52:A:THR:HG22	18	0.26
(3,86)	1:71:A:THR:HA	1:71:A:THR:HG21	7	0.26
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE2	17	0.26
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	4	0.26
(3,75)	1:76:A:TYR:HA	1:76:A:TYR:HD2	3	0.26
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,29)	1:115:A:SER:HA	1:69:A:PHE:HA	3	0.26
(3,29)	1:114:A:ARG:HA	1:69:A:PHE:HA	9	0.26
(3,18)	1:103:A:ASP:HA	1:103:A:ASP:HB2	2	0.26
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	12	0.26
(3,16)	1:26:A:ARG:HB2	1:31:A:ASN:HA	20	0.26
(3,10)	1:20:A:ILE:HG22	1:21:A:LEU:HA	14	0.26
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	3	0.26
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	6	0.26
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	12	0.26
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	15	0.26
(1,2236)	1:73:A:VAL:HG23	1:61:A:PHE:HD2	11	0.26
(1,2235)	1:111:A:ASN:H	1:97:A:ALA:HB1	11	0.26
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	19	0.26
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	14	0.26
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	16	0.26
(1,2048)	1:10:A:VAL:HG21	1:90:A:GLU:H	7	0.26
(1,1962)	1:34:A:VAL:HG23	1:34:A:VAL:HA	1	0.26
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	1	0.26
(1,1955)	1:10:A:VAL:HG22	1:10:A:VAL:HA	14	0.26
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	8	0.26
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG22	14	0.26
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG22	19	0.26
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	6	0.26
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	12	0.26
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG21	19	0.26
(1,1721)	1:57:A:TRP:H	1:76:A:TYR:H	20	0.26
(1,1719)	1:57:A:TRP:H	1:56:A:ARG:HA	7	0.26
(1,1700)	1:88:A:ARG:H	1:87:A:LYS:HA	20	0.26
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	3	0.26
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	2	0.26
(1,1644)	1:70:A:PHE:H	1:69:A:PHE:HA	14	0.26
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	18	0.26
(1,1608)	1:52:A:THR:H	1:50:A:ASP:HA	17	0.26
(1,1595)	1:49:A:ASP:H	1:48:A:LYS:HA	13	0.26
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD12	16	0.26
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG22	11	0.26
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	18	0.26
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	13	0.26
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	14	0.26
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	9	0.26
(1,1333)	1:23:A:TYR:HD2	1:23:A:TYR:HA	11	0.26
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB2	6	0.26
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	5	0.26
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	2	0.26
(1,1243)	1:20:A:ILE:HD12	1:20:A:ILE:HB	1	0.26
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG21	7	0.26
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	14	0.26
(1,1171)	1:1:A:ALA:HB1	1:83:A:PRO:HA	9	0.26
(1,1164)	1:75:A:ALA:HB2	1:9:A:ILE:HG22	8	0.26
(1,1152)	1:15:A:LEU:HA	1:15:A:LEU:HD12	13	0.26
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG21	4	0.26
(1,1141)	1:37:A:LEU:H	1:20:A:ILE:HG22	19	0.26
(1,1140)	1:20:A:ILE:HG23	1:21:A:LEU:H	20	0.26
(1,1105)	1:98:A:ILE:HD11	1:94:A:ARG:H	20	0.26
(1,1097)	1:10:A:VAL:HG21	1:10:A:VAL:HA	8	0.26
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	17	0.26
(1,1055)	1:42:A:THR:HG23	1:11:A:ILE:H	12	0.26
(1,1050)	1:57:A:TRP:HB3	1:75:A:ALA:HB2	3	0.26
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG23	2	0.26
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	18	0.26
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	19	0.26
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	4	0.26
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	11	0.26
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	7	0.26
(1,910)	1:11:A:ILE:H	1:10:A:VAL:HG23	3	0.26
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG21	8	0.26
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG22	16	0.26
(1,890)	1:98:A:ILE:HG21	1:98:A:ILE:HA	2	0.26
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	4	0.26
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	10	0.26
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	5	0.26
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	19	0.26
(1,621)	1:70:A:PHE:H	1:114:A:ARG:H	14	0.26
(1,608)	1:58:A:ASN:HB3	1:59:A:CYS:H	5	0.26
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	10	0.26
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	20	0.26
(1,489)	1:30:A:THR:H	1:30:A:THR:HG22	3	0.26
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG23	18	0.26
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD1	1	0.26
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD2	5	0.26
(1,381)	1:70:A:PHE:HE1	1:70:A:PHE:HA	3	0.26
(1,336)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	7	0.26
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	9	0.26
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	1	0.26
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	10	0.26
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	9	0.26
(1,273)	1:73:A:VAL:HG21	1:73:A:VAL:HA	10	0.26
(1,273)	1:73:A:VAL:HG22	1:73:A:VAL:HA	18	0.26
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB2	15	0.26
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	6	0.26
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	12	0.26
(1,269)	1:98:A:ILE:HB	1:98:A:ILE:HD13	13	0.26
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE2	10	0.26
(1,255)	1:32:A:VAL:HG11	1:47:A:PHE:HE1	11	0.26
(1,244)	1:70:A:PHE:HD1	1:70:A:PHE:HB3	7	0.26
(1,244)	1:70:A:PHE:HD1	1:70:A:PHE:HB3	17	0.26
(1,244)	1:70:A:PHE:HD1	1:70:A:PHE:HB3	20	0.26
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	9	0.26
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	5	0.26
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	6	0.26
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	13	0.26
(1,145)	1:42:A:THR:HG21	1:12:A:LYS:HA	1	0.26
(1,145)	1:42:A:THR:HG21	1:12:A:LYS:HA	16	0.26
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	5	0.26
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	3	0.26
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	5	0.26
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	3	0.26
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	10	0.26
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	11	0.26
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	14	0.26
(1,117)	1:20:A:ILE:HD11	1:39:A:PHE:H	1	0.26
(1,94)	1:9:A:ILE:HG21	1:75:A:ALA:HA	7	0.26
(1,76)	1:36:A:TYR:HA	1:20:A:ILE:HG21	4	0.26
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB3	13	0.26
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	9	0.26
(1,65)	1:34:A:VAL:HG23	1:34:A:VAL:HA	20	0.26
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	2	0.26
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	8	0.26
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	16	0.26
(1,54)	1:7:A:ILE:HG23	1:8:A:GLU:H	9	0.26
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG21	11	0.26
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG23	20	0.26
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG21	19	0.26
(1,45)	1:9:A:ILE:HD13	1:7:A:ILE:HG21	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD13	9	0.26
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	3	0.26
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	16	0.26
(1,19)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	2	0.26
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	14	0.26
(1,15)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	14	0.26
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG22	7	0.26
(4,26)	1:35:A:GLN:H	1:23:A:TYR:O	18	0.25
(4,23)	1:21:A:LEU:H	1:37:A:LEU:O	18	0.25
(3,311)	1:105:A:ARG:HG2	1:105:A:ARG:H	20	0.25
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	13	0.25
(3,287)	1:4:A:CYS:HB3	1:5:A:LYS:H	3	0.25
(3,258)	1:76:A:TYR:HB3	1:75:A:ALA:HB3	20	0.25
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG13	7	0.25
(3,251)	1:99:A:TYR:HA	1:110:A:LEU:HB2	16	0.25
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	19	0.25
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	2	0.25
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	13	0.25
(3,227)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	16	0.25
(3,223)	1:92:A:SER:HB2	1:99:A:TYR:HB2	4	0.25
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	17	0.25
(3,212)	1:47:A:PHE:H	1:8:A:GLU:HG3	2	0.25
(3,212)	1:8:A:GLU:HG2	1:47:A:PHE:H	8	0.25
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG2	7	0.25
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG2	1	0.25
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG3	16	0.25
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	1	0.25
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	2	0.25
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	8	0.25
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	10	0.25
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	15	0.25
(3,203)	1:105:A:ARG:H	1:103:A:ASP:HB2	10	0.25
(3,197)	1:91:A:LEU:H	1:91:A:LEU:HB2	3	0.25
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB2	2	0.25
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	19	0.25
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	2	0.25
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	8	0.25
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	13	0.25
(3,169)	1:48:A:LYS:HB3	1:6:A:GLU:H	12	0.25
(3,161)	1:7:A:ILE:HG23	1:84:A:LEU:HB3	6	0.25
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	14	0.25
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG21	20	0.25
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG21	6	0.25
(3,145)	1:29:A:ASN:H	1:56:A:ARG:HA	2	0.25
(3,98)	1:57:A:TRP:HB3	1:75:A:ALA:HB2	3	0.25
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	9	0.25
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	1	0.25
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	10	0.25
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	5	0.25
(3,51)	1:18:A:SER:HA	1:20:A:ILE:HD12	12	0.25
(3,50)	1:10:A:VAL:HG21	1:10:A:VAL:HA	9	0.25
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	9	0.25
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	4	0.25
(3,34)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	16	0.25
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	12	0.25
(3,29)	1:114:A:ARG:HA	1:69:A:PHE:HA	18	0.25
(3,16)	1:26:A:ARG:HB2	1:31:A:ASN:HA	3	0.25
(3,16)	1:31:A:ASN:HA	1:26:A:ARG:HB3	4	0.25
(3,15)	1:85:A:CYS:HB3	1:4:A:CYS:HA	6	0.25
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG23	19	0.25
(3,4)	1:45:A:ILE:HG13	1:45:A:ILE:HB	16	0.25
(1,2246)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	18	0.25
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG22	11	0.25
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	5	0.25
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	5	0.25
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE1	9	0.25
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	13	0.25
(1,2096)	1:73:A:VAL:HG23	1:72:A:GLU:HA	6	0.25
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	6	0.25
(1,2050)	1:73:A:VAL:HG22	1:73:A:VAL:HA	17	0.25
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	19	0.25
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	20	0.25
(1,1982)	1:47:A:PHE:HD2	1:30:A:THR:HB	5	0.25
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	10	0.25
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	6	0.25
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	3	0.25
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG11	7	0.25
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	20	0.25
(1,1930)	1:98:A:ILE:HG21	1:61:A:PHE:HE2	1	0.25
(1,1913)	1:9:A:ILE:HD12	1:9:A:ILE:HA	3	0.25
(1,1913)	1:9:A:ILE:HD11	1:9:A:ILE:HA	13	0.25
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD12	19	0.25
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	10	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG23	15	0.25
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	14	0.25
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	13	0.25
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	4	0.25
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	14	0.25
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	16	0.25
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD12	4	0.25
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD11	6	0.25
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD11	17	0.25
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	13	0.25
(1,1503)	1:30:A:THR:H	1:27:A:SER:H	12	0.25
(1,1397)	1:108:A:GLN:HG2	1:108:A:GLN:H	12	0.25
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	8	0.25
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	14	0.25
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB1	18	0.25
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	4	0.25
(1,1242)	1:20:A:ILE:HD12	1:39:A:PHE:H	6	0.25
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG22	6	0.25
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG22	7	0.25
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	17	0.25
(1,1168)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	18	0.25
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	1	0.25
(1,1145)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	3	0.25
(1,1145)	1:76:A:TYR:HD1	1:7:A:ILE:HG23	4	0.25
(1,1110)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	4	0.25
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	3	0.25
(1,1105)	1:98:A:ILE:HD13	1:94:A:ARG:H	5	0.25
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	13	0.25
(1,1105)	1:98:A:ILE:HD13	1:94:A:ARG:H	17	0.25
(1,1061)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	11	0.25
(1,1061)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	16	0.25
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	13	0.25
(1,982)	1:73:A:VAL:HG23	1:72:A:GLU:HA	15	0.25
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	14	0.25
(1,950)	1:101:A:LYS:HB2	1:107:A:PRO:HA	20	0.25
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	10	0.25
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	6	0.25
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG22	14	0.25
(1,880)	1:11:A:ILE:H	1:11:A:ILE:HG21	17	0.25
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	6	0.25
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	13	0.25
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:90:A:GLU:H	1:89:A:TYR:HB3	7	0.25
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG22	1	0.25
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG22	16	0.25
(1,736)	1:102:A:MET:H	1:101:A:LYS:HB2	14	0.25
(1,693)	1:57:A:TRP:H	1:56:A:ARG:HA	7	0.25
(1,686)	1:90:A:GLU:HG3	1:90:A:GLU:H	11	0.25
(1,679)	1:88:A:ARG:H	1:87:A:LYS:HA	20	0.25
(1,678)	1:87:A:LYS:HB3	1:88:A:ARG:H	19	0.25
(1,668)	1:85:A:CYS:H	1:84:A:LEU:HA	6	0.25
(1,668)	1:85:A:CYS:H	1:84:A:LEU:HA	18	0.25
(1,575)	1:49:A:ASP:H	1:48:A:LYS:HA	13	0.25
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	2	0.25
(1,488)	1:29:A:ASN:HB2	1:30:A:THR:H	16	0.25
(1,465)	1:23:A:TYR:H	1:34:A:VAL:HG13	5	0.25
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	13	0.25
(1,424)	1:13:A:ASN:HB3	1:13:A:ASN:H	4	0.25
(1,413)	1:10:A:VAL:HG21	1:10:A:VAL:H	20	0.25
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	3	0.25
(1,306)	1:30:A:THR:HB	1:47:A:PHE:HE2	8	0.25
(1,299)	1:23:A:TYR:HE2	1:45:A:ILE:HD11	1	0.25
(1,298)	1:34:A:VAL:HG22	1:24:A:HIS:HE1	12	0.25
(1,286)	1:45:A:ILE:HG22	1:9:A:ILE:HG12	4	0.25
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	11	0.25
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	14	0.25
(1,194)	1:71:A:THR:HB	1:71:A:THR:HA	2	0.25
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	7	0.25
(1,156)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	16	0.25
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	6	0.25
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	19	0.25
(1,129)	1:15:A:LEU:H	1:15:A:LEU:HG	8	0.25
(1,113)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	18	0.25
(1,106)	1:9:A:ILE:HD12	1:9:A:ILE:HA	19	0.25
(1,74)	1:1:A:ALA:HB2	1:83:A:PRO:HA	5	0.25
(1,73)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	3	0.25
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG22	8	0.25
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	7	0.25
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB1	17	0.25
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD11	12	0.25
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG22	11	0.25
(1,48)	1:37:A:LEU:H	1:20:A:ILE:HG22	3	0.25
(1,47)	1:20:A:ILE:HG23	1:21:A:LEU:H	8	0.25
(1,45)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	12	0.25
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	20	0.25
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	6	0.25
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	12	0.25
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	15	0.25
(1,19)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	1	0.25
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	3	0.25
(1,15)	1:98:A:ILE:HD12	1:61:A:PHE:HE1	17	0.25
(1,8)	1:10:A:VAL:HG21	1:10:A:VAL:HA	5	0.25
(1,8)	1:10:A:VAL:HG21	1:10:A:VAL:HA	16	0.25
(1,6)	1:71:A:THR:HA	1:71:A:THR:HG22	2	0.25
(4,23)	1:21:A:LEU:H	1:37:A:LEU:O	1	0.24
(4,23)	1:21:A:LEU:H	1:37:A:LEU:O	2	0.24
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	1	0.24
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	19	0.24
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	12	0.24
(3,317)	1:47:A:PHE:H	1:8:A:GLU:HG3	17	0.24
(3,315)	1:104:A:GLU:H	1:104:A:GLU:HG2	20	0.24
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	12	0.24
(3,257)	1:93:A:ALA:HB1	1:98:A:ILE:HG21	1	0.24
(3,248)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	9	0.24
(3,216)	1:19:A:ARG:HG3	1:95:A:MET:H	1	0.24
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	16	0.24
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	7	0.24
(3,207)	1:7:A:ILE:H	1:6:A:GLU:HG3	15	0.24
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	12	0.24
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	20	0.24
(3,204)	1:105:A:ARG:HG2	1:105:A:ARG:H	20	0.24
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	13	0.24
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	19	0.24
(3,185)	1:47:A:PHE:HB3	1:48:A:LYS:H	18	0.24
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	4	0.24
(3,179)	1:29:A:ASN:H	1:56:A:ARG:HA	5	0.24
(3,167)	1:5:A:LYS:HG2	1:6:A:GLU:H	19	0.24
(3,165)	1:4:A:CYS:HB2	1:5:A:LYS:H	9	0.24
(3,161)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	3	0.24
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG21	17	0.24
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	13	0.24
(3,148)	1:111:A:ASN:H	1:110:A:LEU:HB2	18	0.24
(3,134)	1:36:A:TYR:HD1	1:22:A:GLN:HA	14	0.24
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	4	0.24
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,92)	1:52:A:THR:HB	1:52:A:THR:HG22	19	0.24
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG21	20	0.24
(3,78)	1:39:A:PHE:HD1	1:16:A:GLY:HA2	17	0.24
(3,75)	1:39:A:PHE:HA	1:39:A:PHE:HD1	18	0.24
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	1	0.24
(3,50)	1:10:A:VAL:HG22	1:10:A:VAL:HA	11	0.24
(3,49)	1:98:A:ILE:HG22	1:98:A:ILE:HA	19	0.24
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	19	0.24
(3,31)	1:92:A:SER:HB3	1:92:A:SER:H	3	0.24
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB3	8	0.24
(3,4)	1:45:A:ILE:HG13	1:45:A:ILE:HB	18	0.24
(1,2274)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	2	0.24
(1,2263)	1:37:A:LEU:HA	1:37:A:LEU:HB2	20	0.24
(1,2255)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	8	0.24
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	7	0.24
(1,2237)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	10	0.24
(1,2234)	1:30:A:THR:HA	1:30:A:THR:HG22	18	0.24
(1,2228)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	19	0.24
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	3	0.24
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	4	0.24
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	5	0.24
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG23	7	0.24
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG22	10	0.24
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	16	0.24
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	1	0.24
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG22	13	0.24
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	20	0.24
(1,2124)	1:36:A:TYR:HA	1:36:A:TYR:HD1	5	0.24
(1,2096)	1:73:A:VAL:HG22	1:72:A:GLU:HA	12	0.24
(1,2094)	1:90:A:GLU:HB3	1:90:A:GLU:HA	3	0.24
(1,2089)	1:46:A:LYS:HB2	1:46:A:LYS:HA	2	0.24
(1,2050)	1:73:A:VAL:HG22	1:73:A:VAL:HA	8	0.24
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	14	0.24
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG22	1	0.24
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	4	0.24
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	6	0.24
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	7	0.24
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG22	8	0.24
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	12	0.24
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG22	18	0.24
(1,1956)	1:10:A:VAL:HG23	1:42:A:THR:HB	1	0.24
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG13	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	4	0.24
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG11	6	0.24
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	9	0.24
(1,1910)	1:7:A:ILE:HD11	1:84:A:LEU:HB3	19	0.24
(1,1850)	1:71:A:THR:H	1:70:A:PHE:HE1	2	0.24
(1,1796)	1:32:A:VAL:H	1:26:A:ARG:HA	4	0.24
(1,1699)	1:7:A:ILE:HD11	1:87:A:LYS:H	16	0.24
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	4	0.24
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG21	16	0.24
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	5	0.24
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	7	0.24
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	12	0.24
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	13	0.24
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	19	0.24
(1,1600)	1:50:A:ASP:H	1:49:A:ASP:HB2	18	0.24
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD12	8	0.24
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	1	0.24
(1,1541)	1:20:A:ILE:HD13	1:38:A:ASN:H	15	0.24
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	10	0.24
(1,1503)	1:30:A:THR:H	1:27:A:SER:H	8	0.24
(1,1356)	1:98:A:ILE:HD11	1:71:A:THR:HG22	14	0.24
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	4	0.24
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	12	0.24
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	18	0.24
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	1	0.24
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	12	0.24
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	9	0.24
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD13	17	0.24
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	15	0.24
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	10	0.24
(1,1210)	1:32:A:VAL:HA	1:32:A:VAL:HG13	10	0.24
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	9	0.24
(1,1166)	1:47:A:PHE:HD2	1:30:A:THR:HG21	18	0.24
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB3	5	0.24
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	2	0.24
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	4	0.24
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	12	0.24
(1,1148)	1:94:A:ARG:H	1:93:A:ALA:HB2	18	0.24
(1,1145)	1:76:A:TYR:HD1	1:7:A:ILE:HG21	6	0.24
(1,1141)	1:37:A:LEU:H	1:20:A:ILE:HG22	8	0.24
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG21	6	0.24
(1,1105)	1:98:A:ILE:HD11	1:94:A:ARG:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	9	0.24
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	1	0.24
(1,1058)	1:11:A:ILE:HD12	1:61:A:PHE:HE1	19	0.24
(1,1036)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	14	0.24
(1,1034)	1:103:A:ASP:HA	1:103:A:ASP:HB2	12	0.24
(1,974)	1:39:A:PHE:HA	1:39:A:PHE:HD1	10	0.24
(1,950)	1:101:A:LYS:HB2	1:107:A:PRO:HA	3	0.24
(1,948)	1:10:A:VAL:HG21	1:90:A:GLU:H	18	0.24
(1,913)	1:15:A:LEU:HD13	1:19:A:ARG:HB3	12	0.24
(1,913)	1:15:A:LEU:HD11	1:19:A:ARG:HB3	17	0.24
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	20	0.24
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG21	2	0.24
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE1	17	0.24
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	9	0.24
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	5	0.24
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	9	0.24
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG22	19	0.24
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	20	0.24
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	10	0.24
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	12	0.24
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG21	19	0.24
(1,695)	1:57:A:TRP:H	1:76:A:TYR:H	20	0.24
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	3	0.24
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	2	0.24
(1,619)	1:70:A:PHE:H	1:69:A:PHE:HA	14	0.24
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	18	0.24
(1,587)	1:52:A:THR:H	1:50:A:ASP:HA	17	0.24
(1,489)	1:30:A:THR:H	1:30:A:THR:HG22	11	0.24
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	14	0.24
(1,336)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	8	0.24
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	6	0.24
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	17	0.24
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	5	0.24
(1,306)	1:30:A:THR:HB	1:47:A:PHE:HE1	20	0.24
(1,292)	1:43:A:ARG:HB2	1:43:A:ARG:HA	8	0.24
(1,291)	1:73:A:VAL:HG23	1:71:A:THR:HG23	14	0.24
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	13	0.24
(1,273)	1:73:A:VAL:HG22	1:73:A:VAL:HA	5	0.24
(1,255)	1:32:A:VAL:HG12	1:47:A:PHE:HE1	2	0.24
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	12	0.24
(1,209)	1:32:A:VAL:HG21	1:32:A:VAL:HA	8	0.24
(1,209)	1:32:A:VAL:HG23	1:32:A:VAL:HA	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	4	0.24
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	19	0.24
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	18	0.24
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	19	0.24
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	1	0.24
(1,145)	1:42:A:THR:HG22	1:12:A:LYS:HA	7	0.24
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	10	0.24
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	18	0.24
(1,117)	1:20:A:ILE:HD13	1:39:A:PHE:H	9	0.24
(1,94)	1:9:A:ILE:HG22	1:75:A:ALA:HA	10	0.24
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG23	17	0.24
(1,65)	1:34:A:VAL:HG22	1:34:A:VAL:HA	3	0.24
(1,65)	1:34:A:VAL:HG22	1:34:A:VAL:HA	8	0.24
(1,65)	1:34:A:VAL:HG23	1:34:A:VAL:HA	14	0.24
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	2	0.24
(1,51)	1:98:A:ILE:HG22	1:92:A:SER:H	20	0.24
(1,48)	1:37:A:LEU:H	1:20:A:ILE:HG22	15	0.24
(1,25)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	18	0.24
(1,23)	1:9:A:ILE:HD13	1:75:A:ALA:HB3	6	0.24
(1,19)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	17	0.24
(1,11)	1:73:A:VAL:HG21	1:98:A:ILE:HD13	2	0.24
(1,8)	1:10:A:VAL:HG22	1:10:A:VAL:HA	6	0.24
(3,319)	1:19:A:ARG:HG2	1:95:A:MET:H	2	0.23
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	18	0.23
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	2	0.23
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB3	4	0.23
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB3	8	0.23
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	4	0.23
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	18	0.23
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	6	0.23
(3,219)	1:9:A:ILE:HG22	1:57:A:TRP:HB2	9	0.23
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	18	0.23
(3,214)	1:108:A:GLN:H	1:100:A:PHE:HB3	10	0.23
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	11	0.23
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	4	0.23
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	12	0.23
(3,167)	1:5:A:LYS:HG2	1:6:A:GLU:H	12	0.23
(3,165)	1:4:A:CYS:HB3	1:5:A:LYS:H	3	0.23
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG23	9	0.23
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	14	0.23
(3,137)	1:11:A:ILE:H	1:11:A:ILE:HD12	14	0.23
(3,118)	1:90:A:GLU:HB2	1:10:A:VAL:HG13	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,97)	1:19:A:ARG:HB3	1:39:A:PHE:HB2	5	0.23
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	12	0.23
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG21	13	0.23
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG21	15	0.23
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	16	0.23
(3,76)	1:34:A:VAL:HA	1:24:A:HIS:HD1	2	0.23
(3,60)	1:6:A:GLU:HB2	1:48:A:LYS:HA	17	0.23
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	18	0.23
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	20	0.23
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	3	0.23
(1,2263)	1:37:A:LEU:HA	1:37:A:LEU:HB2	17	0.23
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	2	0.23
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	5	0.23
(1,2246)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	13	0.23
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	16	0.23
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	17	0.23
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	7	0.23
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB1	6	0.23
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	1	0.23
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	9	0.23
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG21	19	0.23
(1,2161)	1:71:A:THR:HB	1:71:A:THR:HA	2	0.23
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG22	9	0.23
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	15	0.23
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG23	18	0.23
(1,2126)	1:23:A:TYR:HE1	1:36:A:TYR:HA	7	0.23
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	1	0.23
(1,2096)	1:73:A:VAL:HG21	1:72:A:GLU:HA	18	0.23
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	8	0.23
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	3	0.23
(1,2071)	1:35:A:GLN:HG3	1:35:A:GLN:HA	15	0.23
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	4	0.23
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	18	0.23
(1,2043)	1:8:A:GLU:HB3	1:8:A:GLU:HA	17	0.23
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	2	0.23
(1,2019)	1:4:A:CYS:HB3	1:4:A:CYS:HA	10	0.23
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	5	0.23
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG22	9	0.23
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	11	0.23
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	14	0.23
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	20	0.23
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:34:A:VAL:HG23	1:34:A:VAL:HA	20	0.23
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG23	18	0.23
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	1	0.23
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	20	0.23
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	10	0.23
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG13	11	0.23
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG11	16	0.23
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG13	19	0.23
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	7	0.23
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	11	0.23
(1,1930)	1:98:A:ILE:HG22	1:61:A:PHE:HE1	18	0.23
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	13	0.23
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	7	0.23
(1,1927)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	14	0.23
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	15	0.23
(1,1918)	1:11:A:ILE:HG22	1:11:A:ILE:HD11	18	0.23
(1,1913)	1:9:A:ILE:HD13	1:9:A:ILE:HA	7	0.23
(1,1913)	1:9:A:ILE:HD13	1:9:A:ILE:HA	15	0.23
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	19	0.23
(1,1786)	1:115:A:SER:H	1:114:A:ARG:HB2	8	0.23
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG21	11	0.23
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	12	0.23
(1,1719)	1:57:A:TRP:H	1:56:A:ARG:HA	15	0.23
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	8	0.23
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	20	0.23
(1,1631)	1:58:A:ASN:HB3	1:59:A:CYS:H	12	0.23
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	1	0.23
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	15	0.23
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	17	0.23
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG13	3	0.23
(1,1503)	1:30:A:THR:H	1:27:A:SER:H	4	0.23
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	17	0.23
(1,1472)	1:22:A:GLN:HG3	1:23:A:TYR:H	11	0.23
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	7	0.23
(1,1397)	1:108:A:GLN:HG2	1:108:A:GLN:H	3	0.23
(1,1310)	1:98:A:ILE:HD13	1:71:A:THR:HG21	2	0.23
(1,1308)	1:109:A:PRO:HA	1:97:A:ALA:HB1	19	0.23
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	17	0.23
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD11	13	0.23
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG22	4	0.23
(1,1225)	1:7:A:ILE:HG12	1:7:A:ILE:HG23	12	0.23
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	1	0.23
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	19	0.23
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	5	0.23
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	7	0.23
(1,1134)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	15	0.23
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	11	0.23
(1,1110)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	7	0.23
(1,1072)	1:20:A:ILE:HG22	1:20:A:ILE:HG12	20	0.23
(1,1071)	1:44:A:ILE:HD13	1:44:A:ILE:HG12	8	0.23
(1,1071)	1:44:A:ILE:HD11	1:44:A:ILE:HG12	12	0.23
(1,1061)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	10	0.23
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	12	0.23
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	6	0.23
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG22	3	0.23
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG21	19	0.23
(1,1037)	1:73:A:VAL:HG23	1:91:A:LEU:HB3	5	0.23
(1,1037)	1:73:A:VAL:HG23	1:91:A:LEU:HB3	17	0.23
(1,982)	1:73:A:VAL:HG22	1:72:A:GLU:HA	13	0.23
(1,982)	1:73:A:VAL:HG22	1:72:A:GLU:HA	20	0.23
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	6	0.23
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	7	0.23
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	3	0.23
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG22	1	0.23
(1,890)	1:98:A:ILE:HG22	1:98:A:ILE:HA	19	0.23
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD12	19	0.23
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	8	0.23
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	10	0.23
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG23	15	0.23
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	14	0.23
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	13	0.23
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	4	0.23
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	7	0.23
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	12	0.23
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	14	0.23
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	16	0.23
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	19	0.23
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD11	6	0.23
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD12	16	0.23
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD11	17	0.23
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	13	0.23
(1,490)	1:30:A:THR:H	1:27:A:SER:H	12	0.23
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	18	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,404)	1:108:A:GLN:HG2	1:108:A:GLN:H	12	0.23
(1,327)	1:7:A:ILE:HD12	1:8:A:GLU:H	17	0.23
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	12	0.23
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	7	0.23
(1,293)	1:47:A:PHE:HA	1:47:A:PHE:HD1	20	0.23
(1,292)	1:43:A:ARG:HB2	1:43:A:ARG:HA	3	0.23
(1,292)	1:43:A:ARG:HB2	1:43:A:ARG:HA	10	0.23
(1,292)	1:43:A:ARG:HB2	1:43:A:ARG:HA	13	0.23
(1,286)	1:45:A:ILE:HG21	1:9:A:ILE:HG12	6	0.23
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	16	0.23
(1,273)	1:73:A:VAL:HG23	1:73:A:VAL:HA	7	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG22	1	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	4	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	5	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	6	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	7	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG22	8	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	11	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG22	18	0.23
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	20	0.23
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	2	0.23
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	6	0.23
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	16	0.23
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	2	0.23
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	12	0.23
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	14	0.23
(1,182)	1:61:A:PHE:HE2	1:93:A:ALA:HB1	11	0.23
(1,169)	1:61:A:PHE:HA	1:61:A:PHE:HD1	18	0.23
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	20	0.23
(1,157)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	2	0.23
(1,145)	1:42:A:THR:HG23	1:12:A:LYS:HA	4	0.23
(1,145)	1:42:A:THR:HG23	1:12:A:LYS:HA	8	0.23
(1,145)	1:42:A:THR:HG23	1:12:A:LYS:HA	10	0.23
(1,144)	1:95:A:MET:H	1:14:A:THR:HG23	20	0.23
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	2	0.23
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	8	0.23
(1,65)	1:34:A:VAL:HG22	1:34:A:VAL:HA	5	0.23
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG21	14	0.23
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG23	18	0.23
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	3	0.23
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG23	3	0.23
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG23	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:20:A:ILE:HG22	1:21:A:LEU:H	7	0.23
(1,37)	1:75:A:ALA:HB2	1:9:A:ILE:HG21	17	0.23
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	5	0.23
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	7	0.23
(1,9)	1:98:A:ILE:HD13	1:98:A:ILE:HA	13	0.23
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	20	0.23
(3,317)	1:47:A:PHE:H	1:8:A:GLU:HG3	19	0.22
(3,272)	1:92:A:SER:HB3	1:93:A:ALA:H	12	0.22
(3,253)	1:110:A:LEU:HB3	1:100:A:PHE:HB3	14	0.22
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	5	0.22
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	19	0.22
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG22	15	0.22
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	8	0.22
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	10	0.22
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	14	0.22
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	6	0.22
(3,212)	1:47:A:PHE:H	1:8:A:GLU:HG3	17	0.22
(3,159)	1:57:A:TRP:HB2	1:75:A:ALA:HB3	4	0.22
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	6	0.22
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	4	0.22
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG23	10	0.22
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	18	0.22
(3,125)	1:73:A:VAL:HG12	1:73:A:VAL:HG22	6	0.22
(3,108)	1:44:A:ILE:HG23	1:8:A:GLU:HB2	13	0.22
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	7	0.22
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	12	0.22
(3,65)	1:6:A:GLU:HG2	1:48:A:LYS:HA	3	0.22
(3,65)	1:6:A:GLU:HG2	1:48:A:LYS:HA	10	0.22
(3,50)	1:10:A:VAL:HG23	1:10:A:VAL:HA	17	0.22
(3,38)	1:36:A:TYR:HD1	1:36:A:TYR:HB2	18	0.22
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB3	12	0.22
(3,27)	1:5:A:LYS:HG3	1:5:A:LYS:HA	7	0.22
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	13	0.22
(3,6)	1:10:A:VAL:H	1:9:A:ILE:HG21	14	0.22
(1,2250)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	8	0.22
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	20	0.22
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB1	19	0.22
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG23	13	0.22
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG23	15	0.22
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE1	2	0.22
(1,2096)	1:73:A:VAL:HG21	1:72:A:GLU:HA	4	0.22
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	8	0.22
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	2	0.22
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	3	0.22
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	10	0.22
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	15	0.22
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG21	16	0.22
(1,1957)	1:10:A:VAL:HG23	1:10:A:VAL:HB	2	0.22
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	8	0.22
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	12	0.22
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	16	0.22
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG22	16	0.22
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG21	18	0.22
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	6	0.22
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD11	14	0.22
(1,1839)	1:57:A:TRP:H	1:56:A:ARG:HB3	15	0.22
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.22
(1,1827)	1:9:A:ILE:H	1:9:A:ILE:HG23	18	0.22
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	3	0.22
(1,1771)	1:105:A:ARG:HB3	1:105:A:ARG:H	20	0.22
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	20	0.22
(1,1631)	1:58:A:ASN:HB3	1:59:A:CYS:H	7	0.22
(1,1614)	1:53:A:GLU:HB3	1:53:A:GLU:H	3	0.22
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD11	14	0.22
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD12	20	0.22
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD1	18	0.22
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	12	0.22
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	3	0.22
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG21	16	0.22
(1,1430)	1:14:A:THR:H	1:93:A:ALA:H	13	0.22
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	6	0.22
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	18	0.22
(1,1308)	1:109:A:PRO:HA	1:97:A:ALA:HB2	14	0.22
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	6	0.22
(1,1293)	1:45:A:ILE:HD13	1:9:A:ILE:HD11	17	0.22
(1,1242)	1:20:A:ILE:HD13	1:39:A:PHE:H	11	0.22
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	14	0.22
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG23	16	0.22
(1,1171)	1:1:A:ALA:HB2	1:83:A:PRO:HA	16	0.22
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	5	0.22
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	8	0.22
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	10	0.22
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	5	0.22
(1,1143)	1:98:A:ILE:HG22	1:92:A:SER:H	14	0.22
(1,1137)	1:9:A:ILE:HD13	1:7:A:ILE:HG21	16	0.22
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	16	0.22
(1,1118)	1:45:A:ILE:HD13	1:45:A:ILE:HB	5	0.22
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD12	2	0.22
(1,1110)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	20	0.22
(1,1107)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	10	0.22
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	2	0.22
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	18	0.22
(1,1097)	1:10:A:VAL:HG23	1:10:A:VAL:HA	2	0.22
(1,1072)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	17	0.22
(1,1057)	1:23:A:TYR:HD2	1:11:A:ILE:HD13	9	0.22
(1,982)	1:73:A:VAL:HG22	1:72:A:GLU:HA	7	0.22
(1,924)	1:47:A:PHE:HD1	1:30:A:THR:HB	9	0.22
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG11	7	0.22
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	8	0.22
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG23	10	0.22
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG21	13	0.22
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	7	0.22
(1,889)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	15	0.22
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	12	0.22
(1,817)	1:71:A:THR:H	1:70:A:PHE:HE1	2	0.22
(1,809)	1:57:A:TRP:H	1:56:A:ARG:HB3	15	0.22
(1,804)	1:25:A:CYS:H	1:59:A:CYS:HB3	4	0.22
(1,769)	1:32:A:VAL:H	1:26:A:ARG:HA	4	0.22
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	12	0.22
(1,712)	1:96:A:ASP:H	1:95:A:MET:HB3	14	0.22
(1,677)	1:7:A:ILE:HD11	1:87:A:LYS:H	16	0.22
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	4	0.22
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	8	0.22
(1,668)	1:85:A:CYS:H	1:84:A:LEU:HA	12	0.22
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG21	16	0.22
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	5	0.22
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	13	0.22
(1,580)	1:50:A:ASP:H	1:49:A:ASP:HB2	18	0.22
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	1	0.22
(1,525)	1:20:A:ILE:HD13	1:38:A:ASN:H	15	0.22
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	10	0.22
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG13	3	0.22
(1,490)	1:30:A:THR:H	1:27:A:SER:H	8	0.22
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:61:A:PHE:HD2	1:23:A:TYR:HA	14	0.22
(1,305)	1:61:A:PHE:HD2	1:23:A:TYR:HA	18	0.22
(1,301)	1:23:A:TYR:HD1	1:36:A:TYR:HA	18	0.22
(1,298)	1:34:A:VAL:HG22	1:24:A:HIS:HE1	5	0.22
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	11	0.22
(1,294)	1:35:A:GLN:HA	1:36:A:TYR:HD1	13	0.22
(1,270)	1:21:A:LEU:HB2	1:21:A:LEU:HA	5	0.22
(1,262)	1:93:A:ALA:HB3	1:13:A:ASN:HB2	11	0.22
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	14	0.22
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	19	0.22
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE1	19	0.22
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	3	0.22
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG22	9	0.22
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	10	0.22
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	14	0.22
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	16	0.22
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	7	0.22
(1,209)	1:32:A:VAL:HG23	1:32:A:VAL:HA	9	0.22
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	7	0.22
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	3	0.22
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	14	0.22
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	8	0.22
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	9	0.22
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	17	0.22
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	5	0.22
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	9	0.22
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD11	16	0.22
(1,105)	1:9:A:ILE:H	1:9:A:ILE:HD12	10	0.22
(1,94)	1:9:A:ILE:HG22	1:75:A:ALA:HA	18	0.22
(1,74)	1:1:A:ALA:HB2	1:83:A:PRO:HA	12	0.22
(1,65)	1:34:A:VAL:HG23	1:34:A:VAL:HA	4	0.22
(1,65)	1:34:A:VAL:HG23	1:34:A:VAL:HA	15	0.22
(1,64)	1:112:A:LYS:HA	1:97:A:ALA:HB3	9	0.22
(1,54)	1:7:A:ILE:HG22	1:8:A:GLU:H	13	0.22
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	7	0.22
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	15	0.22
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	2	0.22
(1,25)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	13	0.22
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	16	0.22
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	17	0.22
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	20	0.22
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,327)	1:10:A:VAL:HG21	1:10:A:VAL:HA	5	0.21
(3,327)	1:10:A:VAL:HG21	1:10:A:VAL:HA	16	0.21
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	19	0.21
(3,309)	1:103:A:ASP:HB3	1:104:A:GLU:H	15	0.21
(3,284)	1:69:A:PHE:HA	1:115:A:SER:HB3	10	0.21
(3,264)	1:76:A:TYR:HB2	1:75:A:ALA:HB1	11	0.21
(3,256)	1:32:A:VAL:HG22	1:45:A:ILE:HG12	3	0.21
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	2	0.21
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	2	0.21
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	11	0.21
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	12	0.21
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	12	0.21
(3,224)	1:92:A:SER:HB2	1:99:A:TYR:HB3	4	0.21
(3,216)	1:19:A:ARG:HG2	1:95:A:MET:H	2	0.21
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	18	0.21
(3,209)	1:104:A:GLU:H	1:104:A:GLU:HG2	20	0.21
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	2	0.21
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB3	4	0.21
(3,193)	1:86:A:GLY:H	1:5:A:LYS:HB2	1	0.21
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG23	8	0.21
(3,154)	1:19:A:ARG:H	1:20:A:ILE:HG12	11	0.21
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	13	0.21
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	12	0.21
(3,134)	1:36:A:TYR:HD2	1:22:A:GLN:HA	8	0.21
(3,119)	1:90:A:GLU:HB2	1:10:A:VAL:HG13	7	0.21
(3,107)	1:44:A:ILE:HG23	1:8:A:GLU:HB2	13	0.21
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	3	0.21
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	9	0.21
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG23	10	0.21
(3,68)	1:19:A:ARG:HB3	1:14:A:THR:HA	17	0.21
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	10	0.21
(3,50)	1:10:A:VAL:HA	1:10:A:VAL:HG13	3	0.21
(3,8)	1:76:A:TYR:HB3	1:75:A:ALA:HB3	20	0.21
(1,2246)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	19	0.21
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB2	1	0.21
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB3	13	0.21
(1,2228)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	4	0.21
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG22	2	0.21
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG23	20	0.21
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	4	0.21
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	14	0.21
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	3	0.21
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG22	8	0.21
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	20	0.21
(1,2111)	1:23:A:TYR:HD2	1:23:A:TYR:HA	14	0.21
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	9	0.21
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	3	0.21
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	11	0.21
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	20	0.21
(1,2051)	1:101:A:LYS:HB2	1:107:A:PRO:HA	2	0.21
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	1	0.21
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	2	0.21
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	12	0.21
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	15	0.21
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG22	13	0.21
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG23	17	0.21
(1,2017)	1:52:A:THR:HB	1:52:A:THR:HG22	19	0.21
(1,1976)	1:112:A:LYS:HA	1:97:A:ALA:HB1	12	0.21
(1,1962)	1:34:A:VAL:HG22	1:34:A:VAL:HA	3	0.21
(1,1962)	1:34:A:VAL:HG22	1:34:A:VAL:HA	8	0.21
(1,1962)	1:34:A:VAL:HG23	1:34:A:VAL:HA	14	0.21
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG22	13	0.21
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG21	15	0.21
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG23	17	0.21
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	11	0.21
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	14	0.21
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	19	0.21
(1,1955)	1:10:A:VAL:HG21	1:10:A:VAL:HA	5	0.21
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG11	12	0.21
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD13	14	0.21
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	5	0.21
(1,1928)	1:98:A:ILE:HG22	1:98:A:ILE:HA	20	0.21
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	9	0.21
(1,1901)	1:37:A:LEU:H	1:20:A:ILE:HD13	6	0.21
(1,1898)	1:89:A:TYR:H	1:10:A:VAL:H	11	0.21
(1,1762)	1:102:A:MET:H	1:101:A:LYS:HB2	10	0.21
(1,1738)	1:94:A:ARG:HB3	1:96:A:ASP:H	6	0.21
(1,1737)	1:96:A:ASP:HB3	1:96:A:ASP:H	17	0.21
(1,1721)	1:57:A:TRP:H	1:76:A:TYR:H	4	0.21
(1,1698)	1:86:A:GLY:H	1:85:A:CYS:HB2	1	0.21
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	9	0.21
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	13	0.21
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD11	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD12	19	0.21
(1,1541)	1:20:A:ILE:HD11	1:38:A:ASN:H	13	0.21
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	16	0.21
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	19	0.21
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD1	12	0.21
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	16	0.21
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	5	0.21
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	14	0.21
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	18	0.21
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	7	0.21
(1,1332)	1:36:A:TYR:HA	1:36:A:TYR:HD1	5	0.21
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG22	11	0.21
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	15	0.21
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	16	0.21
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	11	0.21
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD11	8	0.21
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	4	0.21
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	16	0.21
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB2	3	0.21
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	6	0.21
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	7	0.21
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB3	9	0.21
(1,1162)	1:98:A:ILE:HG12	1:93:A:ALA:HB1	15	0.21
(1,1146)	1:7:A:ILE:HG21	1:8:A:GLU:H	19	0.21
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	6	0.21
(1,1135)	1:7:A:ILE:HD12	1:7:A:ILE:HG21	3	0.21
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	12	0.21
(1,1107)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	11	0.21
(1,1105)	1:98:A:ILE:HD11	1:94:A:ARG:H	6	0.21
(1,1003)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	12	0.21
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	8	0.21
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	10	0.21
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	11	0.21
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	20	0.21
(1,987)	1:90:A:GLU:HG3	1:91:A:LEU:HA	3	0.21
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	6	0.21
(1,919)	1:70:A:PHE:HE1	1:70:A:PHE:HA	13	0.21
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	6	0.21
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG11	20	0.21
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	4	0.21
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG11	6	0.21
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	20	0.21
(1,892)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	8	0.21
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	1	0.21
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	19	0.21
(1,760)	1:115:A:SER:H	1:114:A:ARG:HB2	8	0.21
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG21	11	0.21
(1,693)	1:57:A:TRP:H	1:56:A:ARG:HA	15	0.21
(1,676)	1:86:A:GLY:H	1:85:A:CYS:HB2	1	0.21
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	20	0.21
(1,608)	1:58:A:ASN:HB3	1:59:A:CYS:H	12	0.21
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	1	0.21
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	15	0.21
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	17	0.21
(1,490)	1:30:A:THR:H	1:27:A:SER:H	4	0.21
(1,463)	1:22:A:GLN:HG3	1:23:A:TYR:H	11	0.21
(1,404)	1:108:A:GLN:HG2	1:108:A:GLN:H	3	0.21
(1,348)	1:74:A:GLU:HB2	1:74:A:GLU:H	5	0.21
(1,328)	1:9:A:ILE:HB	1:9:A:ILE:HD13	17	0.21
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	10	0.21
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	16	0.21
(1,305)	1:61:A:PHE:HD2	1:23:A:TYR:HA	17	0.21
(1,292)	1:43:A:ARG:HB2	1:43:A:ARG:HA	12	0.21
(1,286)	1:45:A:ILE:HG23	1:9:A:ILE:HG12	20	0.21
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	9	0.21
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	20	0.21
(1,262)	1:93:A:ALA:HB1	1:13:A:ASN:HB2	14	0.21
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	4	0.21
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	6	0.21
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	17	0.21
(1,245)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	16	0.21
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	2	0.21
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG21	15	0.21
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG23	17	0.21
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG22	19	0.21
(1,209)	1:32:A:VAL:HG22	1:32:A:VAL:HA	17	0.21
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	8	0.21
(1,189)	1:50:A:ASP:HA	1:50:A:ASP:HB2	18	0.21
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	2	0.21
(1,145)	1:42:A:THR:HG23	1:12:A:LYS:HA	17	0.21
(1,142)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	16	0.21
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	14	0.21
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	15	0.21
(1,94)	1:9:A:ILE:HG21	1:75:A:ALA:HA	17	0.21
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	12	0.21
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	7	0.21
(1,54)	1:7:A:ILE:HG21	1:8:A:GLU:H	8	0.21
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	8	0.21
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	1	0.21
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG21	16	0.21
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	11	0.21
(1,47)	1:20:A:ILE:HG23	1:21:A:LEU:H	6	0.21
(1,47)	1:20:A:ILE:HG23	1:21:A:LEU:H	13	0.21
(1,19)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	8	0.21
(1,8)	1:10:A:VAL:HG21	1:10:A:VAL:HA	9	0.21
(1,8)	1:10:A:VAL:HG22	1:10:A:VAL:HA	11	0.21
(3,327)	1:10:A:VAL:HG22	1:10:A:VAL:HA	6	0.2
(3,311)	1:105:A:ARG:HG2	1:105:A:ARG:H	7	0.2
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	20	0.2
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	18	0.2
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	2	0.2
(3,212)	1:47:A:PHE:H	1:8:A:GLU:HG3	19	0.2
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	6	0.2
(3,202)	1:103:A:ASP:HB3	1:104:A:GLU:H	15	0.2
(3,197)	1:91:A:LEU:H	1:91:A:LEU:HB2	16	0.2
(3,189)	1:74:A:GLU:HA	1:76:A:TYR:H	9	0.2
(3,179)	1:29:A:ASN:H	1:56:A:ARG:HA	15	0.2
(3,167)	1:5:A:LYS:HG2	1:6:A:GLU:H	13	0.2
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG23	10	0.2
(3,157)	1:45:A:ILE:HA	1:44:A:ILE:HG23	18	0.2
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	7	0.2
(3,145)	1:29:A:ASN:H	1:56:A:ARG:HA	18	0.2
(3,118)	1:73:A:VAL:HG22	1:59:A:CYS:HB2	13	0.2
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	4	0.2
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	13	0.2
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG21	6	0.2
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG21	7	0.2
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG23	11	0.2
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE2	18	0.2
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	7	0.2
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB2	20	0.2
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	16	0.2
(3,16)	1:26:A:ARG:HB2	1:31:A:ASN:HA	15	0.2
(3,16)	1:26:A:ARG:HB2	1:31:A:ASN:HA	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:11:A:ILE:H	1:11:A:ILE:HD11	12	0.2
(1,2255)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	14	0.2
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	9	0.2
(1,2236)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	16	0.2
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB3	17	0.2
(1,2229)	1:75:A:ALA:HB2	1:9:A:ILE:HG22	4	0.2
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG22	8	0.2
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG23	6	0.2
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	9	0.2
(1,2134)	1:15:A:LEU:H	1:95:A:MET:HA	13	0.2
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	20	0.2
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	3	0.2
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	13	0.2
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	8	0.2
(1,2071)	1:35:A:GLN:HG3	1:35:A:GLN:HA	10	0.2
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	12	0.2
(1,2038)	1:7:A:ILE:HD12	1:7:A:ILE:HG21	3	0.2
(1,2038)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	9	0.2
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD12	6	0.2
(1,2019)	1:4:A:CYS:HB3	1:4:A:CYS:HA	1	0.2
(1,1982)	1:47:A:PHE:HD2	1:30:A:THR:HB	18	0.2
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD11	18	0.2
(1,1962)	1:34:A:VAL:HG22	1:34:A:VAL:HA	5	0.2
(1,1962)	1:34:A:VAL:HG23	1:34:A:VAL:HA	15	0.2
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	9	0.2
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	10	0.2
(1,1957)	1:10:A:VAL:HG23	1:10:A:VAL:HB	13	0.2
(1,1957)	1:10:A:VAL:HG23	1:10:A:VAL:HB	17	0.2
(1,1956)	1:10:A:VAL:HG21	1:42:A:THR:HB	13	0.2
(1,1955)	1:10:A:VAL:HG22	1:10:A:VAL:HA	6	0.2
(1,1955)	1:10:A:VAL:HG21	1:10:A:VAL:HA	16	0.2
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG13	5	0.2
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG21	4	0.2
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	16	0.2
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	10	0.2
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG23	12	0.2
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	10	0.2
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	13	0.2
(1,1927)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	12	0.2
(1,1927)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	16	0.2
(1,1913)	1:9:A:ILE:HD12	1:9:A:ILE:HA	18	0.2
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD13	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD11	12	0.2
(1,1850)	1:71:A:THR:H	1:70:A:PHE:HE1	9	0.2
(1,1826)	1:9:A:ILE:H	1:9:A:ILE:HB	13	0.2
(1,1826)	1:9:A:ILE:H	1:9:A:ILE:HB	16	0.2
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	1	0.2
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG23	8	0.2
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	13	0.2
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	17	0.2
(1,1729)	1:95:A:MET:HG2	1:95:A:MET:H	14	0.2
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	6	0.2
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	14	0.2
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG22	5	0.2
(1,1548)	1:39:A:PHE:HA	1:40:A:LYS:H	6	0.2
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	5	0.2
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	11	0.2
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	18	0.2
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	18	0.2
(1,1452)	1:19:A:ARG:HB3	1:19:A:ARG:H	18	0.2
(1,1431)	1:15:A:LEU:H	1:14:A:THR:H	18	0.2
(1,1408)	1:10:A:VAL:HG23	1:10:A:VAL:H	14	0.2
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	17	0.2
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	1	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	2	0.2
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	3	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	4	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	7	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	8	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	9	0.2
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	11	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	12	0.2
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	13	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	15	0.2
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	16	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	17	0.2
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	19	0.2
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	20	0.2
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG23	6	0.2
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	3	0.2
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	4	0.2
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	5	0.2
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG22	10	0.2
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB1	17	0.2
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD11	4	0.2
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD12	14	0.2
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD13	20	0.2
(1,1229)	1:9:A:ILE:H	1:9:A:ILE:HD13	16	0.2
(1,1172)	1:20:A:ILE:HG23	1:20:A:ILE:HG13	14	0.2
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	2	0.2
(1,1160)	1:34:A:VAL:HG22	1:34:A:VAL:HA	16	0.2
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	16	0.2
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	12	0.2
(1,1140)	1:20:A:ILE:HG21	1:21:A:LEU:H	17	0.2
(1,1135)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	9	0.2
(1,1135)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	10	0.2
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG22	8	0.2
(1,1118)	1:45:A:ILE:HD11	1:45:A:ILE:HB	7	0.2
(1,1072)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	2	0.2
(1,1071)	1:44:A:ILE:HD12	1:44:A:ILE:HG12	9	0.2
(1,1064)	1:37:A:LEU:HA	1:37:A:LEU:HB2	20	0.2
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	14	0.2
(1,1052)	1:73:A:VAL:HG21	1:111:A:ASN:HB2	19	0.2
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	12	0.2
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	14	0.2
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG21	20	0.2
(1,1037)	1:73:A:VAL:HG21	1:91:A:LEU:HB3	1	0.2
(1,1037)	1:73:A:VAL:HG23	1:91:A:LEU:HB3	11	0.2
(1,1005)	1:97:A:ALA:HB1	1:109:A:PRO:HB2	6	0.2
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	4	0.2
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	5	0.2
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	7	0.2
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	17	0.2
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	18	0.2
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	19	0.2
(1,978)	1:90:A:GLU:HB3	1:90:A:GLU:HA	3	0.2
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	20	0.2
(1,928)	1:69:A:PHE:HA	1:115:A:SER:HB3	18	0.2
(1,924)	1:47:A:PHE:HD2	1:30:A:THR:HB	5	0.2
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	1	0.2
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG13	3	0.2
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG13	11	0.2
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG11	16	0.2
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG22	4	0.2
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG22	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	20	0.2
(1,877)	1:11:A:ILE:HG22	1:11:A:ILE:HD11	18	0.2
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD11	14	0.2
(1,804)	1:25:A:CYS:H	1:59:A:CYS:HB3	3	0.2
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	6	0.2
(1,797)	1:9:A:ILE:H	1:9:A:ILE:HG23	18	0.2
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	17	0.2
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	3	0.2
(1,746)	1:105:A:ARG:HB3	1:105:A:ARG:H	20	0.2
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	20	0.2
(1,608)	1:58:A:ASN:HB3	1:59:A:CYS:H	7	0.2
(1,592)	1:53:A:GLU:HB3	1:53:A:GLU:H	3	0.2
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD1	18	0.2
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	12	0.2
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	3	0.2
(1,489)	1:30:A:THR:H	1:30:A:THR:HG21	16	0.2
(1,472)	1:26:A:ARG:H	1:57:A:TRP:HB2	17	0.2
(1,429)	1:14:A:THR:H	1:93:A:ALA:H	13	0.2
(1,349)	1:85:A:CYS:H	1:84:A:LEU:HA	16	0.2
(1,336)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	19	0.2
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	18	0.2
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	11	0.2
(1,306)	1:30:A:THR:HB	1:47:A:PHE:HE2	7	0.2
(1,298)	1:34:A:VAL:HG23	1:24:A:HIS:HE1	17	0.2
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	15	0.2
(1,262)	1:93:A:ALA:HB3	1:13:A:ASN:HB2	7	0.2
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	3	0.2
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	7	0.2
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	12	0.2
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	15	0.2
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	20	0.2
(1,244)	1:70:A:PHE:HD1	1:70:A:PHE:HB3	2	0.2
(1,238)	1:36:A:TYR:HA	1:36:A:TYR:HD1	11	0.2
(1,211)	1:52:A:THR:HB	1:52:A:THR:HG22	13	0.2
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	15	0.2
(1,182)	1:61:A:PHE:HE2	1:93:A:ALA:HB1	3	0.2
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD1	15	0.2
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	13	0.2
(1,156)	1:73:A:VAL:HG23	1:61:A:PHE:HE1	19	0.2
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	20	0.2
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG21	4	0.2
(1,147)	1:33:A:GLY:H	1:34:A:VAL:HG23	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:42:A:THR:HG23	1:12:A:LYS:HA	20	0.2
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD12	6	0.2
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD12	3	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	2	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	3	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	6	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	7	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	14	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	15	0.2
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	19	0.2
(1,65)	1:34:A:VAL:HG23	1:34:A:VAL:HA	11	0.2
(1,65)	1:34:A:VAL:HG22	1:34:A:VAL:HA	19	0.2
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD13	14	0.2
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	15	0.2
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG23	17	0.2
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	5	0.2
(1,25)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	19	0.2
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	2	0.2
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG22	4	0.2
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	18	0.2
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	3	0.2
(1,5)	1:42:A:THR:HG21	1:42:A:THR:HB	4	0.2
(1,5)	1:42:A:THR:HG21	1:42:A:THR:HB	10	0.2
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	9	0.19
(3,319)	1:19:A:ARG:HG3	1:95:A:MET:H	13	0.19
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG2	12	0.19
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB2	9	0.19
(3,303)	1:88:A:ARG:HB3	1:88:A:ARG:H	13	0.19
(3,295)	1:36:A:TYR:H	1:35:A:GLN:HB2	3	0.19
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	15	0.19
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB2	20	0.19
(3,228)	1:7:A:ILE:HG22	1:84:A:LEU:HB3	2	0.19
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	19	0.19
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	1	0.19
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	6	0.19
(3,179)	1:29:A:ASN:H	1:56:A:ARG:HA	6	0.19
(3,171)	1:11:A:ILE:H	1:11:A:ILE:HD13	13	0.19
(3,160)	1:114:A:ARG:HB3	1:61:A:PHE:HB3	14	0.19
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG21	6	0.19
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	2	0.19
(3,94)	1:87:A:LYS:HB2	1:87:A:LYS:HA	7	0.19
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG23	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG23	8	0.19
(3,60)	1:6:A:GLU:HB2	1:48:A:LYS:HA	6	0.19
(3,60)	1:6:A:GLU:HB2	1:48:A:LYS:HA	12	0.19
(3,50)	1:10:A:VAL:HG21	1:10:A:VAL:HA	12	0.19
(3,42)	1:47:A:PHE:HB2	1:47:A:PHE:HA	11	0.19
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	15	0.19
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	1	0.19
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	8	0.19
(3,4)	1:45:A:ILE:HG13	1:45:A:ILE:HB	6	0.19
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	14	0.19
(1,2237)	1:73:A:VAL:HG21	1:61:A:PHE:HE1	4	0.19
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB1	12	0.19
(1,2228)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	7	0.19
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	12	0.19
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	10	0.19
(1,2147)	1:62:A:ARG:HA	1:70:A:PHE:HA	18	0.19
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE1	19	0.19
(1,2111)	1:23:A:TYR:HD1	1:23:A:TYR:HA	16	0.19
(1,2096)	1:73:A:VAL:HG22	1:72:A:GLU:HA	2	0.19
(1,2096)	1:73:A:VAL:HG21	1:72:A:GLU:HA	16	0.19
(1,2096)	1:73:A:VAL:HG21	1:72:A:GLU:HA	17	0.19
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	14	0.19
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	2	0.19
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	7	0.19
(1,2050)	1:73:A:VAL:HG22	1:73:A:VAL:HA	4	0.19
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	9	0.19
(1,2050)	1:73:A:VAL:HG21	1:73:A:VAL:HA	10	0.19
(1,2050)	1:73:A:VAL:HG22	1:73:A:VAL:HA	18	0.19
(1,2038)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	10	0.19
(1,2019)	1:4:A:CYS:HB3	1:4:A:CYS:HA	17	0.19
(1,2009)	1:30:A:THR:HA	1:30:A:THR:HG22	18	0.19
(1,1982)	1:47:A:PHE:HD2	1:30:A:THR:HB	14	0.19
(1,1962)	1:34:A:VAL:HG23	1:34:A:VAL:HA	4	0.19
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG22	11	0.19
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG21	19	0.19
(1,1958)	1:11:A:ILE:H	1:10:A:VAL:HG22	11	0.19
(1,1957)	1:10:A:VAL:HG23	1:10:A:VAL:HB	18	0.19
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG11	2	0.19
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	13	0.19
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG11	14	0.19
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG22	7	0.19
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG23	8	0.19
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG23	8	0.19
(1,1928)	1:98:A:ILE:HG22	1:98:A:ILE:HA	8	0.19
(1,1928)	1:98:A:ILE:HG22	1:98:A:ILE:HA	14	0.19
(1,1926)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	20	0.19
(1,1918)	1:11:A:ILE:HG23	1:11:A:ILE:HD11	20	0.19
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD12	2	0.19
(1,1883)	1:113:A:TRP:HB3	1:114:A:ARG:H	3	0.19
(1,1839)	1:57:A:TRP:H	1:56:A:ARG:HB3	13	0.19
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	20	0.19
(1,1787)	1:115:A:SER:H	1:114:A:ARG:HB3	9	0.19
(1,1787)	1:115:A:SER:H	1:114:A:ARG:HB3	16	0.19
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	5	0.19
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	19	0.19
(1,1757)	1:101:A:LYS:H	1:100:A:PHE:HA	12	0.19
(1,1721)	1:57:A:TRP:H	1:76:A:TYR:H	11	0.19
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	16	0.19
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG22	3	0.19
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	13	0.19
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG21	20	0.19
(1,1602)	1:51:A:GLY:H	1:50:A:ASP:H	15	0.19
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	1	0.19
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	7	0.19
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	12	0.19
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG21	6	0.19
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	17	0.19
(1,1420)	1:12:A:LYS:HG2	1:12:A:LYS:H	1	0.19
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	18	0.19
(1,1344)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	6	0.19
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	1	0.19
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	10	0.19
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	20	0.19
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	1	0.19
(1,1333)	1:23:A:TYR:HD2	1:23:A:TYR:HA	15	0.19
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG23	17	0.19
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	1	0.19
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG23	7	0.19
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	16	0.19
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD11	15	0.19
(1,1257)	1:45:A:ILE:HG21	1:45:A:ILE:HD13	12	0.19
(1,1257)	1:45:A:ILE:HG23	1:45:A:ILE:HD11	18	0.19
(1,1243)	1:20:A:ILE:HD12	1:20:A:ILE:HB	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1242)	1:20:A:ILE:HD13	1:39:A:PHE:H	16	0.19
(1,1152)	1:15:A:LEU:HA	1:15:A:LEU:HD13	14	0.19
(1,1143)	1:98:A:ILE:HG22	1:92:A:SER:H	15	0.19
(1,1143)	1:98:A:ILE:HG21	1:92:A:SER:H	16	0.19
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	9	0.19
(1,1082)	1:30:A:THR:HA	1:30:A:THR:HG22	18	0.19
(1,1061)	1:73:A:VAL:HG22	1:59:A:CYS:HB3	1	0.19
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG23	8	0.19
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	3	0.19
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	13	0.19
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	14	0.19
(1,998)	1:104:A:GLU:HA	1:104:A:GLU:HB3	15	0.19
(1,982)	1:73:A:VAL:HG23	1:72:A:GLU:HA	6	0.19
(1,976)	1:46:A:LYS:HB2	1:46:A:LYS:HA	2	0.19
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	4	0.19
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	18	0.19
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	14	0.19
(1,913)	1:15:A:LEU:HD11	1:19:A:ARG:HB3	4	0.19
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	20	0.19
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	10	0.19
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG13	19	0.19
(1,892)	1:98:A:ILE:HG21	1:61:A:PHE:HE2	1	0.19
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	7	0.19
(1,863)	1:37:A:LEU:H	1:20:A:ILE:HD13	6	0.19
(1,860)	1:89:A:TYR:H	1:10:A:VAL:H	11	0.19
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	18	0.19
(1,796)	1:9:A:ILE:H	1:9:A:ILE:HB	13	0.19
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	7	0.19
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	15	0.19
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	20	0.19
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	1	0.19
(1,736)	1:102:A:MET:H	1:101:A:LYS:HB2	10	0.19
(1,711)	1:94:A:ARG:HB3	1:96:A:ASP:H	6	0.19
(1,709)	1:96:A:ASP:HB3	1:96:A:ASP:H	17	0.19
(1,695)	1:57:A:TRP:H	1:76:A:TYR:H	4	0.19
(1,678)	1:87:A:LYS:HB3	1:88:A:ARG:H	3	0.19
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	9	0.19
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	13	0.19
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD12	19	0.19
(1,525)	1:20:A:ILE:HD11	1:38:A:ASN:H	13	0.19
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	16	0.19
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD1	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:10:A:VAL:HG23	1:10:A:VAL:H	14	0.19
(1,391)	1:112:A:LYS:H	1:98:A:ILE:HB	7	0.19
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	4	0.19
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	1	0.19
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	15	0.19
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	7	0.19
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	9	0.19
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	2	0.19
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	6	0.19
(1,298)	1:34:A:VAL:HG21	1:24:A:HIS:HE1	19	0.19
(1,291)	1:73:A:VAL:HG23	1:71:A:THR:HG22	2	0.19
(1,291)	1:73:A:VAL:HG21	1:71:A:THR:HG22	17	0.19
(1,290)	1:20:A:ILE:HD12	1:20:A:ILE:HB	13	0.19
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	13	0.19
(1,209)	1:32:A:VAL:HG21	1:32:A:VAL:HA	6	0.19
(1,190)	1:52:A:THR:HB	1:52:A:THR:HA	11	0.19
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	6	0.19
(1,156)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	1	0.19
(1,145)	1:42:A:THR:HG21	1:12:A:LYS:HA	13	0.19
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	10	0.19
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD11	9	0.19
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	1	0.19
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	5	0.19
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	12	0.19
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	16	0.19
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	10	0.19
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG23	18	0.19
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	6	0.19
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG23	10	0.19
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG21	9	0.19
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG21	5	0.19
(1,47)	1:20:A:ILE:HG21	1:21:A:LEU:H	4	0.19
(1,42)	1:7:A:ILE:HD11	1:84:A:LEU:HB3	9	0.19
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	9	0.19
(1,19)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	6	0.19
(1,8)	1:10:A:VAL:HG23	1:10:A:VAL:HA	17	0.19
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	1	0.19
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	7	0.19
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	14	0.19
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	15	0.19
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	17	0.19
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,329)	1:6:A:GLU:HG2	1:6:A:GLU:HA	3	0.18
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	20	0.18
(3,316)	1:54:A:ARG:H	1:53:A:GLU:HG3	11	0.18
(3,309)	1:104:A:GLU:H	1:103:A:ASP:HB2	7	0.18
(3,297)	1:47:A:PHE:HB3	1:48:A:LYS:H	10	0.18
(3,262)	1:45:A:ILE:HG13	1:45:A:ILE:HB	12	0.18
(3,251)	1:99:A:TYR:HA	1:109:A:PRO:HB3	5	0.18
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	18	0.18
(3,246)	1:5:A:LYS:HG3	1:5:A:LYS:HA	18	0.18
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	4	0.18
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	11	0.18
(3,243)	1:25:A:CYS:HA	1:59:A:CYS:HB2	6	0.18
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	7	0.18
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	3	0.18
(3,218)	1:11:A:ILE:HG22	1:37:A:LEU:HB2	14	0.18
(3,204)	1:105:A:ARG:HG2	1:105:A:ARG:H	7	0.18
(3,197)	1:91:A:LEU:H	1:91:A:LEU:HB2	7	0.18
(3,195)	1:88:A:ARG:HB3	1:88:A:ARG:H	13	0.18
(3,184)	1:47:A:PHE:H	1:8:A:GLU:HB3	1	0.18
(3,164)	1:5:A:LYS:HB2	1:5:A:LYS:H	7	0.18
(3,161)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	11	0.18
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	4	0.18
(3,139)	1:98:A:ILE:HG23	1:98:A:ILE:HD12	12	0.18
(3,134)	1:36:A:TYR:HD1	1:22:A:GLN:HA	11	0.18
(3,60)	1:6:A:GLU:HB2	1:48:A:LYS:HA	11	0.18
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	5	0.18
(3,49)	1:98:A:ILE:HG22	1:98:A:ILE:HA	20	0.18
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	8	0.18
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	15	0.18
(3,28)	1:19:A:ARG:HA	1:19:A:ARG:HG3	18	0.18
(3,24)	1:10:A:VAL:H	1:9:A:ILE:HB	16	0.18
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	20	0.18
(3,17)	1:87:A:LYS:HB2	1:87:A:LYS:HA	1	0.18
(3,16)	1:31:A:ASN:HA	1:26:A:ARG:HB3	12	0.18
(3,8)	1:76:A:TYR:HB2	1:75:A:ALA:HB2	15	0.18
(1,2278)	1:15:A:LEU:HA	1:15:A:LEU:HD12	13	0.18
(1,2263)	1:37:A:LEU:HA	1:37:A:LEU:HB2	7	0.18
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	4	0.18
(1,2246)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	8	0.18
(1,2228)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	20	0.18
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	16	0.18
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG23	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG22	12	0.18
(1,2150)	1:62:A:ARG:HA	1:70:A:PHE:HB3	13	0.18
(1,2148)	1:70:A:PHE:HB2	1:62:A:ARG:HA	17	0.18
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	16	0.18
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	6	0.18
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	15	0.18
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	3	0.18
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	4	0.18
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	8	0.18
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	13	0.18
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	20	0.18
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	8	0.18
(1,2019)	1:4:A:CYS:HB3	1:4:A:CYS:HA	3	0.18
(1,2007)	1:78:A:PRO:HA	1:78:A:PRO:HB2	6	0.18
(1,1982)	1:47:A:PHE:HD1	1:30:A:THR:HB	15	0.18
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	7	0.18
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG23	3	0.18
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG23	7	0.18
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG22	9	0.18
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	3	0.18
(1,1957)	1:10:A:VAL:HG21	1:10:A:VAL:HB	5	0.18
(1,1957)	1:10:A:VAL:HG22	1:10:A:VAL:HB	15	0.18
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	20	0.18
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG13	17	0.18
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG21	6	0.18
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG22	15	0.18
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	11	0.18
(1,1928)	1:98:A:ILE:HG22	1:98:A:ILE:HA	15	0.18
(1,1928)	1:98:A:ILE:HG21	1:98:A:ILE:HA	16	0.18
(1,1923)	1:23:A:TYR:HE2	1:11:A:ILE:HG22	20	0.18
(1,1898)	1:89:A:TYR:H	1:10:A:VAL:H	7	0.18
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD12	3	0.18
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	7	0.18
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	1	0.18
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	4	0.18
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	11	0.18
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	15	0.18
(1,1843)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	17	0.18
(1,1839)	1:57:A:TRP:H	1:56:A:ARG:HB3	2	0.18
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	5	0.18
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	19	0.18
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	2	0.18
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	14	0.18
(1,1631)	1:58:A:ASN:HB3	1:59:A:CYS:H	8	0.18
(1,1600)	1:50:A:ASP:H	1:49:A:ASP:HB2	4	0.18
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	6	0.18
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	6	0.18
(1,1501)	1:29:A:ASN:HB2	1:30:A:THR:H	5	0.18
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	18	0.18
(1,1452)	1:19:A:ARG:HB3	1:19:A:ARG:H	19	0.18
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD1	13	0.18
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	18	0.18
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	19	0.18
(1,1344)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	10	0.18
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	2	0.18
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	4	0.18
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	7	0.18
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	8	0.18
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	11	0.18
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	14	0.18
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	15	0.18
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	17	0.18
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	18	0.18
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	10	0.18
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	15	0.18
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	18	0.18
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	20	0.18
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG22	2	0.18
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	9	0.18
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG23	15	0.18
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG21	19	0.18
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	10	0.18
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD13	9	0.18
(1,1206)	1:30:A:THR:HA	1:30:A:THR:HG22	18	0.18
(1,1173)	1:20:A:ILE:HG23	1:20:A:ILE:HG12	4	0.18
(1,1171)	1:1:A:ALA:HB1	1:83:A:PRO:HA	17	0.18
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	6	0.18
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	7	0.18
(1,1166)	1:47:A:PHE:HD2	1:30:A:THR:HG21	14	0.18
(1,1160)	1:34:A:VAL:HG23	1:34:A:VAL:HA	1	0.18
(1,1160)	1:34:A:VAL:HG21	1:34:A:VAL:HA	10	0.18
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD12	6	0.18
(1,1147)	1:61:A:PHE:HD1	1:71:A:THR:HG21	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1143)	1:98:A:ILE:HG22	1:92:A:SER:H	8	0.18
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	18	0.18
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG22	14	0.18
(1,1118)	1:45:A:ILE:HD11	1:45:A:ILE:HB	1	0.18
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	1	0.18
(1,1109)	1:9:A:ILE:HD12	1:9:A:ILE:HG23	11	0.18
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	15	0.18
(1,1103)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	18	0.18
(1,1102)	1:98:A:ILE:HD12	1:71:A:THR:HG22	6	0.18
(1,1097)	1:10:A:VAL:HG23	1:10:A:VAL:HA	1	0.18
(1,1097)	1:10:A:VAL:HG22	1:10:A:VAL:HA	14	0.18
(1,1064)	1:37:A:LEU:HA	1:37:A:LEU:HB2	17	0.18
(1,1058)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	8	0.18
(1,1055)	1:42:A:THR:HG21	1:11:A:ILE:H	11	0.18
(1,1036)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	16	0.18
(1,982)	1:73:A:VAL:HG22	1:72:A:GLU:HA	12	0.18
(1,974)	1:39:A:PHE:HA	1:39:A:PHE:HD1	3	0.18
(1,962)	1:35:A:GLN:HG3	1:35:A:GLN:HA	15	0.18
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	8	0.18
(1,948)	1:10:A:VAL:HG21	1:90:A:GLU:H	7	0.18
(1,944)	1:8:A:GLU:HB3	1:8:A:GLU:HA	17	0.18
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	2	0.18
(1,935)	1:4:A:CYS:HB3	1:4:A:CYS:HA	10	0.18
(1,908)	1:10:A:VAL:HG23	1:10:A:VAL:HB	2	0.18
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	8	0.18
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	11	0.18
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	12	0.18
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	16	0.18
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	19	0.18
(1,907)	1:10:A:VAL:HG23	1:42:A:THR:HB	1	0.18
(1,905)	1:24:A:HIS:HB3	1:34:A:VAL:HG12	3	0.18
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG11	12	0.18
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG11	7	0.18
(1,903)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	11	0.18
(1,889)	1:98:A:ILE:HG22	1:91:A:LEU:HB2	14	0.18
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	15	0.18
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD13	11	0.18
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	9	0.18
(1,817)	1:71:A:THR:H	1:70:A:PHE:HE1	9	0.18
(1,809)	1:57:A:TRP:H	1:56:A:ARG:HB3	2	0.18
(1,796)	1:9:A:ILE:H	1:9:A:ILE:HB	16	0.18
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	4	0.18
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	8	0.18
(1,758)	1:111:A:ASN:H	1:98:A:ILE:HG23	8	0.18
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	13	0.18
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	17	0.18
(1,730)	1:101:A:LYS:H	1:100:A:PHE:HA	12	0.18
(1,702)	1:95:A:MET:HG2	1:95:A:MET:H	14	0.18
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	6	0.18
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	14	0.18
(1,622)	1:71:A:THR:H	1:71:A:THR:HG22	5	0.18
(1,532)	1:39:A:PHE:HA	1:40:A:LYS:H	6	0.18
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	5	0.18
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	19	0.18
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	18	0.18
(1,448)	1:19:A:ARG:HB3	1:19:A:ARG:H	18	0.18
(1,430)	1:15:A:LEU:H	1:14:A:THR:H	18	0.18
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	17	0.18
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	18	0.18
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	6	0.18
(1,335)	1:109:A:PRO:HB3	1:97:A:ALA:HB2	14	0.18
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	5	0.18
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	19	0.18
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	2	0.18
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	19	0.18
(1,302)	1:23:A:TYR:HD2	1:59:A:CYS:HB3	18	0.18
(1,290)	1:20:A:ILE:HD11	1:20:A:ILE:HB	18	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD12	1	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	2	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	3	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	4	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD12	5	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	6	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	7	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	8	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	9	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD12	10	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD12	11	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	12	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD12	14	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	15	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	16	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	18	0.18
(1,268)	1:98:A:ILE:HD11	1:98:A:ILE:HD13	19	0.18
(1,268)	1:98:A:ILE:HD12	1:98:A:ILE:HD13	20	0.18
(1,249)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	18	0.18
(1,244)	1:70:A:PHE:HD1	1:70:A:PHE:HB3	9	0.18
(1,169)	1:61:A:PHE:HA	1:61:A:PHE:HD2	14	0.18
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD2	18	0.18
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	2	0.18
(1,145)	1:42:A:THR:HG21	1:12:A:LYS:HA	2	0.18
(1,144)	1:95:A:MET:H	1:14:A:THR:HG21	12	0.18
(1,131)	1:94:A:ARG:HA	1:15:A:LEU:HG	15	0.18
(1,90)	1:50:A:ASP:HA	1:50:A:ASP:HB3	13	0.18
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG22	13	0.18
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG21	15	0.18
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG23	17	0.18
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	17	0.18
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	2	0.18
(1,50)	1:99:A:TYR:H	1:98:A:ILE:HG23	13	0.18
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	13	0.18
(1,38)	1:45:A:ILE:HD11	1:45:A:ILE:HG13	16	0.18
(1,36)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	4	0.18
(1,33)	1:9:A:ILE:HG12	1:9:A:ILE:HG22	12	0.18
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	14	0.18
(1,23)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	15	0.18
(1,19)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	4	0.18
(1,9)	1:98:A:ILE:HD13	1:98:A:ILE:HA	14	0.18
(1,5)	1:42:A:THR:HG21	1:42:A:THR:HB	5	0.18
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	6	0.18
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	8	0.18
(1,5)	1:42:A:THR:HG21	1:42:A:THR:HB	13	0.18
(1,5)	1:42:A:THR:HG21	1:42:A:THR:HB	18	0.18
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	19	0.18
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	20	0.18
(1,2)	1:30:A:THR:HA	1:30:A:THR:HG22	5	0.18
(4,13)	1:90:A:GLU:H	1:101:A:LYS:O	10	0.17
(3,327)	1:10:A:VAL:HG21	1:10:A:VAL:HA	9	0.17
(3,327)	1:10:A:VAL:HG22	1:10:A:VAL:HA	11	0.17
(3,326)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	3	0.17
(3,326)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	19	0.17
(3,309)	1:103:A:ASP:HB3	1:104:A:GLU:H	4	0.17
(3,298)	1:48:A:LYS:HB2	1:48:A:LYS:H	7	0.17
(3,246)	1:5:A:LYS:HG3	1:5:A:LYS:HA	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	6	0.17
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	7	0.17
(3,243)	1:25:A:CYS:HA	1:26:A:ARG:HB3	10	0.17
(3,231)	1:14:A:THR:HB	1:12:A:LYS:HG3	4	0.17
(3,216)	1:19:A:ARG:HG3	1:95:A:MET:H	13	0.17
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG2	12	0.17
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB2	9	0.17
(3,205)	1:111:A:ASN:H	1:98:A:ILE:HB	9	0.17
(3,202)	1:104:A:GLU:H	1:103:A:ASP:HB2	7	0.17
(3,185)	1:47:A:PHE:HB3	1:48:A:LYS:H	10	0.17
(3,181)	1:36:A:TYR:H	1:35:A:GLN:HB2	3	0.17
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	19	0.17
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	17	0.17
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	20	0.17
(3,125)	1:73:A:VAL:HG11	1:73:A:VAL:HG23	8	0.17
(3,125)	1:73:A:VAL:HG11	1:73:A:VAL:HG22	16	0.17
(3,108)	1:44:A:ILE:HG23	1:8:A:GLU:HB2	1	0.17
(3,107)	1:44:A:ILE:HG23	1:8:A:GLU:HB2	1	0.17
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG22	14	0.17
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	11	0.17
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	5	0.17
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	18	0.17
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	10	0.17
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	13	0.17
(3,36)	1:61:A:PHE:HE2	1:93:A:ALA:HA	5	0.17
(3,35)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	3	0.17
(3,31)	1:92:A:SER:HB3	1:92:A:SER:H	11	0.17
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	19	0.17
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	11	0.17
(3,16)	1:31:A:ASN:HA	1:26:A:ARG:HB3	9	0.17
(3,15)	1:85:A:CYS:HB3	1:4:A:CYS:HA	7	0.17
(1,2222)	1:95:A:MET:HG3	1:14:A:THR:HG22	18	0.17
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG21	7	0.17
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG22	17	0.17
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	17	0.17
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	20	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	2	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	6	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	9	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	10	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	11	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	14	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	15	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	17	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	18	0.17
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	19	0.17
(1,2070)	1:35:A:GLN:HA	1:35:A:GLN:HG2	2	0.17
(1,2050)	1:73:A:VAL:HG22	1:73:A:VAL:HA	5	0.17
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD13	1	0.17
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	11	0.17
(1,1982)	1:47:A:PHE:HD1	1:30:A:THR:HB	11	0.17
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD11	12	0.17
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	6	0.17
(1,1962)	1:34:A:VAL:HG23	1:34:A:VAL:HA	11	0.17
(1,1962)	1:34:A:VAL:HG22	1:34:A:VAL:HA	19	0.17
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG23	6	0.17
(1,1955)	1:10:A:VAL:HG21	1:10:A:VAL:HA	9	0.17
(1,1955)	1:10:A:VAL:HG22	1:10:A:VAL:HA	11	0.17
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	15	0.17
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	1	0.17
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	10	0.17
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG23	12	0.17
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	20	0.17
(1,1943)	1:71:A:THR:HA	1:71:A:THR:HG22	2	0.17
(1,1918)	1:11:A:ILE:HG23	1:11:A:ILE:HD12	6	0.17
(1,1898)	1:89:A:TYR:H	1:10:A:VAL:H	18	0.17
(1,1892)	1:30:A:THR:H	1:27:A:SER:H	12	0.17
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	7	0.17
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	10	0.17
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	12	0.17
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	14	0.17
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	18	0.17
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	19	0.17
(1,1839)	1:57:A:TRP:H	1:56:A:ARG:HB3	20	0.17
(1,1826)	1:9:A:ILE:H	1:9:A:ILE:HB	3	0.17
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG23	15	0.17
(1,1796)	1:32:A:VAL:H	1:26:A:ARG:HA	13	0.17
(1,1796)	1:32:A:VAL:H	1:26:A:ARG:HA	20	0.17
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	1	0.17
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	9	0.17
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	3	0.17
(1,1672)	1:79:A:ASP:H	1:78:A:PRO:HA	16	0.17
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:50:A:ASP:H	1:49:A:ASP:HA	15	0.17
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	3	0.17
(1,1548)	1:39:A:PHE:HA	1:40:A:LYS:H	9	0.17
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	4	0.17
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	16	0.17
(1,1452)	1:19:A:ARG:HB3	1:19:A:ARG:H	14	0.17
(1,1430)	1:14:A:THR:H	1:93:A:ALA:H	14	0.17
(1,1408)	1:10:A:VAL:HG21	1:10:A:VAL:H	1	0.17
(1,1406)	1:8:A:GLU:HG2	1:8:A:GLU:H	20	0.17
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	5	0.17
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	12	0.17
(1,1396)	1:108:A:GLN:HG2	1:108:A:GLN:H	12	0.17
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	2	0.17
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	6	0.17
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	9	0.17
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	13	0.17
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	16	0.17
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	19	0.17
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	2	0.17
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	4	0.17
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	7	0.17
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	8	0.17
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	11	0.17
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	14	0.17
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	17	0.17
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	19	0.17
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	13	0.17
(1,1297)	1:95:A:MET:H	1:14:A:THR:HG21	14	0.17
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG23	13	0.17
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	8	0.17
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	10	0.17
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	20	0.17
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD11	3	0.17
(1,1242)	1:20:A:ILE:HD13	1:39:A:PHE:H	7	0.17
(1,1230)	1:9:A:ILE:HD12	1:9:A:ILE:HA	10	0.17
(1,1171)	1:1:A:ALA:HB3	1:83:A:PRO:HA	8	0.17
(1,1171)	1:1:A:ALA:HB1	1:83:A:PRO:HA	13	0.17
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	17	0.17
(1,1165)	1:57:A:TRP:HB3	1:75:A:ALA:HB1	19	0.17
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	13	0.17
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG22	2	0.17
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG23	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD12	17	0.17
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	3	0.17
(1,1052)	1:73:A:VAL:HG23	1:111:A:ASN:HB2	2	0.17
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	5	0.17
(1,1039)	1:73:A:VAL:HB	1:98:A:ILE:HG21	14	0.17
(1,1022)	1:73:A:VAL:HG23	1:91:A:LEU:HB2	11	0.17
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	15	0.17
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE1	9	0.17
(1,982)	1:73:A:VAL:HG21	1:72:A:GLU:HA	18	0.17
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	8	0.17
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	1	0.17
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	20	0.17
(1,913)	1:15:A:LEU:HD12	1:19:A:ARG:HB3	9	0.17
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	9	0.17
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	14	0.17
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG13	5	0.17
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG21	18	0.17
(1,892)	1:98:A:ILE:HG22	1:61:A:PHE:HE1	18	0.17
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG21	13	0.17
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	5	0.17
(1,890)	1:98:A:ILE:HG22	1:98:A:ILE:HA	20	0.17
(1,867)	1:14:A:THR:H	1:19:A:ARG:HB3	1	0.17
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD12	2	0.17
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD11	12	0.17
(1,850)	1:113:A:TRP:HB3	1:114:A:ARG:H	3	0.17
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	10	0.17
(1,809)	1:57:A:TRP:H	1:56:A:ARG:HB3	13	0.17
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	5	0.17
(1,776)	1:56:A:ARG:HB2	1:56:A:ARG:H	20	0.17
(1,761)	1:115:A:SER:H	1:114:A:ARG:HB3	9	0.17
(1,761)	1:115:A:SER:H	1:114:A:ARG:HB3	16	0.17
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	5	0.17
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	19	0.17
(1,734)	1:102:A:MET:H	1:102:A:MET:HG2	2	0.17
(1,695)	1:57:A:TRP:H	1:76:A:TYR:H	11	0.17
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	5	0.17
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	16	0.17
(1,622)	1:71:A:THR:H	1:71:A:THR:HG22	3	0.17
(1,621)	1:70:A:PHE:H	1:114:A:ARG:H	9	0.17
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	13	0.17
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG21	20	0.17
(1,581)	1:51:A:GLY:H	1:50:A:ASP:H	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	1	0.17
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	7	0.17
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	11	0.17
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	12	0.17
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	18	0.17
(1,489)	1:30:A:THR:H	1:30:A:THR:HG21	6	0.17
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	17	0.17
(1,421)	1:12:A:LYS:HG2	1:12:A:LYS:H	1	0.17
(1,349)	1:85:A:CYS:H	1:84:A:LEU:HA	7	0.17
(1,340)	1:87:A:LYS:HB3	1:88:A:ARG:H	11	0.17
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	6	0.17
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	7	0.17
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	10	0.17
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	18	0.17
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	20	0.17
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	4	0.17
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	12	0.17
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	13	0.17
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	16	0.17
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	2	0.17
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	20	0.17
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	20	0.17
(1,154)	1:98:A:ILE:HG13	1:113:A:TRP:H	16	0.17
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	10	0.17
(1,145)	1:42:A:THR:HG21	1:12:A:LYS:HA	5	0.17
(1,144)	1:95:A:MET:H	1:14:A:THR:HG22	11	0.17
(1,138)	1:36:A:TYR:HA	1:23:A:TYR:H	10	0.17
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	9	0.17
(1,126)	1:45:A:ILE:H	1:45:A:ILE:HD13	16	0.17
(1,120)	1:20:A:ILE:HA	1:38:A:ASN:HA	13	0.17
(1,117)	1:20:A:ILE:HD12	1:39:A:PHE:H	5	0.17
(1,71)	1:112:A:LYS:HB3	1:97:A:ALA:HB1	17	0.17
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	3	0.17
(1,70)	1:47:A:PHE:HD1	1:30:A:THR:HG23	13	0.17
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG23	16	0.17
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG21	7	0.17
(1,47)	1:20:A:ILE:HG22	1:21:A:LEU:H	2	0.17
(1,27)	1:20:A:ILE:HA	1:20:A:ILE:HD12	4	0.17
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	4	0.17
(1,25)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	8	0.17
(1,19)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	16	0.17
(1,5)	1:42:A:THR:HG21	1:42:A:THR:HB	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	9	0.17
(1,5)	1:42:A:THR:HG23	1:42:A:THR:HB	12	0.17
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	16	0.17
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	5	0.16
(4,4)	1:7:A:ILE:H	1:47:A:PHE:O	19	0.16
(3,329)	1:6:A:GLU:HA	1:6:A:GLU:HG3	2	0.16
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	18	0.16
(3,309)	1:103:A:ASP:HB3	1:104:A:GLU:H	18	0.16
(3,297)	1:47:A:PHE:HB3	1:48:A:LYS:H	20	0.16
(3,262)	1:45:A:ILE:HG13	1:45:A:ILE:HB	16	0.16
(3,248)	1:114:A:ARG:HB3	1:113:A:TRP:HB2	11	0.16
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	10	0.16
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG23	5	0.16
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB3	2	0.16
(3,215)	1:99:A:TYR:H	1:97:A:ALA:HB1	7	0.16
(3,211)	1:54:A:ARG:H	1:53:A:GLU:HG3	11	0.16
(3,192)	1:86:A:GLY:H	1:87:A:LYS:HB2	9	0.16
(3,186)	1:48:A:LYS:HB2	1:48:A:LYS:H	7	0.16
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG22	4	0.16
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG21	7	0.16
(3,158)	1:12:A:LYS:HB3	1:14:A:THR:HG21	15	0.16
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	1	0.16
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	2	0.16
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	5	0.16
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	16	0.16
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	14	0.16
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	2	0.16
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	19	0.16
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	4	0.16
(3,60)	1:6:A:GLU:HB2	1:48:A:LYS:HA	2	0.16
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	16	0.16
(3,56)	1:85:A:CYS:HB3	1:85:A:CYS:HA	17	0.16
(3,50)	1:10:A:VAL:HG22	1:10:A:VAL:HA	19	0.16
(3,49)	1:98:A:ILE:HG22	1:98:A:ILE:HA	8	0.16
(3,49)	1:98:A:ILE:HG22	1:98:A:ILE:HA	14	0.16
(3,24)	1:10:A:VAL:H	1:9:A:ILE:HB	3	0.16
(1,2239)	1:73:A:VAL:HG23	1:71:A:THR:HG23	14	0.16
(1,2218)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	1	0.16
(1,2148)	1:70:A:PHE:HB2	1:62:A:ARG:HA	9	0.16
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	10	0.16
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE1	6	0.16
(1,2096)	1:73:A:VAL:HG23	1:72:A:GLU:HA	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	10	0.16
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	4	0.16
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	11	0.16
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	14	0.16
(1,2082)	1:45:A:ILE:HA	1:45:A:ILE:HB	16	0.16
(1,2070)	1:35:A:GLN:HA	1:35:A:GLN:HG2	8	0.16
(1,2050)	1:73:A:VAL:HG23	1:73:A:VAL:HA	7	0.16
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	16	0.16
(1,2020)	1:4:A:CYS:HB3	1:4:A:CYS:HA	10	0.16
(1,1998)	1:32:A:VAL:HG22	1:32:A:VAL:HA	2	0.16
(1,1982)	1:47:A:PHE:HD1	1:30:A:THR:HB	13	0.16
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG22	10	0.16
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG21	14	0.16
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	18	0.16
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG21	14	0.16
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	15	0.16
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	3	0.16
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	4	0.16
(1,1917)	1:9:A:ILE:H	1:9:A:ILE:HD11	19	0.16
(1,1908)	1:111:A:ASN:H	1:110:A:LEU:HB3	7	0.16
(1,1892)	1:30:A:THR:H	1:27:A:SER:H	8	0.16
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	2	0.16
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	4	0.16
(1,1826)	1:9:A:ILE:H	1:9:A:ILE:HB	1	0.16
(1,1817)	1:112:A:LYS:H	1:111:A:ASN:HB2	8	0.16
(1,1812)	1:113:A:TRP:H	1:113:A:TRP:HB2	6	0.16
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	11	0.16
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	20	0.16
(1,1765)	1:104:A:GLU:H	1:104:A:GLU:HB2	6	0.16
(1,1721)	1:57:A:TRP:H	1:76:A:TYR:H	8	0.16
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	14	0.16
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	4	0.16
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	5	0.16
(1,1631)	1:58:A:ASN:HB3	1:59:A:CYS:H	9	0.16
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	1	0.16
(1,1610)	1:53:A:GLU:H	1:52:A:THR:HA	13	0.16
(1,1600)	1:50:A:ASP:H	1:49:A:ASP:HB2	10	0.16
(1,1577)	1:9:A:ILE:HG12	1:46:A:LYS:H	18	0.16
(1,1546)	1:38:A:ASN:HB2	1:39:A:PHE:H	7	0.16
(1,1533)	1:36:A:TYR:HB3	1:37:A:LEU:H	19	0.16
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	3	0.16
(1,1520)	1:35:A:GLN:HG3	1:35:A:GLN:H	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:35:A:GLN:H	1:34:A:VAL:HG11	6	0.16
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG23	10	0.16
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	8	0.16
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB1	14	0.16
(1,1342)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	3	0.16
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	5	0.16
(1,1342)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	12	0.16
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	3	0.16
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	5	0.16
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	6	0.16
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	9	0.16
(1,1339)	1:61:A:PHE:HD2	1:61:A:PHE:HE2	12	0.16
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	13	0.16
(1,1339)	1:61:A:PHE:HD1	1:61:A:PHE:HE1	16	0.16
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG22	2	0.16
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG22	8	0.16
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG23	20	0.16
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	2	0.16
(1,1259)	1:45:A:ILE:H	1:45:A:ILE:HD12	10	0.16
(1,1242)	1:20:A:ILE:HD12	1:39:A:PHE:H	4	0.16
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	19	0.16
(1,1172)	1:20:A:ILE:HG22	1:20:A:ILE:HG13	4	0.16
(1,1171)	1:1:A:ALA:HB2	1:83:A:PRO:HA	1	0.16
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	14	0.16
(1,1166)	1:47:A:PHE:HD1	1:30:A:THR:HG21	15	0.16
(1,1163)	1:9:A:ILE:HD12	1:75:A:ALA:HB3	19	0.16
(1,1160)	1:34:A:VAL:HG23	1:34:A:VAL:HA	20	0.16
(1,1143)	1:98:A:ILE:HG23	1:92:A:SER:H	10	0.16
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	6	0.16
(1,1113)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	6	0.16
(1,1113)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	12	0.16
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	15	0.16
(1,1108)	1:7:A:ILE:HD11	1:7:A:ILE:HA	19	0.16
(1,1107)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	9	0.16
(1,1061)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	8	0.16
(1,1037)	1:73:A:VAL:HG22	1:91:A:LEU:HB3	6	0.16
(1,1022)	1:73:A:VAL:HG21	1:91:A:LEU:HB2	1	0.16
(1,1022)	1:73:A:VAL:HG23	1:91:A:LEU:HB2	17	0.16
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	14	0.16
(1,1016)	1:4:A:CYS:HA	1:85:A:CYS:HB2	15	0.16
(1,1014)	1:23:A:TYR:HD2	1:25:A:CYS:HA	18	0.16
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	10	0.16
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	20	0.16
(1,982)	1:73:A:VAL:HG21	1:72:A:GLU:HA	4	0.16
(1,974)	1:39:A:PHE:HA	1:39:A:PHE:HD1	8	0.16
(1,974)	1:39:A:PHE:HA	1:39:A:PHE:HD1	9	0.16
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	3	0.16
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	11	0.16
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	12	0.16
(1,935)	1:4:A:CYS:HB3	1:4:A:CYS:HA	1	0.16
(1,913)	1:15:A:LEU:HD12	1:19:A:ARG:HB3	11	0.16
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	10	0.16
(1,908)	1:10:A:VAL:HG23	1:10:A:VAL:HB	13	0.16
(1,908)	1:10:A:VAL:HG23	1:10:A:VAL:HB	17	0.16
(1,908)	1:10:A:VAL:HG23	1:10:A:VAL:HB	18	0.16
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG11	2	0.16
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	13	0.16
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG11	14	0.16
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG21	18	0.16
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	19	0.16
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG21	20	0.16
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	6	0.16
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	13	0.16
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG21	9	0.16
(1,848)	1:45:A:ILE:H	1:44:A:ILE:HG12	7	0.16
(1,847)	1:7:A:ILE:H	1:48:A:LYS:HA	12	0.16
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	1	0.16
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	4	0.16
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	11	0.16
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	3	0.16
(1,812)	1:113:A:TRP:HE1	1:15:A:LEU:HD13	17	0.16
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	3	0.16
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	9	0.16
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	13	0.16
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	14	0.16
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	3	0.16
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	19	0.16
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	19	0.16
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	2	0.16
(1,620)	1:70:A:PHE:H	1:70:A:PHE:HD1	14	0.16
(1,608)	1:58:A:ASN:HB3	1:59:A:CYS:H	8	0.16
(1,580)	1:50:A:ASP:H	1:49:A:ASP:HB2	4	0.16
(1,579)	1:50:A:ASP:H	1:49:A:ASP:HA	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	4	0.16
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	6	0.16
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	6	0.16
(1,488)	1:29:A:ASN:HB2	1:30:A:THR:H	5	0.16
(1,454)	1:20:A:ILE:H	1:20:A:ILE:HG12	18	0.16
(1,453)	1:20:A:ILE:H	1:19:A:ARG:HB3	18	0.16
(1,448)	1:19:A:ARG:HB3	1:19:A:ARG:H	19	0.16
(1,431)	1:15:A:LEU:H	1:39:A:PHE:HD1	13	0.16
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	18	0.16
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	19	0.16
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	18	0.16
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	14	0.16
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	3	0.16
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	8	0.16
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	10	0.16
(1,307)	1:25:A:CYS:HA	1:24:A:HIS:HD1	20	0.16
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	14	0.16
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	13	0.16
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	18	0.16
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	19	0.16
(1,272)	1:52:A:THR:HG22	1:52:A:THR:HA	8	0.16
(1,272)	1:52:A:THR:HG21	1:52:A:THR:HA	15	0.16
(1,260)	1:17:A:PRO:HB2	1:17:A:PRO:HA	8	0.16
(1,250)	1:61:A:PHE:HB3	1:61:A:PHE:HD2	11	0.16
(1,249)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	3	0.16
(1,197)	1:92:A:SER:HB2	1:92:A:SER:HA	18	0.16
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	11	0.16
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	2	0.16
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	4	0.16
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	7	0.16
(1,154)	1:98:A:ILE:HG13	1:113:A:TRP:H	6	0.16
(1,152)	1:61:A:PHE:HD2	1:98:A:ILE:HD12	14	0.16
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	3	0.16
(1,141)	1:64:A:GLY:HA2	1:65:A:ILE:HG21	9	0.16
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG22	11	0.16
(1,65)	1:34:A:VAL:HG22	1:34:A:VAL:HA	12	0.16
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	15	0.16
(1,43)	1:7:A:ILE:HD12	1:7:A:ILE:HG22	7	0.16
(1,23)	1:9:A:ILE:HD13	1:75:A:ALA:HB3	14	0.16
(1,8)	1:10:A:VAL:HG21	1:10:A:VAL:HA	12	0.16
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	18	0.15
(3,337)	1:53:A:GLU:HG3	1:53:A:GLU:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,327)	1:10:A:VAL:HG23	1:10:A:VAL:HA	17	0.15
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	3	0.15
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	13	0.15
(3,251)	1:99:A:TYR:HA	1:110:A:LEU:HB2	8	0.15
(3,245)	1:81:A:LYS:HA	1:81:A:LYS:HB2	16	0.15
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	4	0.15
(3,202)	1:103:A:ASP:HB3	1:104:A:GLU:H	4	0.15
(3,202)	1:103:A:ASP:HB3	1:104:A:GLU:H	18	0.15
(3,192)	1:86:A:GLY:H	1:5:A:LYS:HB3	5	0.15
(3,185)	1:47:A:PHE:HB3	1:48:A:LYS:H	20	0.15
(3,184)	1:48:A:LYS:HB2	1:47:A:PHE:H	7	0.15
(3,183)	1:46:A:LYS:H	1:45:A:ILE:HB	8	0.15
(3,155)	1:91:A:LEU:H	1:91:A:LEU:HB2	3	0.15
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	8	0.15
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	10	0.15
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	15	0.15
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG23	2	0.15
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG22	11	0.15
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG23	12	0.15
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	19	0.15
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	6	0.15
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	11	0.15
(3,85)	1:53:A:GLU:HG3	1:53:A:GLU:HA	6	0.15
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	5	0.15
(3,78)	1:39:A:PHE:HD2	1:16:A:GLY:HA2	15	0.15
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	4	0.15
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	11	0.15
(3,49)	1:98:A:ILE:HG22	1:98:A:ILE:HA	15	0.15
(3,49)	1:98:A:ILE:HG21	1:98:A:ILE:HA	16	0.15
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	12	0.15
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG22	2	0.15
(3,33)	1:76:A:TYR:HD2	1:7:A:ILE:HG21	7	0.15
(3,29)	1:115:A:SER:HA	1:69:A:PHE:HA	5	0.15
(3,27)	1:5:A:LYS:HG3	1:5:A:LYS:HA	9	0.15
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	5	0.15
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	7	0.15
(3,17)	1:87:A:LYS:HB2	1:87:A:LYS:HA	3	0.15
(1,2268)	1:108:A:GLN:HG3	1:108:A:GLN:HA	17	0.15
(1,2249)	1:23:A:TYR:HD2	1:11:A:ILE:HD11	3	0.15
(1,2236)	1:73:A:VAL:HG21	1:61:A:PHE:HD1	8	0.15
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB3	10	0.15
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	18	0.15
(1,2096)	1:73:A:VAL:HG23	1:72:A:GLU:HA	19	0.15
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	10	0.15
(1,2066)	1:79:A:ASP:HB2	1:79:A:ASP:HA	16	0.15
(1,2040)	1:84:A:LEU:HB2	1:7:A:ILE:HD11	4	0.15
(1,2038)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	12	0.15
(1,2022)	1:95:A:MET:HA	1:15:A:LEU:HD11	12	0.15
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	11	0.15
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	13	0.15
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	20	0.15
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	17	0.15
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG21	1	0.15
(1,1957)	1:10:A:VAL:HG23	1:10:A:VAL:HB	4	0.15
(1,1952)	1:34:A:VAL:HB	1:34:A:VAL:HG12	1	0.15
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	5	0.15
(1,1942)	1:95:A:MET:HA	1:15:A:LEU:HD12	17	0.15
(1,1928)	1:98:A:ILE:HG21	1:98:A:ILE:HA	1	0.15
(1,1914)	1:9:A:ILE:HB	1:9:A:ILE:HD13	12	0.15
(1,1908)	1:111:A:ASN:H	1:110:A:LEU:HB3	18	0.15
(1,1898)	1:89:A:TYR:H	1:10:A:VAL:H	12	0.15
(1,1892)	1:30:A:THR:H	1:27:A:SER:H	4	0.15
(1,1881)	1:54:A:ARG:H	1:52:A:THR:HG21	4	0.15
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	3	0.15
(1,1850)	1:71:A:THR:H	1:70:A:PHE:HE1	13	0.15
(1,1788)	1:13:A:ASN:H	1:12:A:LYS:HB2	18	0.15
(1,1787)	1:115:A:SER:H	1:114:A:ARG:HB3	3	0.15
(1,1782)	1:111:A:ASN:HB3	1:111:A:ASN:H	18	0.15
(1,1762)	1:102:A:MET:H	1:101:A:LYS:HB2	4	0.15
(1,1742)	1:113:A:TRP:HE1	1:97:A:ALA:H	6	0.15
(1,1721)	1:57:A:TRP:H	1:76:A:TYR:H	9	0.15
(1,1672)	1:79:A:ASP:H	1:78:A:PRO:HA	8	0.15
(1,1667)	1:57:A:TRP:H	1:76:A:TYR:H	16	0.15
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG22	12	0.15
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	8	0.15
(1,1628)	1:55:A:SER:H	1:56:A:ARG:HB3	12	0.15
(1,1618)	1:54:A:ARG:H	1:52:A:THR:HB	9	0.15
(1,1618)	1:54:A:ARG:H	1:52:A:THR:HB	13	0.15
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	5	0.15
(1,1596)	1:49:A:ASP:HB3	1:49:A:ASP:H	15	0.15
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	11	0.15
(1,1548)	1:39:A:PHE:HA	1:40:A:LYS:H	3	0.15
(1,1548)	1:39:A:PHE:HA	1:40:A:LYS:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1548)	1:39:A:PHE:HA	1:40:A:LYS:H	10	0.15
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	8	0.15
(1,1545)	1:38:A:ASN:HB3	1:39:A:PHE:H	5	0.15
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	17	0.15
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	1	0.15
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	14	0.15
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG23	14	0.15
(1,1463)	1:21:A:LEU:HB2	1:22:A:GLN:H	11	0.15
(1,1457)	1:20:A:ILE:H	1:20:A:ILE:HG21	2	0.15
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	14	0.15
(1,1397)	1:108:A:GLN:HG2	1:108:A:GLN:H	9	0.15
(1,1396)	1:108:A:GLN:HG2	1:108:A:GLN:H	3	0.15
(1,1387)	1:4:A:CYS:HA	1:5:A:LYS:H	14	0.15
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	14	0.15
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	1	0.15
(1,1308)	1:109:A:PRO:HA	1:97:A:ALA:HB2	10	0.15
(1,1308)	1:109:A:PRO:HA	1:97:A:ALA:HB3	20	0.15
(1,1298)	1:42:A:THR:HG21	1:12:A:LYS:HA	11	0.15
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG23	19	0.15
(1,1277)	1:1:A:ALA:HB1	1:83:A:PRO:HA	20	0.15
(1,1243)	1:20:A:ILE:HD13	1:20:A:ILE:HB	8	0.15
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	2	0.15
(1,1230)	1:9:A:ILE:HD11	1:9:A:ILE:HA	5	0.15
(1,1173)	1:20:A:ILE:HG21	1:20:A:ILE:HG12	14	0.15
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	9	0.15
(1,1168)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	8	0.15
(1,1160)	1:34:A:VAL:HG21	1:34:A:VAL:HA	9	0.15
(1,1152)	1:15:A:LEU:HA	1:15:A:LEU:HD12	17	0.15
(1,1135)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	12	0.15
(1,1113)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	18	0.15
(1,1110)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	16	0.15
(1,1107)	1:7:A:ILE:HD12	1:5:A:LYS:HB3	2	0.15
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB1	6	0.15
(1,995)	1:23:A:TYR:HE1	1:36:A:TYR:HA	7	0.15
(1,980)	1:12:A:LYS:HB2	1:92:A:SER:HA	18	0.15
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	1	0.15
(1,962)	1:35:A:GLN:HG3	1:35:A:GLN:HA	10	0.15
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	7	0.15
(1,950)	1:101:A:LYS:HB2	1:107:A:PRO:HA	2	0.15
(1,924)	1:47:A:PHE:HD2	1:30:A:THR:HB	18	0.15
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD11	18	0.15
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,908)	1:10:A:VAL:HG21	1:10:A:VAL:HB	5	0.15
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG13	17	0.15
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG21	4	0.15
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	16	0.15
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG23	3	0.15
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	4	0.15
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	6	0.15
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG21	9	0.15
(1,892)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	10	0.15
(1,890)	1:98:A:ILE:HG22	1:98:A:ILE:HA	8	0.15
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	10	0.15
(1,890)	1:98:A:ILE:HG22	1:98:A:ILE:HA	14	0.15
(1,889)	1:98:A:ILE:HG23	1:91:A:LEU:HB2	12	0.15
(1,889)	1:98:A:ILE:HG21	1:91:A:LEU:HB2	16	0.15
(1,877)	1:11:A:ILE:HG23	1:11:A:ILE:HD11	20	0.15
(1,870)	1:111:A:ASN:H	1:110:A:LEU:HB3	7	0.15
(1,860)	1:89:A:TYR:H	1:10:A:VAL:H	7	0.15
(1,860)	1:89:A:TYR:H	1:10:A:VAL:H	18	0.15
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD12	3	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	7	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	10	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	12	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	14	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	15	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	18	0.15
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	19	0.15
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	2	0.15
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	7	0.15
(1,809)	1:57:A:TRP:H	1:56:A:ARG:HB3	20	0.15
(1,796)	1:9:A:ILE:H	1:9:A:ILE:HB	1	0.15
(1,796)	1:9:A:ILE:H	1:9:A:ILE:HB	3	0.15
(1,787)	1:113:A:TRP:H	1:112:A:LYS:HB3	12	0.15
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG23	15	0.15
(1,769)	1:32:A:VAL:H	1:26:A:ARG:HA	13	0.15
(1,769)	1:32:A:VAL:H	1:26:A:ARG:HA	20	0.15
(1,761)	1:115:A:SER:H	1:114:A:ARG:HB3	3	0.15
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	1	0.15
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	9	0.15
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	20	0.15
(1,739)	1:104:A:GLU:H	1:104:A:GLU:HB2	6	0.15
(1,734)	1:102:A:MET:H	1:102:A:MET:HG2	14	0.15
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	5	0.15
(1,650)	1:79:A:ASP:H	1:78:A:PRO:HA	16	0.15
(1,644)	1:76:A:TYR:H	1:74:A:GLU:HB3	20	0.15
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	6	0.15
(1,588)	1:53:A:GLU:H	1:52:A:THR:HA	13	0.15
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	3	0.15
(1,532)	1:39:A:PHE:HA	1:40:A:LYS:H	9	0.15
(1,530)	1:38:A:ASN:HB2	1:39:A:PHE:H	7	0.15
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	3	0.15
(1,453)	1:20:A:ILE:H	1:19:A:ARG:HB3	16	0.15
(1,448)	1:19:A:ARG:HB3	1:19:A:ARG:H	14	0.15
(1,429)	1:14:A:THR:H	1:93:A:ALA:H	14	0.15
(1,413)	1:10:A:VAL:HG21	1:10:A:VAL:H	1	0.15
(1,411)	1:8:A:GLU:HG2	1:8:A:GLU:H	20	0.15
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	5	0.15
(1,410)	1:88:A:ARG:HA	1:8:A:GLU:H	12	0.15
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	2	0.15
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG21	13	0.15
(1,349)	1:85:A:CYS:H	1:84:A:LEU:HA	6	0.15
(1,349)	1:85:A:CYS:H	1:84:A:LEU:HA	18	0.15
(1,340)	1:87:A:LYS:HB3	1:88:A:ARG:H	12	0.15
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	2	0.15
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	15	0.15
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	10	0.15
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	5	0.15
(1,299)	1:23:A:TYR:HE2	1:45:A:ILE:HD13	20	0.15
(1,298)	1:34:A:VAL:HG21	1:24:A:HIS:HE1	7	0.15
(1,298)	1:34:A:VAL:HG22	1:24:A:HIS:HE1	8	0.15
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	8	0.15
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	17	0.15
(1,272)	1:52:A:THR:HG22	1:52:A:THR:HA	18	0.15
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB1	6	0.15
(1,209)	1:32:A:VAL:HG21	1:32:A:VAL:HA	19	0.15
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	5	0.15
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	6	0.15
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	7	0.15
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	9	0.15
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	13	0.15
(1,188)	1:115:A:SER:HB3	1:115:A:SER:HA	20	0.15
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	9	0.15
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	8	0.15
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD2	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	16	0.15
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	7	0.15
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	16	0.15
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD11	14	0.15
(1,94)	1:9:A:ILE:HG21	1:75:A:ALA:HA	1	0.15
(1,70)	1:47:A:PHE:HD2	1:30:A:THR:HG21	2	0.15
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG23	3	0.15
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG21	19	0.15
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB1	4	0.15
(1,65)	1:34:A:VAL:HG21	1:34:A:VAL:HA	13	0.15
(1,47)	1:20:A:ILE:HG23	1:21:A:LEU:H	9	0.15
(1,39)	1:45:A:ILE:HA	1:45:A:ILE:HG12	12	0.15
(1,23)	1:9:A:ILE:HD13	1:75:A:ALA:HB1	9	0.15
(4,23)	1:21:A:LEU:H	1:37:A:LEU:O	9	0.14
(4,21)	1:58:A:ASN:H	1:26:A:ARG:O	14	0.14
(4,10)	1:95:A:MET:H	1:14:A:THR:O	13	0.14
(3,332)	1:69:A:PHE:HA	1:115:A:SER:HB3	8	0.14
(3,327)	1:10:A:VAL:HA	1:10:A:VAL:HG13	3	0.14
(3,315)	1:104:A:GLU:HG3	1:104:A:GLU:H	14	0.14
(3,314)	1:57:A:TRP:HE1	1:47:A:PHE:HB2	17	0.14
(3,304)	1:89:A:TYR:H	1:88:A:ARG:HB3	3	0.14
(3,294)	1:28:A:GLY:H	1:27:A:SER:HB3	10	0.14
(3,289)	1:48:A:LYS:HB2	1:6:A:GLU:H	8	0.14
(3,262)	1:45:A:ILE:HG13	1:45:A:ILE:HB	18	0.14
(3,245)	1:5:A:LYS:HA	1:5:A:LYS:HB3	12	0.14
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG22	8	0.14
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG3	5	0.14
(3,233)	1:6:A:GLU:HA	1:48:A:LYS:HB3	11	0.14
(3,232)	1:6:A:GLU:HG2	1:6:A:GLU:HA	3	0.14
(3,227)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	18	0.14
(3,222)	1:92:A:SER:HB3	1:12:A:LYS:HB2	6	0.14
(3,220)	1:44:A:ILE:HG22	1:8:A:GLU:HG2	15	0.14
(3,219)	1:9:A:ILE:HG22	1:76:A:TYR:HB2	10	0.14
(3,189)	1:74:A:GLU:HA	1:76:A:TYR:H	8	0.14
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	14	0.14
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	12	0.14
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	20	0.14
(3,145)	1:55:A:SER:HB2	1:29:A:ASN:H	3	0.14
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	13	0.14
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	3	0.14
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	4	0.14
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	13	0.14
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	20	0.14
(3,92)	1:14:A:THR:HB	1:14:A:THR:HG21	17	0.14
(3,84)	1:95:A:MET:HB3	1:95:A:MET:HA	12	0.14
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD13	10	0.14
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	5	0.14
(3,65)	1:6:A:GLU:HG3	1:48:A:LYS:HA	12	0.14
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	8	0.14
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	15	0.14
(3,44)	1:56:A:ARG:HA	1:28:A:GLY:HA2	6	0.14
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	9	0.14
(3,24)	1:9:A:ILE:H	1:9:A:ILE:HB	6	0.14
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	6	0.14
(3,15)	1:85:A:CYS:HB3	1:4:A:CYS:HA	10	0.14
(1,2276)	1:19:A:ARG:HB2	1:14:A:THR:HA	16	0.14
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	10	0.14
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	11	0.14
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	13	0.14
(1,2236)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	10	0.14
(1,2236)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	20	0.14
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	11	0.14
(1,2176)	1:41:A:GLY:HA3	1:40:A:LYS:HB3	14	0.14
(1,2169)	1:4:A:CYS:HA	1:85:A:CYS:HB2	3	0.14
(1,2160)	1:71:A:THR:HA	1:71:A:THR:HG23	14	0.14
(1,2150)	1:62:A:ARG:HA	1:70:A:PHE:HB3	12	0.14
(1,2150)	1:62:A:ARG:HA	1:70:A:PHE:HB3	14	0.14
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	14	0.14
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	4	0.14
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	9	0.14
(1,2074)	1:113:A:TRP:HA	1:71:A:THR:HG23	12	0.14
(1,2063)	1:73:A:VAL:HG23	1:73:A:VAL:HA	20	0.14
(1,2024)	1:48:A:LYS:HA	1:6:A:GLU:HA	7	0.14
(1,1998)	1:32:A:VAL:HG22	1:32:A:VAL:HA	14	0.14
(1,1991)	1:115:A:SER:HB2	1:115:A:SER:HA	18	0.14
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	5	0.14
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	6	0.14
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	7	0.14
(1,1990)	1:115:A:SER:HB3	1:115:A:SER:HA	9	0.14
(1,1976)	1:112:A:LYS:HA	1:97:A:ALA:HB3	6	0.14
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD13	2	0.14
(1,1962)	1:34:A:VAL:HG22	1:34:A:VAL:HA	12	0.14
(1,1959)	1:34:A:VAL:HB	1:34:A:VAL:HG23	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:10:A:VAL:HG23	1:10:A:VAL:HB	7	0.14
(1,1955)	1:10:A:VAL:HG23	1:10:A:VAL:HA	17	0.14
(1,1951)	1:22:A:GLN:HG3	1:34:A:VAL:HG12	1	0.14
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG22	19	0.14
(1,1941)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	19	0.14
(1,1929)	1:91:A:LEU:HA	1:98:A:ILE:HG21	5	0.14
(1,1910)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	15	0.14
(1,1908)	1:111:A:ASN:H	1:110:A:LEU:HB3	13	0.14
(1,1898)	1:89:A:TYR:H	1:10:A:VAL:H	17	0.14
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	9	0.14
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	8	0.14
(1,1828)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.14
(1,1826)	1:9:A:ILE:H	1:9:A:ILE:HB	15	0.14
(1,1765)	1:104:A:GLU:H	1:104:A:GLU:HB2	16	0.14
(1,1755)	1:99:A:TYR:HB3	1:100:A:PHE:H	14	0.14
(1,1752)	1:99:A:TYR:HB2	1:99:A:TYR:H	19	0.14
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	5	0.14
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	6	0.14
(1,1731)	1:94:A:ARG:HB3	1:95:A:MET:H	6	0.14
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	18	0.14
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	20	0.14
(1,1675)	1:79:A:ASP:H	1:78:A:PRO:HB3	7	0.14
(1,1615)	1:53:A:GLU:H	1:52:A:THR:HG23	9	0.14
(1,1590)	1:26:A:ARG:H	1:58:A:ASN:H	6	0.14
(1,1577)	1:9:A:ILE:HG12	1:46:A:LYS:H	7	0.14
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD12	2	0.14
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD2	3	0.14
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD1	13	0.14
(1,1545)	1:38:A:ASN:HB3	1:39:A:PHE:H	4	0.14
(1,1545)	1:38:A:ASN:HB3	1:39:A:PHE:H	20	0.14
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	5	0.14
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	16	0.14
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	4	0.14
(1,1502)	1:30:A:THR:H	1:30:A:THR:HG22	2	0.14
(1,1500)	1:30:A:THR:HB	1:30:A:THR:H	4	0.14
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	4	0.14
(1,1472)	1:22:A:GLN:HG3	1:23:A:TYR:H	16	0.14
(1,1412)	1:11:A:ILE:H	1:11:A:ILE:HG13	1	0.14
(1,1390)	1:85:A:CYS:HB3	1:5:A:LYS:H	16	0.14
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	18	0.14
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	12	0.14
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	16	0.14
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	17	0.14
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	19	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	1	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	2	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	3	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	4	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	5	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	7	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	9	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	12	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	13	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	14	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	16	0.14
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	17	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	18	0.14
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	19	0.14
(1,1356)	1:98:A:ILE:HD11	1:71:A:THR:HG23	9	0.14
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	17	0.14
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	7	0.14
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	9	0.14
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	20	0.14
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	3	0.14
(1,1242)	1:20:A:ILE:HD12	1:39:A:PHE:H	15	0.14
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD11	2	0.14
(1,1163)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	4	0.14
(1,1160)	1:34:A:VAL:HG22	1:34:A:VAL:HA	8	0.14
(1,1160)	1:34:A:VAL:HG23	1:34:A:VAL:HA	14	0.14
(1,1145)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	12	0.14
(1,1143)	1:98:A:ILE:HG21	1:92:A:SER:H	17	0.14
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG23	10	0.14
(1,1137)	1:9:A:ILE:HD12	1:7:A:ILE:HG22	14	0.14
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	5	0.14
(1,1116)	1:20:A:ILE:HA	1:20:A:ILE:HD11	20	0.14
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	5	0.14
(1,1113)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	7	0.14
(1,1107)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	1	0.14
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	3	0.14
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	14	0.14
(1,1105)	1:98:A:ILE:HD12	1:94:A:ARG:H	14	0.14
(1,1103)	1:98:A:ILE:HD12	1:61:A:PHE:HE2	14	0.14
(1,1103)	1:98:A:ILE:HD12	1:61:A:PHE:HE1	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:98:A:ILE:HD13	1:71:A:THR:HG22	7	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG22	1	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	4	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	6	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	7	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG22	8	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	11	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	12	0.14
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG22	18	0.14
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB2	1	0.14
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB1	19	0.14
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE1	2	0.14
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	13	0.14
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	2	0.14
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	4	0.14
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	5	0.14
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	6	0.14
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	7	0.14
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	13	0.14
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	18	0.14
(1,935)	1:4:A:CYS:HB3	1:4:A:CYS:HA	3	0.14
(1,935)	1:4:A:CYS:HB3	1:4:A:CYS:HA	17	0.14
(1,928)	1:69:A:PHE:HA	1:115:A:SER:HB3	5	0.14
(1,924)	1:47:A:PHE:HD2	1:30:A:THR:HB	14	0.14
(1,917)	1:95:A:MET:HG2	1:15:A:LEU:HD12	6	0.14
(1,913)	1:15:A:LEU:HD11	1:19:A:ARG:HB3	3	0.14
(1,910)	1:11:A:ILE:H	1:10:A:VAL:HG22	11	0.14
(1,908)	1:10:A:VAL:HG22	1:10:A:VAL:HB	15	0.14
(1,907)	1:10:A:VAL:HG21	1:42:A:THR:HB	13	0.14
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	15	0.14
(1,901)	1:98:A:ILE:HB	1:71:A:THR:HG21	12	0.14
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	7	0.14
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG23	8	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG23	1	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG21	2	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	5	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG23	7	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	8	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG23	11	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG21	12	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	13	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	16	0.14
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	17	0.14
(1,890)	1:98:A:ILE:HG22	1:98:A:ILE:HA	15	0.14
(1,890)	1:98:A:ILE:HG21	1:98:A:ILE:HA	16	0.14
(1,888)	1:91:A:LEU:HB3	1:98:A:ILE:HG23	20	0.14
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	2	0.14
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	4	0.14
(1,798)	1:9:A:ILE:H	1:9:A:ILE:HG12	5	0.14
(1,798)	1:9:A:ILE:H	1:9:A:ILE:HG12	15	0.14
(1,788)	1:112:A:LYS:H	1:111:A:ASN:HB2	8	0.14
(1,783)	1:113:A:TRP:H	1:113:A:TRP:HB2	6	0.14
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	11	0.14
(1,729)	1:99:A:TYR:HB3	1:100:A:PHE:H	14	0.14
(1,695)	1:57:A:TRP:H	1:76:A:TYR:H	8	0.14
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	14	0.14
(1,621)	1:70:A:PHE:H	1:114:A:ARG:H	2	0.14
(1,608)	1:58:A:ASN:HB3	1:59:A:CYS:H	9	0.14
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	1	0.14
(1,580)	1:50:A:ASP:H	1:49:A:ASP:HB2	10	0.14
(1,558)	1:9:A:ILE:HG12	1:46:A:LYS:H	18	0.14
(1,532)	1:39:A:PHE:HA	1:40:A:LYS:H	3	0.14
(1,518)	1:36:A:TYR:HB3	1:37:A:LEU:H	19	0.14
(1,506)	1:35:A:GLN:HG3	1:35:A:GLN:H	9	0.14
(1,504)	1:35:A:GLN:H	1:34:A:VAL:HG11	6	0.14
(1,489)	1:30:A:THR:H	1:30:A:THR:HG23	10	0.14
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	8	0.14
(1,427)	1:14:A:THR:H	1:93:A:ALA:HB1	14	0.14
(1,398)	1:85:A:CYS:HB3	1:5:A:LYS:H	16	0.14
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	8	0.14
(1,381)	1:70:A:PHE:HE1	1:70:A:PHE:HA	10	0.14
(1,364)	1:113:A:TRP:H	1:112:A:LYS:HB3	18	0.14
(1,352)	1:57:A:TRP:HE1	1:56:A:ARG:HA	14	0.14
(1,340)	1:87:A:LYS:HB3	1:88:A:ARG:H	19	0.14
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	4	0.14
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	11	0.14
(1,292)	1:43:A:ARG:HB2	1:43:A:ARG:HA	14	0.14
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	14	0.14
(1,272)	1:52:A:THR:HG21	1:52:A:THR:HA	11	0.14
(1,272)	1:52:A:THR:HG23	1:52:A:THR:HA	12	0.14
(1,262)	1:93:A:ALA:HB3	1:13:A:ASN:HB2	3	0.14
(1,242)	1:39:A:PHE:HD2	1:17:A:PRO:HA	1	0.14
(1,242)	1:39:A:PHE:HD2	1:17:A:PRO:HA	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	5	0.14
(1,181)	1:61:A:PHE:HD2	1:21:A:LEU:HB2	19	0.14
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	9	0.14
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD1	20	0.14
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	8	0.14
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	16	0.14
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	17	0.14
(1,154)	1:98:A:ILE:HG13	1:113:A:TRP:H	3	0.14
(1,144)	1:95:A:MET:H	1:14:A:THR:HG22	8	0.14
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	11	0.14
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	11	0.14
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD12	10	0.14
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD11	12	0.14
(1,112)	1:12:A:LYS:H	1:11:A:ILE:HD13	17	0.14
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG23	6	0.14
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG23	7	0.14
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG22	9	0.14
(1,62)	1:95:A:MET:HA	1:15:A:LEU:HD12	17	0.14
(1,38)	1:45:A:ILE:HD11	1:45:A:ILE:HG13	1	0.14
(4,13)	1:90:A:GLU:H	1:101:A:LYS:O	7	0.13
(4,9)	1:14:A:THR:H	1:93:A:ALA:O	4	0.13
(3,309)	1:103:A:ASP:HB3	1:104:A:GLU:H	6	0.13
(3,295)	1:35:A:GLN:HB3	1:36:A:TYR:H	12	0.13
(3,295)	1:36:A:TYR:H	1:35:A:GLN:HB2	16	0.13
(3,246)	1:5:A:LYS:HG3	1:5:A:LYS:HA	16	0.13
(3,245)	1:5:A:LYS:HA	1:5:A:LYS:HB3	13	0.13
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG21	16	0.13
(3,222)	1:92:A:SER:HB3	1:12:A:LYS:HB2	14	0.13
(3,222)	1:92:A:SER:HB3	1:12:A:LYS:HB2	18	0.13
(3,210)	1:44:A:ILE:H	1:44:A:ILE:HG23	9	0.13
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	3	0.13
(3,200)	1:14:A:THR:H	1:93:A:ALA:H	13	0.13
(3,197)	1:91:A:LEU:H	1:91:A:LEU:HB2	12	0.13
(3,178)	1:28:A:GLY:H	1:27:A:SER:HB3	10	0.13
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	8	0.13
(3,169)	1:48:A:LYS:HB2	1:6:A:GLU:H	13	0.13
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	11	0.13
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	13	0.13
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	5	0.13
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	15	0.13
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	16	0.13
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG21	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	2	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	6	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	9	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	10	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	11	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	12	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	14	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	15	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	17	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	18	0.13
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	19	0.13
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	17	0.13
(3,56)	1:85:A:CYS:HB3	1:85:A:CYS:HA	10	0.13
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	3	0.13
(3,49)	1:98:A:ILE:HG23	1:98:A:ILE:HA	4	0.13
(3,31)	1:92:A:SER:HB3	1:92:A:SER:H	10	0.13
(3,30)	1:69:A:PHE:HA	1:115:A:SER:HB2	9	0.13
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	9	0.13
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	10	0.13
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	17	0.13
(3,15)	1:85:A:CYS:HB3	1:4:A:CYS:HA	11	0.13
(3,14)	1:111:A:ASN:HA	1:111:A:ASN:HB2	6	0.13
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	14	0.13
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	15	0.13
(1,2255)	1:73:A:VAL:HG21	1:59:A:CYS:HB3	18	0.13
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	18	0.13
(1,2250)	1:11:A:ILE:HD12	1:61:A:PHE:HE1	6	0.13
(1,2250)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	20	0.13
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	12	0.13
(1,2236)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	7	0.13
(1,2236)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	15	0.13
(1,2234)	1:30:A:THR:HA	1:30:A:THR:HG22	5	0.13
(1,2223)	1:32:A:VAL:HG21	1:32:A:VAL:HA	8	0.13
(1,2223)	1:32:A:VAL:HG23	1:32:A:VAL:HA	13	0.13
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG12	8	0.13
(1,2144)	1:68:A:LYS:HB2	1:65:A:ILE:HG21	14	0.13
(1,2126)	1:23:A:TYR:HE1	1:36:A:TYR:HA	20	0.13
(1,2075)	1:56:A:ARG:HB3	1:56:A:ARG:HA	15	0.13
(1,2071)	1:35:A:GLN:HG3	1:35:A:GLN:HA	14	0.13
(1,2027)	1:7:A:ILE:HD11	1:7:A:ILE:HA	19	0.13
(1,2020)	1:4:A:CYS:HB3	1:4:A:CYS:HA	1	0.13
(1,2019)	1:4:A:CYS:HB3	1:4:A:CYS:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1991)	1:115:A:SER:HB2	1:115:A:SER:HA	10	0.13
(1,1991)	1:115:A:SER:HB2	1:115:A:SER:HA	17	0.13
(1,1966)	1:15:A:LEU:HA	1:15:A:LEU:HD11	15	0.13
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	16	0.13
(1,1936)	1:20:A:ILE:HG22	1:36:A:TYR:HB2	10	0.13
(1,1933)	1:45:A:ILE:H	1:44:A:ILE:HG22	7	0.13
(1,1932)	1:9:A:ILE:HD12	1:9:A:ILE:HG23	11	0.13
(1,1930)	1:98:A:ILE:HG22	1:61:A:PHE:HE2	20	0.13
(1,1928)	1:98:A:ILE:HG21	1:98:A:ILE:HA	17	0.13
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD11	20	0.13
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	13	0.13
(1,1874)	1:7:A:ILE:H	1:7:A:ILE:HG23	17	0.13
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	6	0.13
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	16	0.13
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	17	0.13
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	7	0.13
(1,1828)	1:9:A:ILE:H	1:9:A:ILE:HG12	15	0.13
(1,1800)	1:31:A:ASN:H	1:30:A:THR:HG23	18	0.13
(1,1787)	1:115:A:SER:H	1:114:A:ARG:HB3	17	0.13
(1,1787)	1:115:A:SER:H	1:114:A:ARG:HB3	18	0.13
(1,1762)	1:102:A:MET:H	1:101:A:LYS:HB2	8	0.13
(1,1728)	1:15:A:LEU:HA	1:95:A:MET:H	19	0.13
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	2	0.13
(1,1661)	1:75:A:ALA:H	1:58:A:ASN:HA	4	0.13
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	1	0.13
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	5	0.13
(1,1640)	1:65:A:ILE:H	1:65:A:ILE:HB	2	0.13
(1,1608)	1:52:A:THR:H	1:50:A:ASP:HA	13	0.13
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	3	0.13
(1,1557)	1:42:A:THR:H	1:44:A:ILE:HD13	4	0.13
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD2	7	0.13
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD2	9	0.13
(1,1550)	1:40:A:LYS:H	1:39:A:PHE:HD2	11	0.13
(1,1545)	1:38:A:ASN:HB3	1:39:A:PHE:H	13	0.13
(1,1541)	1:20:A:ILE:HD11	1:38:A:ASN:H	20	0.13
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	13	0.13
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD2	4	0.13
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD1	14	0.13
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB1	9	0.13
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	7	0.13
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	7	0.13
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	1	0.13
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	2	0.13
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	3	0.13
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	4	0.13
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	5	0.13
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	6	0.13
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	8	0.13
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	9	0.13
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	11	0.13
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	13	0.13
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	18	0.13
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	6	0.13
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	8	0.13
(1,1363)	1:76:A:TYR:HE1	1:76:A:TYR:HD1	11	0.13
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	15	0.13
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	20	0.13
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	1	0.13
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	2	0.13
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	3	0.13
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	4	0.13
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	6	0.13
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	7	0.13
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	8	0.13
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	9	0.13
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	13	0.13
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	16	0.13
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	18	0.13
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	19	0.13
(1,1333)	1:23:A:TYR:HD2	1:23:A:TYR:HA	14	0.13
(1,1310)	1:98:A:ILE:HD11	1:71:A:THR:HG21	13	0.13
(1,1298)	1:42:A:THR:HG21	1:12:A:LYS:HA	16	0.13
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	2	0.13
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	17	0.13
(1,1247)	1:20:A:ILE:HA	1:20:A:ILE:HD12	2	0.13
(1,1242)	1:20:A:ILE:HD11	1:39:A:PHE:H	1	0.13
(1,1177)	1:74:A:GLU:HA	1:74:A:GLU:HG2	5	0.13
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG23	5	0.13
(1,1160)	1:34:A:VAL:HG22	1:34:A:VAL:HA	3	0.13
(1,1160)	1:34:A:VAL:HG22	1:34:A:VAL:HA	5	0.13
(1,1154)	1:94:A:ARG:HA	1:15:A:LEU:HD12	13	0.13
(1,1153)	1:95:A:MET:HA	1:15:A:LEU:HD11	12	0.13
(1,1146)	1:7:A:ILE:HG23	1:8:A:GLU:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:20:A:ILE:HG23	1:21:A:LEU:H	8	0.13
(1,1134)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	14	0.13
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	2	0.13
(1,1113)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	13	0.13
(1,1113)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	16	0.13
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	17	0.13
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	20	0.13
(1,1110)	1:9:A:ILE:HD13	1:75:A:ALA:HB3	6	0.13
(1,1107)	1:7:A:ILE:HD11	1:5:A:LYS:HB3	17	0.13
(1,1098)	1:98:A:ILE:HD13	1:98:A:ILE:HA	13	0.13
(1,1097)	1:10:A:VAL:HG21	1:10:A:VAL:HA	5	0.13
(1,1097)	1:10:A:VAL:HG22	1:10:A:VAL:HA	6	0.13
(1,1097)	1:10:A:VAL:HG21	1:10:A:VAL:HA	16	0.13
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	3	0.13
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	5	0.13
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG22	9	0.13
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	14	0.13
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	20	0.13
(1,1064)	1:37:A:LEU:HA	1:37:A:LEU:HB2	7	0.13
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB3	13	0.13
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB3	17	0.13
(1,1042)	1:113:A:TRP:HB3	1:61:A:PHE:HE2	4	0.13
(1,1022)	1:73:A:VAL:HG23	1:91:A:LEU:HB2	18	0.13
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	16	0.13
(1,982)	1:73:A:VAL:HG22	1:72:A:GLU:HA	2	0.13
(1,982)	1:73:A:VAL:HG21	1:72:A:GLU:HA	16	0.13
(1,982)	1:73:A:VAL:HG21	1:72:A:GLU:HA	17	0.13
(1,979)	1:90:A:GLU:HA	1:90:A:GLU:HG2	6	0.13
(1,979)	1:90:A:GLU:HA	1:90:A:GLU:HG2	14	0.13
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	2	0.13
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	3	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	2	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	3	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	4	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	8	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	9	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	10	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	13	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	14	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	18	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	19	0.13
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	3	0.13
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	14	0.13
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	19	0.13
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	20	0.13
(1,933)	1:78:A:PRO:HA	1:78:A:PRO:HB2	6	0.13
(1,928)	1:69:A:PHE:HA	1:115:A:SER:HB3	6	0.13
(1,928)	1:69:A:PHE:HA	1:115:A:SER:HB3	7	0.13
(1,924)	1:47:A:PHE:HD1	1:30:A:THR:HB	15	0.13
(1,918)	1:15:A:LEU:HA	1:15:A:LEU:HD11	12	0.13
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG21	10	0.13
(1,894)	1:44:A:ILE:HB	1:44:A:ILE:HG22	14	0.13
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG23	12	0.13
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	11	0.13
(1,887)	1:98:A:ILE:HB	1:98:A:ILE:HG21	14	0.13
(1,877)	1:11:A:ILE:HG23	1:11:A:ILE:HD12	6	0.13
(1,870)	1:111:A:ASN:H	1:110:A:LEU:HB3	13	0.13
(1,870)	1:111:A:ASN:H	1:110:A:LEU:HB3	18	0.13
(1,860)	1:89:A:TYR:H	1:10:A:VAL:H	12	0.13
(1,849)	1:54:A:ARG:H	1:52:A:THR:HG21	4	0.13
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	3	0.13
(1,817)	1:71:A:THR:H	1:70:A:PHE:HE1	13	0.13
(1,804)	1:25:A:CYS:H	1:59:A:CYS:HB3	8	0.13
(1,804)	1:25:A:CYS:H	1:59:A:CYS:HB3	12	0.13
(1,762)	1:13:A:ASN:H	1:12:A:LYS:HB2	18	0.13
(1,757)	1:111:A:ASN:HB3	1:111:A:ASN:H	18	0.13
(1,736)	1:102:A:MET:H	1:101:A:LYS:HB2	4	0.13
(1,725)	1:99:A:TYR:HB2	1:99:A:TYR:H	19	0.13
(1,717)	1:113:A:TRP:HE1	1:97:A:ALA:H	6	0.13
(1,701)	1:15:A:LEU:HA	1:95:A:MET:H	19	0.13
(1,695)	1:57:A:TRP:H	1:76:A:TYR:H	9	0.13
(1,678)	1:87:A:LYS:HB3	1:88:A:ARG:H	12	0.13
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	18	0.13
(1,650)	1:79:A:ASP:H	1:78:A:PRO:HA	8	0.13
(1,638)	1:75:A:ALA:H	1:58:A:ASN:HA	4	0.13
(1,622)	1:71:A:THR:H	1:71:A:THR:HG22	12	0.13
(1,621)	1:70:A:PHE:H	1:114:A:ARG:H	13	0.13
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	8	0.13
(1,603)	1:55:A:SER:H	1:56:A:ARG:HB3	12	0.13
(1,594)	1:54:A:ARG:H	1:52:A:THR:HB	9	0.13
(1,594)	1:54:A:ARG:H	1:52:A:THR:HB	13	0.13
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	5	0.13
(1,576)	1:49:A:ASP:HB3	1:49:A:ASP:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,546)	1:43:A:ARG:H	1:44:A:ILE:HG13	11	0.13
(1,532)	1:39:A:PHE:HA	1:40:A:LYS:H	7	0.13
(1,532)	1:39:A:PHE:HA	1:40:A:LYS:H	10	0.13
(1,531)	1:39:A:PHE:HD2	1:39:A:PHE:H	8	0.13
(1,529)	1:38:A:ASN:HB3	1:39:A:PHE:H	5	0.13
(1,529)	1:38:A:ASN:HB3	1:39:A:PHE:H	20	0.13
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	5	0.13
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	17	0.13
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	1	0.13
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	14	0.13
(1,489)	1:30:A:THR:H	1:30:A:THR:HG23	14	0.13
(1,487)	1:30:A:THR:HB	1:30:A:THR:H	4	0.13
(1,463)	1:22:A:GLN:HG3	1:23:A:TYR:H	16	0.13
(1,459)	1:21:A:LEU:HB2	1:22:A:GLN:H	11	0.13
(1,455)	1:20:A:ILE:H	1:20:A:ILE:HG21	2	0.13
(1,453)	1:20:A:ILE:H	1:19:A:ARG:HB3	14	0.13
(1,404)	1:108:A:GLN:HG2	1:108:A:GLN:H	9	0.13
(1,395)	1:4:A:CYS:HA	1:5:A:LYS:H	14	0.13
(1,392)	1:112:A:LYS:H	1:112:A:LYS:HB2	14	0.13
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	12	0.13
(1,381)	1:70:A:PHE:HE1	1:70:A:PHE:HA	12	0.13
(1,370)	1:102:A:MET:H	1:102:A:MET:HG2	10	0.13
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	17	0.13
(1,329)	1:5:A:LYS:HA	1:5:A:LYS:HB3	16	0.13
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	17	0.13
(1,294)	1:35:A:GLN:HA	1:36:A:TYR:HD1	19	0.13
(1,278)	1:40:A:LYS:HB2	1:40:A:LYS:HA	10	0.13
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	12	0.13
(1,272)	1:52:A:THR:HG21	1:52:A:THR:HA	16	0.13
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	18	0.13
(1,176)	1:100:A:PHE:HA	1:91:A:LEU:HA	11	0.13
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	19	0.13
(1,154)	1:98:A:ILE:HG13	1:113:A:TRP:H	19	0.13
(1,153)	1:61:A:PHE:HD2	1:71:A:THR:HG22	1	0.13
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	3	0.13
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	3	0.13
(1,74)	1:1:A:ALA:HB2	1:83:A:PRO:HA	19	0.13
(1,67)	1:109:A:PRO:HA	1:97:A:ALA:HB2	1	0.13
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG22	1	0.13
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG21	13	0.13
(1,48)	1:37:A:LEU:H	1:20:A:ILE:HG22	18	0.13
(1,47)	1:20:A:ILE:HG22	1:21:A:LEU:H	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:9:A:ILE:HD13	1:7:A:ILE:HG22	8	0.13
(1,42)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	3	0.13
(1,29)	1:25:A:CYS:HB2	1:45:A:ILE:HD13	5	0.13
(1,8)	1:10:A:VAL:HG22	1:10:A:VAL:HA	19	0.13
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	3	0.12
(3,327)	1:10:A:VAL:HG21	1:10:A:VAL:HA	12	0.12
(3,317)	1:8:A:GLU:HG2	1:47:A:PHE:H	18	0.12
(3,312)	1:7:A:ILE:H	1:6:A:GLU:HB3	3	0.12
(3,311)	1:105:A:ARG:HG3	1:105:A:ARG:H	4	0.12
(3,310)	1:103:A:ASP:HB3	1:105:A:ARG:H	12	0.12
(3,265)	1:26:A:ARG:HB2	1:31:A:ASN:HA	14	0.12
(3,265)	1:26:A:ARG:HB2	1:31:A:ASN:HA	20	0.12
(3,238)	1:46:A:LYS:HA	1:44:A:ILE:HG21	17	0.12
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG21	1	0.12
(3,236)	1:93:A:ALA:HA	1:98:A:ILE:HG21	17	0.12
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	9	0.12
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	20	0.12
(3,232)	1:6:A:GLU:HA	1:6:A:GLU:HG3	2	0.12
(3,228)	1:9:A:ILE:HG12	1:7:A:ILE:HG22	5	0.12
(3,226)	1:87:A:LYS:HB3	1:7:A:ILE:HG21	3	0.12
(3,226)	1:87:A:LYS:HB2	1:7:A:ILE:HG21	19	0.12
(3,224)	1:92:A:SER:HB3	1:99:A:TYR:HB3	15	0.12
(3,209)	1:104:A:GLU:HG3	1:104:A:GLU:H	14	0.12
(3,208)	1:57:A:TRP:HE1	1:47:A:PHE:HB2	17	0.12
(3,196)	1:89:A:TYR:H	1:88:A:ARG:HB3	3	0.12
(3,189)	1:74:A:GLU:HA	1:76:A:TYR:H	20	0.12
(3,181)	1:35:A:GLN:HB3	1:36:A:TYR:H	12	0.12
(3,159)	1:57:A:TRP:HB2	1:75:A:ALA:HB1	6	0.12
(3,147)	1:5:A:LYS:HG2	1:6:A:GLU:H	19	0.12
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	2	0.12
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	4	0.12
(3,140)	1:47:A:PHE:H	1:8:A:GLU:HB3	8	0.12
(3,135)	1:82:A:HIS:HD1	1:79:A:ASP:HA	9	0.12
(3,132)	1:38:A:ASN:HB3	1:38:A:ASN:HA	6	0.12
(3,131)	1:89:A:TYR:HB2	1:89:A:TYR:HA	19	0.12
(3,96)	1:45:A:ILE:HA	1:45:A:ILE:HB	16	0.12
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	1	0.12
(3,67)	1:44:A:ILE:HB	1:44:A:ILE:HA	13	0.12
(3,49)	1:98:A:ILE:HG21	1:98:A:ILE:HA	1	0.12
(3,42)	1:47:A:PHE:HB3	1:47:A:PHE:HA	17	0.12
(3,31)	1:92:A:SER:HB3	1:92:A:SER:H	15	0.12
(3,29)	1:114:A:ARG:HA	1:69:A:PHE:HA	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	1	0.12
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	2	0.12
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	14	0.12
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	19	0.12
(3,15)	1:85:A:CYS:HB3	1:4:A:CYS:HA	17	0.12
(3,11)	1:74:A:GLU:HA	1:74:A:GLU:HG2	5	0.12
(1,2278)	1:15:A:LEU:HA	1:15:A:LEU:HD13	14	0.12
(1,2276)	1:19:A:ARG:HB2	1:14:A:THR:HA	19	0.12
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	4	0.12
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	17	0.12
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	20	0.12
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	2	0.12
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	5	0.12
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	8	0.12
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	9	0.12
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	11	0.12
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	19	0.12
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	20	0.12
(1,2250)	1:11:A:ILE:HD13	1:61:A:PHE:HE1	3	0.12
(1,2246)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	11	0.12
(1,2239)	1:73:A:VAL:HG23	1:71:A:THR:HG22	2	0.12
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE1	9	0.12
(1,2236)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	1	0.12
(1,2236)	1:73:A:VAL:HG22	1:61:A:PHE:HD1	12	0.12
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB2	7	0.12
(1,2231)	1:74:A:GLU:HA	1:75:A:ALA:HB1	14	0.12
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	7	0.12
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG12	4	0.12
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG11	7	0.12
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG12	20	0.12
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	20	0.12
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	18	0.12
(1,2150)	1:62:A:ARG:HA	1:70:A:PHE:HB3	6	0.12
(1,2148)	1:70:A:PHE:HB2	1:62:A:ARG:HA	2	0.12
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	16	0.12
(1,2126)	1:23:A:TYR:HE1	1:36:A:TYR:HA	17	0.12
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	11	0.12
(1,2075)	1:56:A:ARG:HB3	1:56:A:ARG:HA	2	0.12
(1,2070)	1:35:A:GLN:HA	1:35:A:GLN:HG2	1	0.12
(1,2063)	1:73:A:VAL:HG21	1:73:A:VAL:HA	3	0.12
(1,2020)	1:4:A:CYS:HB3	1:4:A:CYS:HA	3	0.12
(1,2020)	1:4:A:CYS:HB3	1:4:A:CYS:HA	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2007)	1:78:A:PRO:HA	1:78:A:PRO:HB2	7	0.12
(1,1991)	1:115:A:SER:HB2	1:115:A:SER:HA	19	0.12
(1,1989)	1:14:A:THR:HB	1:14:A:THR:HA	13	0.12
(1,1976)	1:112:A:LYS:HA	1:97:A:ALA:HB3	20	0.12
(1,1962)	1:34:A:VAL:HG21	1:34:A:VAL:HA	13	0.12
(1,1953)	1:24:A:HIS:HB3	1:34:A:VAL:HG13	8	0.12
(1,1930)	1:98:A:ILE:HG23	1:61:A:PHE:HE2	4	0.12
(1,1917)	1:9:A:ILE:H	1:9:A:ILE:HD11	12	0.12
(1,1908)	1:111:A:ASN:H	1:110:A:LEU:HB3	12	0.12
(1,1898)	1:89:A:TYR:H	1:10:A:VAL:H	5	0.12
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	5	0.12
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	8	0.12
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	11	0.12
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	17	0.12
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	18	0.12
(1,1801)	1:56:A:ARG:H	1:55:A:SER:H	9	0.12
(1,1740)	1:97:A:ALA:H	1:94:A:ARG:HB2	20	0.12
(1,1738)	1:94:A:ARG:HB3	1:96:A:ASP:H	2	0.12
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	5	0.12
(1,1695)	1:86:A:GLY:H	1:85:A:CYS:HA	12	0.12
(1,1692)	1:85:A:CYS:H	1:85:A:CYS:HB3	19	0.12
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	7	0.12
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	11	0.12
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	6	0.12
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	12	0.12
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	16	0.12
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	17	0.12
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG21	6	0.12
(1,1644)	1:70:A:PHE:H	1:69:A:PHE:HA	18	0.12
(1,1640)	1:65:A:ILE:H	1:65:A:ILE:HB	17	0.12
(1,1618)	1:54:A:ARG:H	1:52:A:THR:HB	11	0.12
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD13	17	0.12
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	16	0.12
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	20	0.12
(1,1548)	1:39:A:PHE:HA	1:40:A:LYS:H	11	0.12
(1,1545)	1:38:A:ASN:HB3	1:39:A:PHE:H	17	0.12
(1,1541)	1:20:A:ILE:HD13	1:38:A:ASN:H	11	0.12
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	2	0.12
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	14	0.12
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	7	0.12
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	9	0.12
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1503)	1:30:A:THR:H	1:27:A:SER:H	18	0.12
(1,1503)	1:30:A:THR:H	1:27:A:SER:H	20	0.12
(1,1498)	1:29:A:ASN:H	1:28:A:GLY:H	13	0.12
(1,1486)	1:26:A:ARG:HB2	1:27:A:SER:H	1	0.12
(1,1452)	1:19:A:ARG:HB3	1:19:A:ARG:H	16	0.12
(1,1444)	1:16:A:GLY:H	1:39:A:PHE:HD1	18	0.12
(1,1432)	1:15:A:LEU:H	1:39:A:PHE:HD1	1	0.12
(1,1408)	1:10:A:VAL:HG21	1:10:A:VAL:H	2	0.12
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	6	0.12
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	1	0.12
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	5	0.12
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	9	0.12
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	20	0.12
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	12	0.12
(1,1372)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	14	0.12
(1,1372)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	20	0.12
(1,1363)	1:76:A:TYR:HE2	1:76:A:TYR:HD2	10	0.12
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	5	0.12
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	11	0.12
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	12	0.12
(1,1341)	1:36:A:TYR:HE2	1:36:A:TYR:HD2	14	0.12
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	20	0.12
(1,1298)	1:42:A:THR:HG21	1:12:A:LYS:HA	1	0.12
(1,1296)	1:95:A:MET:HG3	1:14:A:THR:HG22	18	0.12
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	17	0.12
(1,1272)	1:92:A:SER:HA	1:93:A:ALA:HB3	12	0.12
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	6	0.12
(1,1243)	1:20:A:ILE:HD11	1:20:A:ILE:HB	11	0.12
(1,1232)	1:9:A:ILE:HB	1:9:A:ILE:HD13	6	0.12
(1,1211)	1:32:A:VAL:HG22	1:32:A:VAL:HA	2	0.12
(1,1167)	1:112:A:LYS:HB3	1:97:A:ALA:HB3	13	0.12
(1,1166)	1:47:A:PHE:HD2	1:30:A:THR:HG22	8	0.12
(1,1160)	1:34:A:VAL:HG23	1:34:A:VAL:HA	4	0.12
(1,1160)	1:34:A:VAL:HG23	1:34:A:VAL:HA	15	0.12
(1,1137)	1:9:A:ILE:HD13	1:7:A:ILE:HG21	2	0.12
(1,1132)	1:98:A:ILE:HD11	1:61:A:PHE:HB2	18	0.12
(1,1127)	1:9:A:ILE:HD12	1:9:A:ILE:HG23	11	0.12
(1,1122)	1:68:A:LYS:HB2	1:65:A:ILE:HG23	20	0.12
(1,1091)	1:71:A:THR:HA	1:71:A:THR:HG22	2	0.12
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	2	0.12
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	10	0.12
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG21	16	0.12
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG23	17	0.12
(1,1061)	1:73:A:VAL:HG23	1:59:A:CYS:HB3	14	0.12
(1,1013)	1:100:A:PHE:HA	1:98:A:ILE:HG21	10	0.12
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	9	0.12
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	4	0.12
(1,980)	1:12:A:LYS:HB2	1:92:A:SER:HA	6	0.12
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	15	0.12
(1,974)	1:39:A:PHE:HA	1:39:A:PHE:HD1	14	0.12
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	6	0.12
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	11	0.12
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	12	0.12
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	15	0.12
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	16	0.12
(1,971)	1:45:A:ILE:HA	1:45:A:ILE:HB	17	0.12
(1,968)	1:56:A:ARG:HA	1:28:A:GLY:HA2	8	0.12
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	9	0.12
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD13	1	0.12
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	11	0.12
(1,913)	1:15:A:LEU:HD11	1:19:A:ARG:HB3	6	0.12
(1,912)	1:19:A:ARG:HB2	1:15:A:LEU:HD11	19	0.12
(1,904)	1:34:A:VAL:HB	1:34:A:VAL:HG12	1	0.12
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	1	0.12
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG23	12	0.12
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	20	0.12
(1,891)	1:91:A:LEU:HA	1:98:A:ILE:HG23	8	0.12
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	3	0.12
(1,890)	1:98:A:ILE:HG23	1:98:A:ILE:HA	4	0.12
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	8	0.12
(1,796)	1:9:A:ILE:H	1:9:A:ILE:HB	15	0.12
(1,761)	1:115:A:SER:H	1:114:A:ARG:HB3	17	0.12
(1,761)	1:115:A:SER:H	1:114:A:ARG:HB3	18	0.12
(1,739)	1:104:A:GLU:H	1:104:A:GLU:HB2	16	0.12
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	5	0.12
(1,715)	1:97:A:ALA:H	1:94:A:ARG:HB2	6	0.12
(1,710)	1:96:A:ASP:H	1:94:A:ARG:HB2	6	0.12
(1,704)	1:94:A:ARG:HB3	1:95:A:MET:H	6	0.12
(1,678)	1:87:A:LYS:HB3	1:88:A:ARG:H	9	0.12
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	20	0.12
(1,668)	1:85:A:CYS:H	1:84:A:LEU:HA	1	0.12
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	2	0.12
(1,653)	1:79:A:ASP:H	1:78:A:PRO:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,593)	1:53:A:GLU:H	1:52:A:THR:HG23	9	0.12
(1,587)	1:52:A:THR:H	1:50:A:ASP:HA	13	0.12
(1,570)	1:26:A:ARG:H	1:58:A:ASN:H	6	0.12
(1,546)	1:43:A:ARG:H	1:44:A:ILE:HG13	3	0.12
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD2	3	0.12
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD2	9	0.12
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD1	13	0.12
(1,529)	1:38:A:ASN:HB3	1:39:A:PHE:H	4	0.12
(1,529)	1:38:A:ASN:HB3	1:39:A:PHE:H	13	0.12
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	16	0.12
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	4	0.12
(1,489)	1:30:A:THR:H	1:30:A:THR:HG22	2	0.12
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	4	0.12
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD2	4	0.12
(1,392)	1:112:A:LYS:H	1:112:A:LYS:HB2	18	0.12
(1,391)	1:112:A:LYS:H	1:98:A:ILE:HB	4	0.12
(1,391)	1:112:A:LYS:H	1:98:A:ILE:HB	6	0.12
(1,391)	1:112:A:LYS:H	1:98:A:ILE:HB	18	0.12
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	7	0.12
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	17	0.12
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG23	12	0.12
(1,364)	1:113:A:TRP:H	1:112:A:LYS:HB3	10	0.12
(1,352)	1:57:A:TRP:HE1	1:56:A:ARG:HA	4	0.12
(1,349)	1:85:A:CYS:H	1:84:A:LEU:HA	12	0.12
(1,302)	1:23:A:TYR:HD2	1:59:A:CYS:HB3	6	0.12
(1,299)	1:23:A:TYR:HE2	1:45:A:ILE:HD13	8	0.12
(1,280)	1:39:A:PHE:HB3	1:19:A:ARG:HB2	8	0.12
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	4	0.12
(1,272)	1:52:A:THR:HG21	1:52:A:THR:HA	20	0.12
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB3	1	0.12
(1,271)	1:13:A:ASN:HA	1:93:A:ALA:HB2	12	0.12
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE1	6	0.12
(1,249)	1:59:A:CYS:HB3	1:61:A:PHE:HE1	2	0.12
(1,232)	1:104:A:GLU:HA	1:104:A:GLU:HB2	12	0.12
(1,194)	1:71:A:THR:HB	1:71:A:THR:HA	14	0.12
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	14	0.12
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	4	0.12
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	14	0.12
(1,144)	1:95:A:MET:H	1:14:A:THR:HG21	16	0.12
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	4	0.12
(1,135)	1:5:A:LYS:HB2	1:5:A:LYS:HA	14	0.12
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG22	10	0.12
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG21	14	0.12
(1,54)	1:7:A:ILE:HG21	1:8:A:GLU:H	3	0.12
(1,52)	1:12:A:LYS:H	1:11:A:ILE:HG22	12	0.12
(1,51)	1:98:A:ILE:HG23	1:92:A:SER:H	4	0.12
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG21	8	0.12
(1,47)	1:20:A:ILE:HG22	1:21:A:LEU:H	3	0.12
(1,42)	1:7:A:ILE:HD12	1:84:A:LEU:HB3	12	0.12
(1,38)	1:45:A:ILE:HD13	1:45:A:ILE:HG13	5	0.12
(1,14)	1:98:A:ILE:HD11	1:71:A:THR:HG23	5	0.12
(1,11)	1:73:A:VAL:HG21	1:98:A:ILE:HD13	9	0.12
(1,9)	1:98:A:ILE:HD11	1:98:A:ILE:HA	17	0.12
(1,5)	1:42:A:THR:HG22	1:42:A:THR:HB	11	0.12
(1,2)	1:30:A:THR:HA	1:30:A:THR:HG21	11	0.12
(4,13)	1:90:A:GLU:H	1:101:A:LYS:O	3	0.11
(3,332)	1:69:A:PHE:HA	1:115:A:SER:HB3	12	0.11
(3,317)	1:47:A:PHE:H	1:8:A:GLU:HG3	1	0.11
(3,313)	1:7:A:ILE:H	1:6:A:GLU:HG3	7	0.11
(3,311)	1:105:A:ARG:HG3	1:105:A:ARG:H	3	0.11
(3,265)	1:26:A:ARG:HB2	1:31:A:ASN:HA	3	0.11
(3,265)	1:31:A:ASN:HA	1:26:A:ARG:HB3	4	0.11
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	1	0.11
(3,246)	1:5:A:LYS:HB2	1:5:A:LYS:HA	5	0.11
(3,235)	1:15:A:LEU:HA	1:19:A:ARG:HG2	10	0.11
(3,210)	1:44:A:ILE:H	1:44:A:ILE:HG21	4	0.11
(3,210)	1:44:A:ILE:H	1:44:A:ILE:HG21	15	0.11
(3,202)	1:103:A:ASP:HB3	1:104:A:GLU:H	6	0.11
(3,181)	1:36:A:TYR:H	1:35:A:GLN:HB2	16	0.11
(3,174)	1:19:A:ARG:H	1:20:A:ILE:HG12	4	0.11
(3,161)	1:7:A:ILE:HG21	1:84:A:LEU:HB3	1	0.11
(3,147)	1:5:A:LYS:HG2	1:6:A:GLU:H	12	0.11
(3,131)	1:38:A:ASN:HB2	1:38:A:ASN:HA	3	0.11
(3,131)	1:38:A:ASN:HB2	1:38:A:ASN:HA	9	0.11
(3,131)	1:38:A:ASN:HB2	1:38:A:ASN:HA	12	0.11
(3,125)	1:73:A:VAL:HG12	1:73:A:VAL:HG21	12	0.11
(3,94)	1:87:A:LYS:HB3	1:87:A:LYS:HA	10	0.11
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD11	15	0.11
(3,60)	1:6:A:GLU:HB3	1:48:A:LYS:HA	14	0.11
(3,56)	1:85:A:CYS:HB3	1:85:A:CYS:HA	7	0.11
(3,31)	1:92:A:SER:HB3	1:92:A:SER:H	8	0.11
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG13	2	0.11
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG12	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,25)	1:65:A:ILE:HD11	1:65:A:ILE:HG13	4	0.11
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG13	5	0.11
(3,25)	1:65:A:ILE:HD13	1:65:A:ILE:HG12	6	0.11
(3,25)	1:65:A:ILE:HD11	1:65:A:ILE:HG12	8	0.11
(3,25)	1:65:A:ILE:HD13	1:65:A:ILE:HG12	10	0.11
(3,25)	1:65:A:ILE:HD11	1:65:A:ILE:HG13	12	0.11
(3,25)	1:65:A:ILE:HD11	1:65:A:ILE:HG12	15	0.11
(3,25)	1:65:A:ILE:HD11	1:65:A:ILE:HG12	16	0.11
(3,25)	1:65:A:ILE:HD13	1:65:A:ILE:HG12	17	0.11
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG13	19	0.11
(3,25)	1:65:A:ILE:HD13	1:65:A:ILE:HG13	20	0.11
(3,24)	1:10:A:VAL:H	1:9:A:ILE:HB	1	0.11
(3,24)	1:9:A:ILE:H	1:9:A:ILE:HB	18	0.11
(3,21)	1:92:A:SER:HB2	1:93:A:ALA:H	15	0.11
(3,18)	1:103:A:ASP:HB3	1:103:A:ASP:HA	18	0.11
(3,6)	1:9:A:ILE:H	1:44:A:ILE:HG21	16	0.11
(1,2276)	1:19:A:ARG:HB2	1:14:A:THR:HA	15	0.11
(1,2261)	1:21:A:LEU:HB2	1:21:A:LEU:HA	18	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	1	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	3	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	4	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	6	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	7	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	10	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	12	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	13	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	14	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	15	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	16	0.11
(1,2254)	1:21:A:LEU:HB3	1:21:A:LEU:HB2	17	0.11
(1,2250)	1:11:A:ILE:HD11	1:61:A:PHE:HE1	10	0.11
(1,2239)	1:73:A:VAL:HG21	1:71:A:THR:HG22	17	0.11
(1,2237)	1:73:A:VAL:HG22	1:61:A:PHE:HE2	3	0.11
(1,2237)	1:73:A:VAL:HG23	1:61:A:PHE:HE2	11	0.11
(1,2228)	1:9:A:ILE:HD11	1:75:A:ALA:HB2	16	0.11
(1,2223)	1:32:A:VAL:HG23	1:32:A:VAL:HA	9	0.11
(1,2223)	1:32:A:VAL:HG22	1:32:A:VAL:HA	17	0.11
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG13	3	0.11
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG11	6	0.11
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG12	9	0.11
(1,2177)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	4	0.11
(1,2150)	1:62:A:ARG:HA	1:70:A:PHE:HB3	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2148)	1:70:A:PHE:HB2	1:62:A:ARG:HA	20	0.11
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	17	0.11
(1,2112)	1:23:A:TYR:HA	1:61:A:PHE:HE1	5	0.11
(1,2095)	1:90:A:GLU:HA	1:90:A:GLU:HG2	2	0.11
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	11	0.11
(1,2090)	1:9:A:ILE:HG12	1:46:A:LYS:HA	14	0.11
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	6	0.11
(1,2086)	1:39:A:PHE:HA	1:39:A:PHE:HD1	7	0.11
(1,2075)	1:56:A:ARG:HB3	1:56:A:ARG:HA	18	0.11
(1,2063)	1:73:A:VAL:HG23	1:73:A:VAL:HA	13	0.11
(1,2043)	1:8:A:GLU:HB3	1:8:A:GLU:HA	19	0.11
(1,1991)	1:115:A:SER:HB2	1:115:A:SER:HA	2	0.11
(1,1955)	1:10:A:VAL:HG21	1:10:A:VAL:HA	12	0.11
(1,1948)	1:61:A:PHE:HD2	1:71:A:THR:HG23	8	0.11
(1,1948)	1:61:A:PHE:HD1	1:71:A:THR:HG22	9	0.11
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	6	0.11
(1,1928)	1:98:A:ILE:HG23	1:98:A:ILE:HA	12	0.11
(1,1925)	1:73:A:VAL:HG23	1:98:A:ILE:HG22	11	0.11
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	2	0.11
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD13	10	0.11
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	1	0.11
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	2	0.11
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	3	0.11
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	14	0.11
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	17	0.11
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	19	0.11
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	2	0.11
(1,1852)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	16	0.11
(1,1812)	1:113:A:TRP:H	1:113:A:TRP:HB2	17	0.11
(1,1812)	1:113:A:TRP:H	1:113:A:TRP:HB2	18	0.11
(1,1803)	1:56:A:ARG:HB2	1:56:A:ARG:H	4	0.11
(1,1802)	1:56:A:ARG:H	1:56:A:ARG:HB3	8	0.11
(1,1796)	1:32:A:VAL:H	1:26:A:ARG:HA	19	0.11
(1,1785)	1:115:A:SER:H	1:114:A:ARG:HA	3	0.11
(1,1784)	1:111:A:ASN:H	1:98:A:ILE:HG22	17	0.11
(1,1755)	1:99:A:TYR:HB3	1:100:A:PHE:H	11	0.11
(1,1707)	1:90:A:GLU:HG3	1:90:A:GLU:H	3	0.11
(1,1693)	1:85:A:CYS:H	1:84:A:LEU:HB2	6	0.11
(1,1693)	1:85:A:CYS:H	1:84:A:LEU:HB2	12	0.11
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	12	0.11
(1,1681)	1:80:A:LEU:HA	1:81:A:LYS:H	17	0.11
(1,1667)	1:57:A:TRP:H	1:76:A:TYR:H	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	1:75:A:ALA:H	1:58:A:ASN:HA	6	0.11
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	7	0.11
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	15	0.11
(1,1645)	1:70:A:PHE:H	1:70:A:PHE:HD1	19	0.11
(1,1630)	1:55:A:SER:H	1:54:A:ARG:HB2	20	0.11
(1,1608)	1:52:A:THR:H	1:50:A:ASP:HA	9	0.11
(1,1606)	1:52:A:THR:H	1:52:A:THR:HG22	17	0.11
(1,1577)	1:9:A:ILE:HG12	1:46:A:LYS:H	1	0.11
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD12	9	0.11
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	7	0.11
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	12	0.11
(1,1547)	1:39:A:PHE:HD2	1:39:A:PHE:H	7	0.11
(1,1541)	1:20:A:ILE:HD12	1:38:A:ASN:H	4	0.11
(1,1528)	1:36:A:TYR:H	1:36:A:TYR:HB2	7	0.11
(1,1519)	1:35:A:GLN:H	1:35:A:GLN:HG2	18	0.11
(1,1483)	1:26:A:ARG:H	1:57:A:TRP:HB2	18	0.11
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB2	20	0.11
(1,1390)	1:85:A:CYS:HB3	1:5:A:LYS:H	14	0.11
(1,1386)	1:5:A:LYS:H	1:5:A:LYS:HB3	3	0.11
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	4	0.11
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	5	0.11
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	10	0.11
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	17	0.11
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	10	0.11
(1,1341)	1:36:A:TYR:HE1	1:36:A:TYR:HD1	20	0.11
(1,1298)	1:42:A:THR:HG22	1:12:A:LYS:HA	7	0.11
(1,1295)	1:69:A:PHE:HB2	1:65:A:ILE:HG22	5	0.11
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG22	6	0.11
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	8	0.11
(1,1276)	1:5:A:LYS:HB2	1:5:A:LYS:HA	9	0.11
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	3	0.11
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	10	0.11
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	11	0.11
(1,1262)	1:15:A:LEU:H	1:15:A:LEU:HG	14	0.11
(1,1171)	1:1:A:ALA:HB2	1:83:A:PRO:HA	5	0.11
(1,1169)	1:36:A:TYR:HB3	1:20:A:ILE:HG22	3	0.11
(1,1166)	1:47:A:PHE:HD1	1:30:A:THR:HG23	17	0.11
(1,1163)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	7	0.11
(1,1147)	1:61:A:PHE:HD2	1:71:A:THR:HG22	16	0.11
(1,1141)	1:37:A:LEU:H	1:20:A:ILE:HG22	3	0.11
(1,1140)	1:20:A:ILE:HG22	1:21:A:LEU:H	7	0.11
(1,1113)	1:20:A:ILE:HD13	1:20:A:ILE:HG13	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:7:A:ILE:HD13	1:5:A:LYS:HB3	5	0.11
(1,1097)	1:10:A:VAL:HG23	1:10:A:VAL:HA	20	0.11
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG22	13	0.11
(1,1090)	1:52:A:THR:HB	1:52:A:THR:HG22	19	0.11
(1,1086)	1:42:A:THR:HG22	1:42:A:THR:HB	3	0.11
(1,1086)	1:42:A:THR:HG21	1:42:A:THR:HB	4	0.11
(1,1051)	1:74:A:GLU:HA	1:75:A:ALA:HB1	12	0.11
(1,1037)	1:73:A:VAL:HG21	1:91:A:LEU:HB3	9	0.11
(1,1036)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	9	0.11
(1,1019)	1:41:A:GLY:HA2	1:40:A:LYS:HB3	12	0.11
(1,999)	1:15:A:LEU:H	1:95:A:MET:HA	13	0.11
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	9	0.11
(1,989)	1:23:A:TYR:HA	1:61:A:PHE:HE1	19	0.11
(1,980)	1:12:A:LYS:HB2	1:92:A:SER:HA	15	0.11
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	17	0.11
(1,974)	1:39:A:PHE:HA	1:39:A:PHE:HD1	11	0.11
(1,964)	1:80:A:LEU:HA	1:80:A:LEU:HB3	16	0.11
(1,961)	1:35:A:GLN:HA	1:35:A:GLN:HG2	2	0.11
(1,958)	1:79:A:ASP:HB2	1:79:A:ASP:HA	16	0.11
(1,941)	1:84:A:LEU:HB2	1:7:A:ILE:HD12	16	0.11
(1,924)	1:47:A:PHE:HD1	1:30:A:THR:HB	11	0.11
(1,924)	1:47:A:PHE:HD1	1:30:A:THR:HB	13	0.11
(1,908)	1:10:A:VAL:HG23	1:10:A:VAL:HB	4	0.11
(1,908)	1:10:A:VAL:HG23	1:10:A:VAL:HB	7	0.11
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	10	0.11
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG21	14	0.11
(1,899)	1:61:A:PHE:HB3	1:71:A:THR:HG22	15	0.11
(1,890)	1:98:A:ILE:HG21	1:98:A:ILE:HA	1	0.11
(1,887)	1:98:A:ILE:HB	1:98:A:ILE:HG21	11	0.11
(1,887)	1:98:A:ILE:HB	1:98:A:ILE:HG21	15	0.11
(1,883)	1:23:A:TYR:HE2	1:11:A:ILE:HG22	20	0.11
(1,860)	1:89:A:TYR:H	1:10:A:VAL:H	17	0.11
(1,855)	1:98:A:ILE:H	1:98:A:ILE:HD11	20	0.11
(1,848)	1:45:A:ILE:H	1:44:A:ILE:HG12	9	0.11
(1,841)	1:7:A:ILE:H	1:7:A:ILE:HG23	17	0.11
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	6	0.11
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	17	0.11
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD2	7	0.11
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	17	0.11
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	18	0.11
(1,819)	1:57:A:TRP:HE1	1:56:A:ARG:HA	11	0.11
(1,804)	1:25:A:CYS:H	1:59:A:CYS:HB3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,804)	1:25:A:CYS:H	1:59:A:CYS:HB3	14	0.11
(1,774)	1:56:A:ARG:H	1:55:A:SER:H	9	0.11
(1,773)	1:31:A:ASN:H	1:30:A:THR:HG23	18	0.11
(1,736)	1:102:A:MET:H	1:101:A:LYS:HB2	8	0.11
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	5	0.11
(1,673)	1:86:A:GLY:H	1:85:A:CYS:HA	12	0.11
(1,671)	1:85:A:CYS:H	1:84:A:LEU:HB2	6	0.11
(1,671)	1:85:A:CYS:H	1:84:A:LEU:HB2	12	0.11
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	7	0.11
(1,638)	1:75:A:ALA:H	1:58:A:ASN:HA	6	0.11
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	1	0.11
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	5	0.11
(1,622)	1:71:A:THR:H	1:71:A:THR:HG21	6	0.11
(1,619)	1:70:A:PHE:H	1:69:A:PHE:HA	18	0.11
(1,615)	1:65:A:ILE:H	1:65:A:ILE:HB	2	0.11
(1,561)	1:46:A:LYS:HB3	1:47:A:PHE:H	4	0.11
(1,558)	1:9:A:ILE:HG12	1:46:A:LYS:H	7	0.11
(1,539)	1:42:A:THR:H	1:44:A:ILE:HD13	4	0.11
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD2	7	0.11
(1,534)	1:40:A:LYS:H	1:39:A:PHE:HD2	11	0.11
(1,532)	1:39:A:PHE:HA	1:40:A:LYS:H	11	0.11
(1,529)	1:38:A:ASN:HB3	1:39:A:PHE:H	17	0.11
(1,525)	1:20:A:ILE:HD11	1:38:A:ASN:H	20	0.11
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	13	0.11
(1,485)	1:29:A:ASN:H	1:28:A:GLY:H	13	0.11
(1,475)	1:26:A:ARG:HB2	1:27:A:SER:H	1	0.11
(1,440)	1:16:A:GLY:H	1:39:A:PHE:HD1	14	0.11
(1,427)	1:14:A:THR:H	1:93:A:ALA:HB1	9	0.11
(1,392)	1:112:A:LYS:H	1:112:A:LYS:HB2	7	0.11
(1,391)	1:112:A:LYS:H	1:98:A:ILE:HB	12	0.11
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	1	0.11
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	5	0.11
(1,336)	1:98:A:ILE:HD11	1:61:A:PHE:HE2	10	0.11
(1,327)	1:7:A:ILE:HD12	1:8:A:GLU:H	4	0.11
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	6	0.11
(1,317)	1:76:A:TYR:H	1:58:A:ASN:HA	14	0.11
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	11	0.11
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	13	0.11
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	15	0.11
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	20	0.11
(1,300)	1:82:A:HIS:HD1	1:79:A:ASP:HB3	7	0.11
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	6	0.11
(1,272)	1:52:A:THR:HG23	1:52:A:THR:HA	7	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	2	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	4	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	5	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	6	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	7	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	8	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	13	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	15	0.11
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	19	0.11
(1,255)	1:32:A:VAL:HG13	1:47:A:PHE:HE1	14	0.11
(1,248)	1:36:A:TYR:HD1	1:36:A:TYR:HB2	20	0.11
(1,245)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	5	0.11
(1,245)	1:70:A:PHE:HB2	1:70:A:PHE:HD1	12	0.11
(1,242)	1:39:A:PHE:HD2	1:17:A:PRO:HA	14	0.11
(1,209)	1:32:A:VAL:HG21	1:32:A:VAL:HA	3	0.11
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	6	0.11
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	10	0.11
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	11	0.11
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	15	0.11
(1,174)	1:42:A:THR:HA	1:12:A:LYS:HA	19	0.11
(1,168)	1:76:A:TYR:HA	1:76:A:TYR:HD2	7	0.11
(1,167)	1:52:A:THR:H	1:51:A:GLY:HA2	17	0.11
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	6	0.11
(1,165)	1:61:A:PHE:H	1:72:A:GLU:HA	15	0.11
(1,154)	1:98:A:ILE:HG13	1:113:A:TRP:H	2	0.11
(1,145)	1:42:A:THR:HG22	1:12:A:LYS:HA	9	0.11
(1,139)	1:25:A:CYS:HB3	1:45:A:ILE:HD11	19	0.11
(1,134)	1:5:A:LYS:HA	1:5:A:LYS:HB3	19	0.11
(1,132)	1:15:A:LEU:HA	1:94:A:ARG:HA	19	0.11
(1,124)	1:45:A:ILE:HG21	1:45:A:ILE:HD12	16	0.11
(1,116)	1:36:A:TYR:HD2	1:20:A:ILE:HD12	1	0.11
(1,106)	1:9:A:ILE:HD12	1:9:A:ILE:HA	17	0.11
(1,94)	1:9:A:ILE:HG22	1:75:A:ALA:HA	6	0.11
(1,78)	1:74:A:GLU:HA	1:74:A:GLU:HB3	6	0.11
(1,78)	1:74:A:GLU:HA	1:74:A:GLU:HB3	9	0.11
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG21	1	0.11
(1,53)	1:76:A:TYR:HD2	1:7:A:ILE:HG23	1	0.11
(1,49)	1:45:A:ILE:H	1:44:A:ILE:HG21	17	0.11
(1,43)	1:7:A:ILE:HD12	1:7:A:ILE:HG23	6	0.11
(1,43)	1:7:A:ILE:HD11	1:7:A:ILE:HG21	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,38)	1:45:A:ILE:HD11	1:45:A:ILE:HG13	7	0.11
(1,25)	1:20:A:ILE:HD12	1:20:A:ILE:HG13	11	0.11
(1,21)	1:7:A:ILE:HD11	1:8:A:GLU:H	12	0.11
(1,20)	1:85:A:CYS:HA	1:7:A:ILE:HD11	8	0.11
(1,14)	1:98:A:ILE:HD13	1:71:A:THR:HG23	3	0.11
(1,13)	1:98:A:ILE:HG23	1:98:A:ILE:HD12	12	0.11
(4,31)	1:89:A:TYR:O	1:10:A:VAL:N	17	0.1
(4,7)	1:10:A:VAL:H	1:89:A:TYR:O	19	0.1
(3,204)	1:105:A:ARG:HG3	1:105:A:ARG:H	4	0.1
(3,203)	1:103:A:ASP:HB3	1:105:A:ARG:H	12	0.1
(3,189)	1:74:A:GLU:HA	1:76:A:TYR:H	16	0.1
(3,148)	1:111:A:ASN:H	1:98:A:ILE:HB	6	0.1
(3,145)	1:29:A:ASN:H	1:56:A:ARG:HA	5	0.1
(3,136)	1:45:A:ILE:HA	1:44:A:ILE:HG23	20	0.1
(3,131)	1:38:A:ASN:HB2	1:38:A:ASN:HA	1	0.1
(3,125)	1:45:A:ILE:HG21	1:45:A:ILE:HD13	14	0.1
(3,80)	1:23:A:TYR:HB3	1:61:A:PHE:HE1	8	0.1
(3,73)	1:9:A:ILE:HB	1:9:A:ILE:HD12	13	0.1
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG12	1	0.1
(3,25)	1:65:A:ILE:HD13	1:65:A:ILE:HG12	7	0.1
(3,25)	1:65:A:ILE:HD12	1:65:A:ILE:HG12	11	0.1
(3,21)	1:92:A:SER:HB3	1:93:A:ALA:H	4	0.1
(3,20)	1:65:A:ILE:HA	1:65:A:ILE:HG13	2	0.1
(1,2272)	1:20:A:ILE:HD13	1:20:A:ILE:HB	7	0.1
(1,2236)	1:73:A:VAL:HG23	1:61:A:PHE:HD1	6	0.1
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG12	10	0.1
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG13	11	0.1
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG11	16	0.1
(1,2212)	1:34:A:VAL:HB	1:34:A:VAL:HG13	19	0.1
(1,2206)	1:107:A:PRO:HB2	1:99:A:TYR:HB3	9	0.1
(1,2161)	1:71:A:THR:HB	1:71:A:THR:HA	14	0.1
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	5	0.1
(1,2140)	1:108:A:GLN:HB2	1:109:A:PRO:HB2	6	0.1
(1,2138)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	19	0.1
(1,2096)	1:73:A:VAL:HG21	1:72:A:GLU:HA	5	0.1
(1,2077)	1:56:A:ARG:HA	1:28:A:GLY:HA2	12	0.1
(1,2071)	1:35:A:GLN:HG3	1:35:A:GLN:HA	20	0.1
(1,2019)	1:4:A:CYS:HB3	1:4:A:CYS:HA	6	0.1
(1,2007)	1:78:A:PRO:HA	1:78:A:PRO:HB2	8	0.1
(1,1979)	1:112:A:LYS:HB3	1:112:A:LYS:HA	11	0.1
(1,1979)	1:112:A:LYS:HB3	1:112:A:LYS:HA	19	0.1
(1,1946)	1:61:A:PHE:HB3	1:71:A:THR:HG21	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1941)	1:36:A:TYR:HB3	1:20:A:ILE:HG21	17	0.1
(1,1918)	1:11:A:ILE:HG22	1:11:A:ILE:HD12	15	0.1
(1,1904)	1:62:A:ARG:H	1:21:A:LEU:HB2	18	0.1
(1,1890)	1:98:A:ILE:H	1:98:A:ILE:HD12	16	0.1
(1,1880)	1:45:A:ILE:H	1:44:A:ILE:HG12	15	0.1
(1,1875)	1:7:A:ILE:H	1:7:A:ILE:HD12	17	0.1
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	5	0.1
(1,1872)	1:60:A:LEU:H	1:61:A:PHE:HA	20	0.1
(1,1828)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.1
(1,1812)	1:113:A:TRP:H	1:113:A:TRP:HB2	1	0.1
(1,1812)	1:113:A:TRP:H	1:113:A:TRP:HB2	2	0.1
(1,1801)	1:56:A:ARG:H	1:55:A:SER:H	20	0.1
(1,1765)	1:104:A:GLU:H	1:104:A:GLU:HB2	1	0.1
(1,1762)	1:102:A:MET:H	1:101:A:LYS:HB2	11	0.1
(1,1657)	1:74:A:GLU:HB3	1:74:A:GLU:H	15	0.1
(1,1648)	1:71:A:THR:H	1:70:A:PHE:HB2	8	0.1
(1,1646)	1:71:A:THR:H	1:71:A:THR:HG21	10	0.1
(1,1631)	1:58:A:ASN:HB3	1:59:A:CYS:H	11	0.1
(1,1608)	1:52:A:THR:H	1:50:A:ASP:HA	15	0.1
(1,1573)	1:45:A:ILE:H	1:45:A:ILE:HD11	13	0.1
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	10	0.1
(1,1564)	1:43:A:ARG:H	1:44:A:ILE:HG13	17	0.1
(1,1503)	1:30:A:THR:H	1:27:A:SER:H	13	0.1
(1,1456)	1:20:A:ILE:H	1:19:A:ARG:HB3	12	0.1
(1,1442)	1:16:A:GLY:H	1:19:A:ARG:HB2	19	0.1
(1,1431)	1:15:A:LEU:H	1:14:A:THR:H	14	0.1
(1,1430)	1:14:A:THR:H	1:93:A:ALA:H	8	0.1
(1,1427)	1:14:A:THR:H	1:93:A:ALA:HB2	12	0.1
(1,1405)	1:88:A:ARG:HA	1:8:A:GLU:H	7	0.1
(1,1384)	1:112:A:LYS:H	1:112:A:LYS:HB2	1	0.1
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	4	0.1
(1,1383)	1:112:A:LYS:H	1:112:A:LYS:HB3	15	0.1
(1,1333)	1:23:A:TYR:HD1	1:23:A:TYR:HA	16	0.1
(1,1294)	1:64:A:GLY:HA2	1:65:A:ILE:HG23	19	0.1
(1,1242)	1:20:A:ILE:HD13	1:39:A:PHE:H	9	0.1
(1,1239)	1:36:A:TYR:HE2	1:20:A:ILE:HG23	18	0.1
(1,1211)	1:32:A:VAL:HG22	1:32:A:VAL:HA	14	0.1
(1,1174)	1:36:A:TYR:HA	1:20:A:ILE:HG21	4	0.1
(1,1163)	1:9:A:ILE:HD11	1:75:A:ALA:HB3	20	0.1
(1,1160)	1:34:A:VAL:HG21	1:34:A:VAL:HA	7	0.1
(1,1142)	1:99:A:TYR:H	1:98:A:ILE:HG23	8	0.1
(1,1137)	1:9:A:ILE:HD11	1:7:A:ILE:HG22	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:7:A:ILE:HD11	1:7:A:ILE:HG23	5	0.1
(1,1125)	1:11:A:ILE:HG22	1:11:A:ILE:HD11	18	0.1
(1,1113)	1:20:A:ILE:HD11	1:20:A:ILE:HG13	9	0.1
(1,1097)	1:10:A:VAL:HG21	1:10:A:VAL:HA	9	0.1
(1,1097)	1:10:A:VAL:HG22	1:10:A:VAL:HA	11	0.1
(1,1086)	1:42:A:THR:HG22	1:42:A:THR:HB	1	0.1
(1,1086)	1:42:A:THR:HG21	1:42:A:THR:HB	10	0.1
(1,1086)	1:42:A:THR:HG23	1:42:A:THR:HB	17	0.1
(1,1002)	1:114:A:ARG:HB3	1:70:A:PHE:HB2	16	0.1
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	3	0.1
(1,994)	1:36:A:TYR:HA	1:22:A:GLN:HG2	14	0.1
(1,982)	1:73:A:VAL:HG23	1:72:A:GLU:HA	3	0.1
(1,980)	1:12:A:LYS:HB2	1:92:A:SER:HA	3	0.1
(1,979)	1:90:A:GLU:HA	1:90:A:GLU:HG2	10	0.1
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	4	0.1
(1,977)	1:9:A:ILE:HG12	1:46:A:LYS:HA	20	0.1
(1,887)	1:98:A:ILE:HB	1:98:A:ILE:HG22	10	0.1
(1,871)	1:9:A:ILE:HB	1:9:A:ILE:HD13	12	0.1
(1,870)	1:111:A:ASN:H	1:110:A:LEU:HB3	12	0.1
(1,848)	1:45:A:ILE:H	1:44:A:ILE:HG12	11	0.1
(1,848)	1:45:A:ILE:H	1:44:A:ILE:HG12	13	0.1
(1,839)	1:60:A:LEU:H	1:61:A:PHE:HA	16	0.1
(1,820)	1:57:A:TRP:HE1	1:47:A:PHE:HD1	2	0.1
(1,798)	1:9:A:ILE:H	1:9:A:ILE:HG12	1	0.1
(1,798)	1:9:A:ILE:H	1:9:A:ILE:HG12	6	0.1
(1,670)	1:85:A:CYS:H	1:85:A:CYS:HB3	19	0.1
(1,659)	1:80:A:LEU:HA	1:81:A:LYS:H	11	0.1
(1,644)	1:76:A:TYR:H	1:74:A:GLU:HB3	12	0.1
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	6	0.1
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	12	0.1
(1,624)	1:71:A:THR:H	1:70:A:PHE:HB2	17	0.1
(1,615)	1:65:A:ILE:H	1:65:A:ILE:HB	17	0.1
(1,546)	1:43:A:ARG:H	1:44:A:ILE:HG13	16	0.1
(1,546)	1:43:A:ARG:H	1:44:A:ILE:HG13	20	0.1
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	2	0.1
(1,514)	1:36:A:TYR:H	1:36:A:TYR:HB2	14	0.1
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	9	0.1
(1,505)	1:35:A:GLN:H	1:35:A:GLN:HG2	12	0.1
(1,448)	1:19:A:ARG:HB3	1:19:A:ARG:H	16	0.1
(1,413)	1:10:A:VAL:HG21	1:10:A:VAL:H	2	0.1
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	9	0.1
(1,390)	1:112:A:LYS:H	1:112:A:LYS:HB3	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,384)	1:43:A:ARG:HB2	1:11:A:ILE:HG22	7	0.1
(1,381)	1:70:A:PHE:HE1	1:70:A:PHE:HA	14	0.1
(1,370)	1:102:A:MET:H	1:102:A:MET:HG2	13	0.1
(1,352)	1:57:A:TRP:HE1	1:56:A:ARG:HA	13	0.1
(1,352)	1:57:A:TRP:HE1	1:56:A:ARG:HA	16	0.1
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	2	0.1
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	5	0.1
(1,339)	1:58:A:ASN:HA	1:74:A:GLU:HA	9	0.1
(1,316)	1:70:A:PHE:HE1	1:62:A:ARG:HA	7	0.1
(1,311)	1:111:A:ASN:H	1:110:A:LEU:HA	19	0.1
(1,301)	1:23:A:TYR:HD1	1:36:A:TYR:HA	9	0.1
(1,294)	1:35:A:GLN:HA	1:36:A:TYR:HD1	17	0.1
(1,277)	1:98:A:ILE:HB	1:112:A:LYS:HA	11	0.1
(1,259)	1:40:A:LYS:HB3	1:40:A:LYS:HA	11	0.1
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	1	0.1
(1,187)	1:30:A:THR:HA	1:30:A:THR:HB	8	0.1
(1,176)	1:100:A:PHE:HA	1:91:A:LEU:HA	12	0.1
(1,68)	1:34:A:VAL:HB	1:34:A:VAL:HG23	16	0.1
(1,54)	1:7:A:ILE:HG22	1:8:A:GLU:H	4	0.1
(1,47)	1:20:A:ILE:HG23	1:21:A:LEU:H	11	0.1
(1,23)	1:9:A:ILE:HD13	1:75:A:ALA:HB2	18	0.1
(1,2)	1:30:A:THR:HA	1:30:A:THR:HG23	6	0.1

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

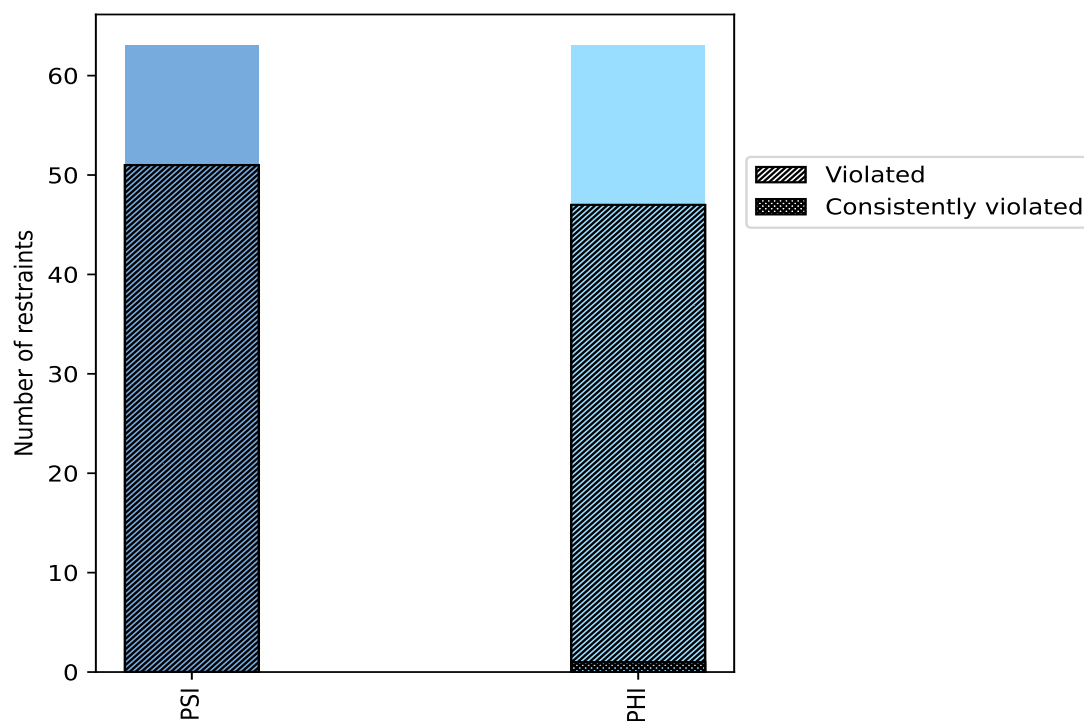
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	63	50.0	51	81.0	40.5	0	0.0	0.0
PHI	63	50.0	47	74.6	37.3	1	1.6	0.8
Total	126	100.0	98	77.8	77.8	1	0.8	0.8

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

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



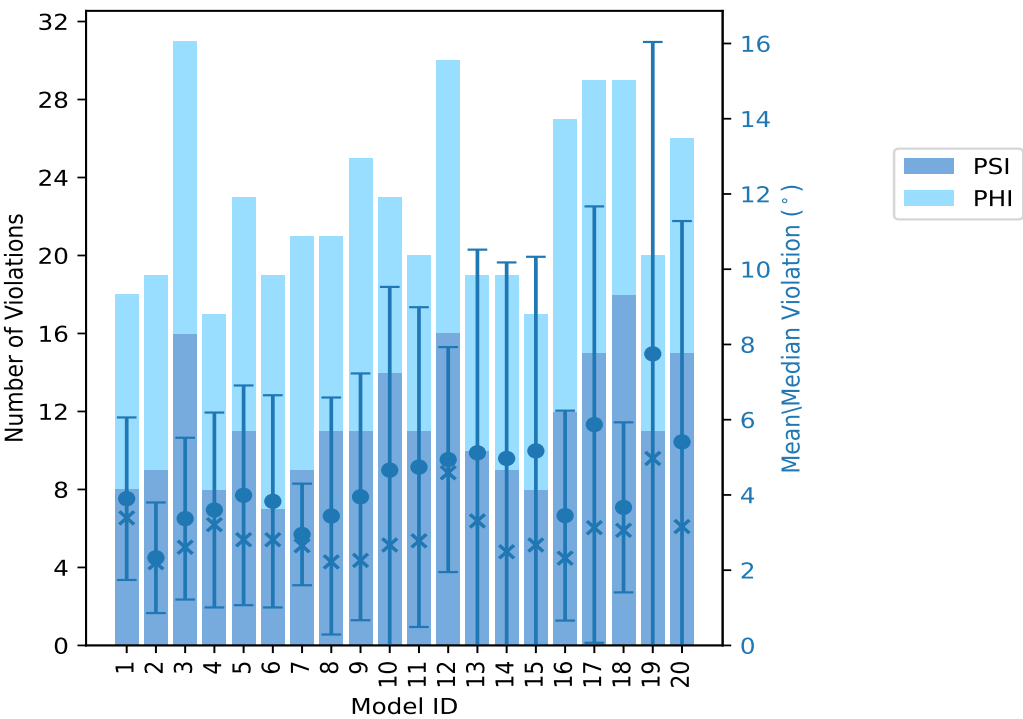
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	8	10	18	3.9	9.53	2.16	3.39
2	9	10	19	2.33	7.21	1.47	2.2
3	16	15	31	3.37	8.28	2.15	2.61
4	8	9	17	3.6	11.87	2.59	3.21
5	11	12	23	3.99	11.03	2.92	2.81
6	7	12	19	3.83	13.33	2.82	2.81
7	9	12	21	2.95	6.23	1.35	2.65
8	11	10	21	3.44	12.2	3.15	2.22
9	11	14	25	3.95	13.98	3.28	2.26
10	14	9	23	4.66	21.67	4.87	2.67
11	11	9	20	4.74	17.05	4.25	2.78
12	16	14	30	4.94	10.82	2.99	4.59
13	10	9	19	5.12	21.61	5.4	3.31
14	9	10	19	4.97	19.99	5.21	2.49
15	8	9	17	5.17	22.03	5.16	2.67
16	12	15	27	3.45	11.26	2.79	2.32
17	15	14	29	5.87	20.23	5.8	3.13
18	18	11	29	3.67	9.46	2.26	3.06
19	11	9	20	7.75	36.99	8.29	4.97
20	15	11	26	5.41	24.79	5.87	3.16

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
12	10	22	1	5.0
10	8	18	2	10.0
6	5	11	3	15.0
5	5	10	4	20.0
4	3	7	5	25.0
1	2	3	6	30.0
3	7	10	7	35.0
2	1	3	8	40.0
2	1	3	9	45.0
0	1	1	10	50.0
0	1	1	11	55.0

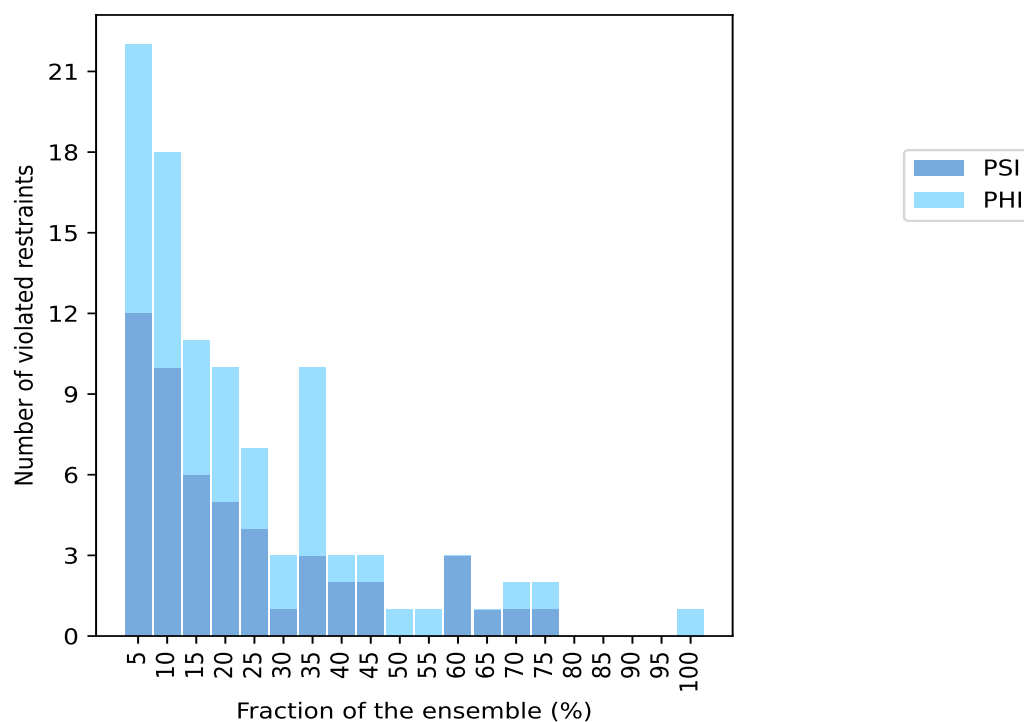
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
3	0	3	12	60.0
1	0	1	13	65.0
1	1	2	14	70.0
1	1	2	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	1	1	20	100.0

¹ Number of models with violations

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

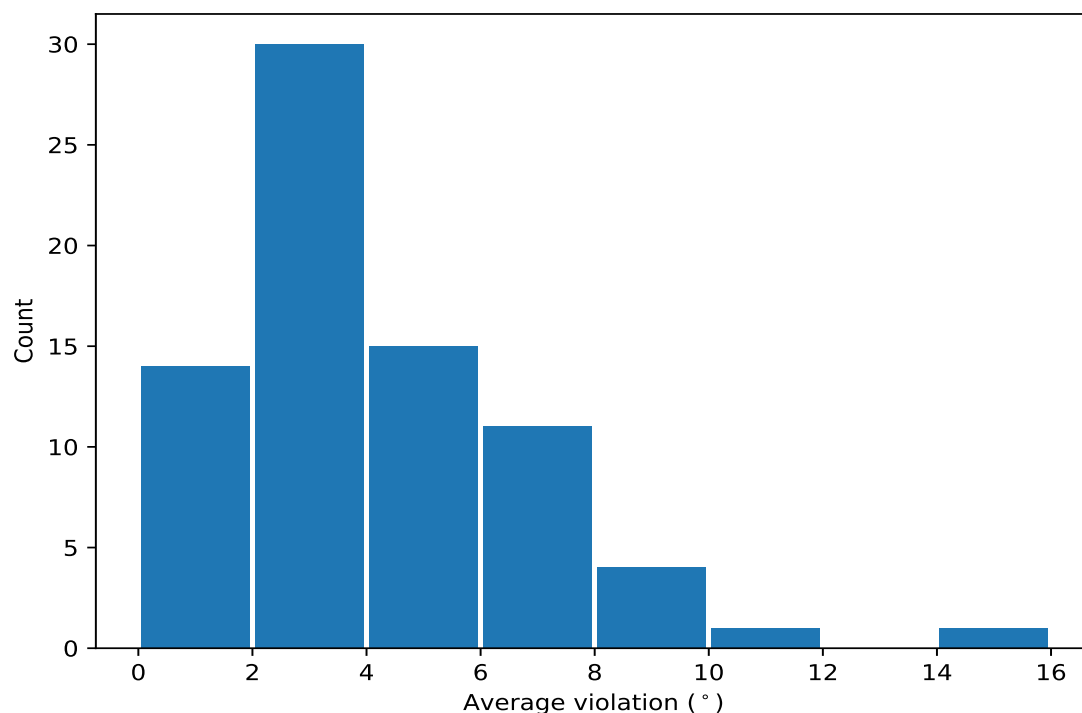


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	20	5.02	1.21	5.29
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	15	4.49	2.05	4.39
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	15	1.75	0.78	1.37
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	14	6.75	4.64	5.69
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	14	4.81	3.12	4.61
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	13	7.36	7.02	3.54
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	12	4.54	3.57	2.92
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	12	3.57	2.43	2.39
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	12	3.22	1.44	2.8
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	11	7.28	3.63	8.29
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	10	4.93	4.34	2.75
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	9	5.28	4.57	4.0
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	9	5.05	3.52	3.2
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	9	2.7	1.86	2.34
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	8	8.74	4.43	8.99
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	8	8.39	7.0	6.76
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	8	2.75	1.88	2.12
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	7	6.38	5.61	4.95
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	7	5.43	2.55	6.2
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	7	4.8	3.75	4.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	7	4.65	6.87	2.0
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	7	2.99	2.16	1.95
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	7	2.63	0.73	2.44
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	7	2.6	0.96	2.71
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	7	2.32	0.73	2.45
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	7	2.08	0.88	1.93
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	7	1.75	0.4	1.75
(1,87)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	6	4.47	4.0	3.1
(1,32)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:SER:N	6	3.67	0.98	3.53
(1,89)	1:80:A:LEU:C	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	6	2.53	1.25	2.06
(1,22)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLN:N	5	9.91	9.77	2.46
(1,98)	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	1:88:A:ARG:N	5	7.41	7.68	3.88
(1,112)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:MET:N	5	3.28	2.51	2.4
(1,65)	1:58:A:ASN:C	1:59:A:CYS:N	1:59:A:CYS:CA	1:59:A:CYS:C	5	2.9	1.59	2.47
(1,84)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:PRO:N	5	2.31	1.2	1.75
(1,17)	1:12:A:LYS:C	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	5	1.97	0.65	1.82
(1,85)	1:78:A:PRO:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	5	1.88	0.79	1.6
(1,73)	1:66:A:ASN:C	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	4	11.47	5.89	12.93
(1,2)	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	1:6:A:GLU:N	4	7.08	4.54	5.95
(1,103)	1:89:A:TYR:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	4	6.2	3.54	5.51
(1,118)	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	1:107:A:PRO:N	4	4.18	2.47	3.56
(1,54)	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	1:46:A:LYS:N	4	3.22	0.82	3.44
(1,19)	1:19:A:ARG:C	1:20:A:ILE:N	1:20:A:ILE:CA	1:20:A:ILE:C	4	2.98	1.26	3.04
(1,92)	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	1:83:A:PRO:N	4	2.62	0.97	2.8
(1,36)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASN:N	4	2.43	0.75	2.35
(1,63)	1:57:A:TRP:C	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	4	2.39	1.45	1.86
(1,23)	1:21:A:LEU:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	4	2.32	0.92	2.15
(1,4)	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	1:7:A:ILE:N	3	15.75	15.03	5.78
(1,3)	1:5:A:LYS:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	3	8.41	3.14	9.9
(1,81)	1:75:A:ALA:C	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	3	6.82	3.1	5.72
(1,88)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:LYS:N	3	6.6	4.92	4.33
(1,62)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ASN:N	3	6.19	5.07	3.13
(1,90)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:HIS:N	3	6.07	3.07	6.26
(1,82)	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	1:77:A:ARG:N	3	5.25	4.25	2.32
(1,83)	1:76:A:TYR:C	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	3	3.71	2.01	2.48
(1,69)	1:61:A:PHE:C	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	3	2.49	0.79	2.88
(1,58)	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	1:48:A:LYS:N	3	2.48	1.25	2.25
(1,1)	1:4:A:CYS:C	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	3	2.33	1.02	1.78
(1,30)	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	1:26:A:ARG:N	2	5.2	1.98	5.2
(1,42)	1:36:A:TYR:N	1:36:A:TYR:CA	1:36:A:TYR:C	1:37:A:LEU:N	2	4.45	0.51	4.45
(1,74)	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	1:68:A:LYS:N	2	2.85	0.08	2.85
(1,70)	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	1:63:A:GLN:N	2	2.33	0.25	2.33
(1,47)	1:41:A:GLY:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	2	2.31	0.88	2.31
(1,117)	1:105:A:ARG:C	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	2	2.3	0.36	2.3
(1,45)	1:37:A:LEU:C	1:38:A:ASN:N	1:38:A:ASN:CA	1:38:A:ASN:C	2	2.13	0.2	2.13
(1,122)	1:108:A:GLN:N	1:108:A:GLN:CA	1:108:A:GLN:C	1:109:A:PRO:N	2	2.06	1.06	2.06
(1,120)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLN:N	2	1.95	0.05	1.95
(1,57)	1:46:A:LYS:C	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	2	1.94	0.26	1.94
(1,113)	1:101:A:LYS:C	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	2	1.86	0.64	1.86
(1,38)	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	1:32:A:VAL:N	2	1.62	0.6	1.62
(1,59)	1:53:A:GLU:C	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	2	1.57	0.07	1.57

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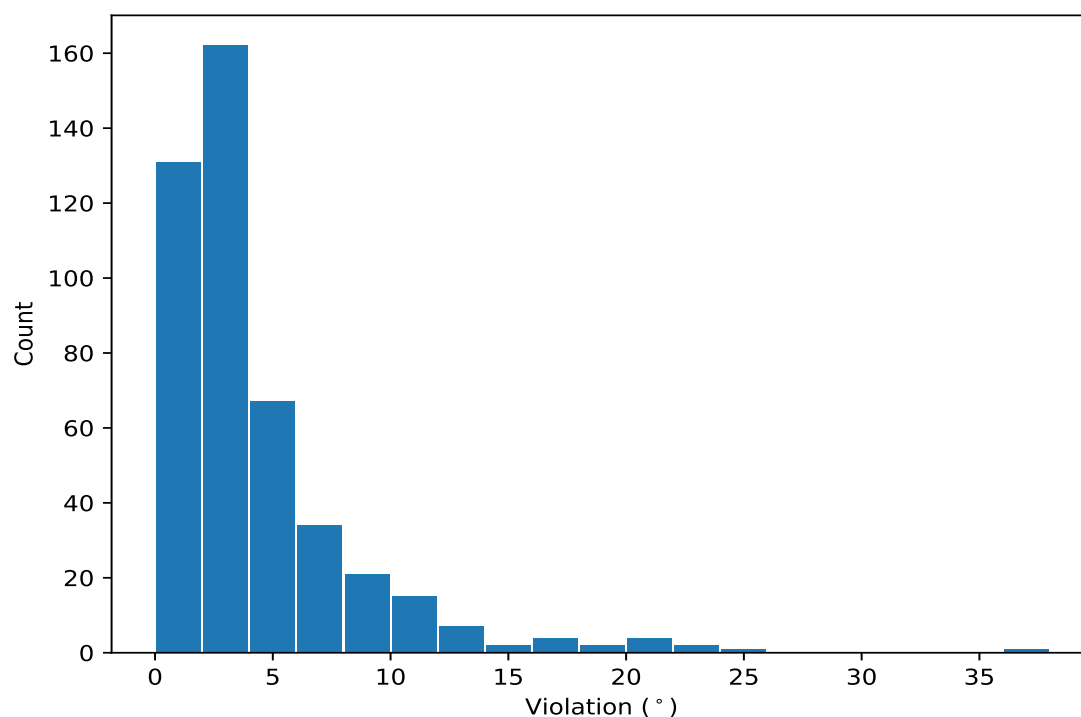
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,11)	1:9:A:ILE:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	2	1.45	0.3	1.45
(1,78)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:GLU:N	2	1.41	0.31	1.41
(1,44)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:ASN:N	2	1.4	0.19	1.4
(1,21)	1:20:A:ILE:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	2	1.39	0.09	1.39
(1,48)	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	1:43:A:ARG:N	2	1.28	0.22	1.28

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	1:7:A:ILE:N	19	36.99
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	20	24.79

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	1:88:A:ARG:N	20	22.49
(1,22)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLN:N	15	22.03
(1,22)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLN:N	10	21.67
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	13	21.61
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	19	21.43
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	17	20.23
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	14	19.99
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	17	18.55
(1,73)	1:66:A:ASN:C	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	13	17.93
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	17	17.17
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	11	17.05
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	14	16.31
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	17	15.27
(1,73)	1:66:A:ASN:C	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	17	14.51
(1,2)	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	1:6:A:GLU:N	9	13.98
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	19	13.61
(1,88)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:LYS:N	10	13.43
(1,62)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ASN:N	6	13.33
(1,87)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	10	13.05
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	15	12.74
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	8	12.2
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	4	11.87
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	11	11.78
(1,103)	1:89:A:TYR:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	17	11.75
(1,73)	1:66:A:ASN:C	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	11	11.35
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	8	11.32
(1,3)	1:5:A:LYS:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	19	11.29
(1,82)	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	1:77:A:ARG:N	16	11.26
(1,81)	1:75:A:ALA:C	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	9	11.05
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	5	11.03
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	16	10.92
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	19	10.82
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	12	10.82
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	14	10.54
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	5	10.52
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	17	10.1
(1,3)	1:5:A:LYS:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	9	9.9
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	20	9.78
(1,90)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:HIS:N	12	9.73
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1	9.53
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	18	9.46
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	12	9.42
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	13	9.41
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	20	9.41
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	5	9.19
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	15	9.17
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	16	9.01
(1,119)	1:106:A:PRO:C	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	12	8.7
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	18	8.61
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	12	8.56
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	12	8.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	19	8.29
(1,2)	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	1:6:A:GLU:N	3	8.28
(1,112)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:MET:N	12	8.18
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	3	8.12
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	18	8.03
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	1	8.0
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	8	7.98
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	15	7.93
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	20	7.93
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	11	7.9
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	11	7.86
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	19	7.83
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	6	7.75
(1,118)	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	1:107:A:PRO:N	12	7.73
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	3	7.64
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	14	7.62
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	3	7.48
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	20	7.32
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	14	7.3
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	12	7.26
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	2	7.21
(1,30)	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	1:26:A:ARG:N	20	7.18
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	18	7.17
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	17	7.17
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	6	7.12
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	12	6.89
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	4	6.83
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	10	6.79
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	1	6.74
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	5	6.73
(1,83)	1:76:A:TYR:C	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	16	6.54
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	8	6.35
(1,90)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:HIS:N	5	6.26
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	7	6.23
(1,98)	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	1:88:A:ARG:N	19	6.22
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	20	6.22
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	12	6.2
(1,103)	1:89:A:TYR:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	3	6.17
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	5	6.09
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	19	6.03
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	12	5.98
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	17	5.96
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	9	5.96
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	9	5.78
(1,4)	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	1:7:A:ILE:N	3	5.78
(1,81)	1:75:A:ALA:C	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	11	5.72
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	18	5.68
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	17	5.65
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	7	5.61
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	18	5.57
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	12	5.55

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	19	5.49
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	5	5.49
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	4	5.44
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	13	5.41
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	9	5.4
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	10	5.4
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	1	5.39
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	16	5.37
(1,32)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:SER:N	20	5.37
(1,118)	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	1:107:A:PRO:N	9	5.24
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	11	5.21
(1,65)	1:58:A:ASN:C	1:59:A:CYS:N	1:59:A:CYS:CA	1:59:A:CYS:C	12	5.15
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	14	5.1
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	12	5.05
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	6	5.05
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	10	5.05
(1,42)	1:36:A:TYR:N	1:36:A:TYR:CA	1:36:A:TYR:C	1:37:A:LEU:N	10	4.96
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	20	4.95
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	4	4.93
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	13	4.88
(1,16)	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1:13:A:ASN:N	18	4.87
(1,103)	1:89:A:TYR:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	7	4.85
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	9	4.82
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	9	4.76
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	15	4.76
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	18	4.76
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	6	4.71
(1,63)	1:57:A:TRP:C	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	20	4.71
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	13	4.63
(1,18)	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1:14:A:THR:N	18	4.55
(1,19)	1:19:A:ARG:C	1:20:A:ILE:N	1:20:A:ILE:CA	1:20:A:ILE:C	13	4.49
(1,4)	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	1:7:A:ILE:N	17	4.49
(1,87)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	2	4.47
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	19	4.46
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	10	4.39
(1,32)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:SER:N	4	4.36
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1	4.34
(1,88)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:LYS:N	15	4.33
(1,65)	1:58:A:ASN:C	1:59:A:CYS:N	1:59:A:CYS:CA	1:59:A:CYS:C	13	4.33
(1,84)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:PRO:N	16	4.3
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	10	4.28
(1,89)	1:80:A:LEU:C	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	14	4.27
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	7	4.24
(1,89)	1:80:A:LEU:C	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	16	4.17
(1,124)	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	1:112:A:LYS:N	3	4.15
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	12	4.13
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	3	4.11
(1,58)	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	1:48:A:LYS:N	19	4.11
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	12	4.1
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1	4.1
(1,54)	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	1:46:A:LYS:N	14	4.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	17	4.06
(1,3)	1:5:A:LYS:C	1:6:A:GLU:N	1:6:A:GLU:CA	1:6:A:GLU:C	3	4.05
(1,87)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	6	4.01
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	17	4.01
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	3	4.0
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	9	3.99
(1,42)	1:36:A:TYR:N	1:36:A:TYR:CA	1:36:A:TYR:C	1:37:A:LEU:N	15	3.94
(1,98)	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	1:88:A:ARG:N	5	3.88
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	15	3.85
(1,19)	1:19:A:ARG:C	1:20:A:ILE:N	1:20:A:ILE:CA	1:20:A:ILE:C	18	3.85
(1,92)	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	1:83:A:PRO:N	20	3.79
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	1	3.76
(1,1)	1:4:A:CYS:C	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	4	3.75
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	1	3.74
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	3	3.72
(1,81)	1:75:A:ALA:C	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	16	3.69
(1,32)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:SER:N	12	3.68
(1,54)	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	1:46:A:LYS:N	4	3.67
(1,23)	1:21:A:LEU:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	18	3.67
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	5	3.66
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	1	3.65
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	18	3.65
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	7	3.64
(1,2)	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	1:6:A:GLU:N	11	3.62
(1,8)	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	1:9:A:ILE:N	19	3.58
(1,36)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASN:N	13	3.56
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	6	3.54
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	17	3.47
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	7	3.43
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	8	3.42
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	3	3.42
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	5	3.4
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	3	3.4
(1,85)	1:78:A:PRO:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	7	3.38
(1,32)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:SER:N	18	3.38
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	16	3.37
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	13	3.31
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	12	3.3
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	4	3.28
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	2	3.26
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	7	3.23
(1,30)	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	1:26:A:ARG:N	4	3.21
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	18	3.2
(1,69)	1:61:A:PHE:C	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	20	3.2
(1,54)	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	1:46:A:LYS:N	11	3.2
(1,47)	1:41:A:GLY:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	6	3.19
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	6	3.18
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1	3.13
(1,62)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ASN:N	17	3.13
(1,122)	1:108:A:GLN:N	1:108:A:GLN:CA	1:108:A:GLN:C	1:109:A:PRO:N	20	3.12
(1,17)	1:12:A:LYS:C	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	17	3.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	7	3.1
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	2	3.06
(1,41)	1:35:A:GLN:C	1:36:A:TYR:N	1:36:A:TYR:CA	1:36:A:TYR:C	18	3.06
(1,84)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:PRO:N	8	3.05
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	18	2.96
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	5	2.94
(1,74)	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	1:68:A:LYS:N	18	2.93
(1,92)	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	1:83:A:PRO:N	10	2.92
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	16	2.92
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	17	2.91
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	8	2.89
(1,69)	1:61:A:PHE:C	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	13	2.88
(1,7)	1:7:A:ILE:C	1:8:A:GLU:N	1:8:A:GLU:CA	1:8:A:GLU:C	7	2.85
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	10	2.84
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	2	2.82
(1,80)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ALA:N	11	2.82
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	6	2.81
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	19	2.81
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	5	2.81
(1,112)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:MET:N	9	2.8
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	9	2.79
(1,74)	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	1:68:A:LYS:N	3	2.77
(1,32)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:SER:N	2	2.76
(1,123)	1:110:A:LEU:C	1:111:A:ASN:N	1:111:A:ASN:CA	1:111:A:ASN:C	3	2.74
(1,24)	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	1:23:A:TYR:N	11	2.73
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	13	2.71
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	1	2.69
(1,92)	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	1:83:A:PRO:N	15	2.67
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	10	2.67
(1,117)	1:105:A:ARG:C	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	7	2.65
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	10	2.65
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	20	2.65
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	7	2.64
(1,23)	1:21:A:LEU:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	3	2.61
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	12	2.6
(1,105)	1:90:A:GLU:C	1:91:A:LEU:N	1:91:A:LEU:CA	1:91:A:LEU:C	3	2.6
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	11	2.58
(1,70)	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	1:63:A:GLN:N	1	2.58
(1,116)	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	1:104:A:GLU:N	14	2.57
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	7	2.56
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	17	2.53
(1,63)	1:57:A:TRP:C	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	16	2.53
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	7	2.52
(1,98)	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	1:88:A:ARG:N	12	2.51
(1,6)	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	1:8:A:GLU:N	19	2.51
(1,113)	1:101:A:LYS:C	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	14	2.49
(1,83)	1:76:A:TYR:C	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	6	2.48
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	16	2.47
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	3	2.47
(1,65)	1:58:A:ASN:C	1:59:A:CYS:N	1:59:A:CYS:CA	1:59:A:CYS:C	8	2.47
(1,32)	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	1:27:A:SER:N	8	2.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLN:N	17	2.46
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	15	2.45
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	10	2.45
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1	2.45
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	4	2.44
(1,2)	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	1:6:A:GLU:N	19	2.44
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	6	2.43
(1,112)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:MET:N	2	2.4
(1,36)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASN:N	16	2.4
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	4	2.37
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	2	2.37
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	5	2.37
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	5	2.36
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	3	2.35
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	8	2.34
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	12	2.34
(1,45)	1:37:A:LEU:C	1:38:A:ASN:N	1:38:A:ASN:CA	1:38:A:ASN:C	6	2.34
(1,22)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLN:N	18	2.34
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	10	2.32
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	16	2.32
(1,82)	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	1:77:A:ARG:N	11	2.32
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	19	2.32
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	1	2.31
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	3	2.31
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	13	2.3
(1,36)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASN:N	18	2.3
(1,89)	1:80:A:LEU:C	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	15	2.29
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	9	2.26
(1,58)	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	1:48:A:LYS:N	1	2.25
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	3	2.24
(1,19)	1:19:A:ARG:C	1:20:A:ILE:N	1:20:A:ILE:CA	1:20:A:ILE:C	2	2.24
(1,38)	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	1:32:A:VAL:N	8	2.22
(1,90)	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	1:82:A:HIS:N	16	2.21
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	20	2.21
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	2	2.2
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	16	2.2
(1,87)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	15	2.2
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	16	2.2
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	14	2.19
(1,57)	1:46:A:LYS:C	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	15	2.19
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	5	2.19
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	2	2.17
(1,82)	1:76:A:TYR:N	1:76:A:TYR:CA	1:76:A:TYR:C	1:77:A:ARG:N	9	2.17
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	15	2.17
(1,83)	1:76:A:TYR:C	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	18	2.11
(1,17)	1:12:A:LYS:C	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	1	2.11
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	6	2.1
(1,73)	1:66:A:ASN:C	1:67:A:MET:N	1:67:A:MET:CA	1:67:A:MET:C	3	2.1
(1,62)	1:57:A:TRP:N	1:57:A:TRP:CA	1:57:A:TRP:C	1:58:A:ASN:N	9	2.1
(1,97)	1:86:A:GLY:C	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	16	2.08
(1,70)	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	1:63:A:GLN:N	14	2.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	9	2.08
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	7	2.07
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	18	2.07
(1,15)	1:11:A:ILE:C	1:12:A:LYS:N	1:12:A:LYS:CA	1:12:A:LYS:C	1	2.07
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	6	2.06
(1,103)	1:89:A:TYR:C	1:90:A:GLU:N	1:90:A:GLU:CA	1:90:A:GLU:C	20	2.03
(1,88)	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	1:81:A:LYS:N	16	2.03
(1,67)	1:60:A:LEU:C	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	17	2.03
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	13	2.03
(1,96)	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	1:87:A:LYS:N	13	2.02
(1,120)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLN:N	20	2.01
(1,115)	1:102:A:MET:C	1:103:A:ASP:N	1:103:A:ASP:CA	1:103:A:ASP:C	8	2.01
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	4	2.0
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	14	2.0
(1,99)	1:87:A:LYS:C	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	9	1.98
(1,98)	1:87:A:LYS:N	1:87:A:LYS:CA	1:87:A:LYS:C	1:88:A:ARG:N	11	1.95
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	20	1.95
(1,117)	1:105:A:ARG:C	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	9	1.94
(1,108)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:ALA:N	12	1.93
(1,45)	1:37:A:LEU:C	1:38:A:ASN:N	1:38:A:ASN:CA	1:38:A:ASN:C	15	1.93
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	6	1.93
(1,85)	1:78:A:PRO:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	5	1.92
(1,54)	1:45:A:ILE:N	1:45:A:ILE:CA	1:45:A:ILE:C	1:46:A:LYS:N	15	1.92
(1,120)	1:107:A:PRO:N	1:107:A:PRO:CA	1:107:A:PRO:C	1:108:A:GLN:N	9	1.9
(1,118)	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	1:107:A:PRO:N	13	1.89
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	8	1.88
(1,118)	1:106:A:PRO:N	1:106:A:PRO:CA	1:106:A:PRO:C	1:107:A:PRO:N	10	1.86
(1,112)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:MET:N	10	1.86
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	5	1.84
(1,87)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	16	1.83
(1,89)	1:80:A:LEU:C	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	6	1.82
(1,17)	1:12:A:LYS:C	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	12	1.82
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	4	1.8
(1,27)	1:23:A:TYR:C	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	18	1.8
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	18	1.8
(1,26)	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	1:24:A:HIS:N	18	1.78
(1,1)	1:4:A:CYS:C	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	7	1.78
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	10	1.76
(1,84)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:PRO:N	3	1.75
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	9	1.75
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	10	1.75
(1,11)	1:9:A:ILE:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	8	1.75
(1,72)	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	1:67:A:MET:N	8	1.73
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	3	1.72
(1,78)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:GLU:N	12	1.72
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	14	1.72
(1,23)	1:21:A:LEU:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	5	1.7
(1,57)	1:46:A:LYS:C	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	11	1.68
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	13	1.67
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	5	1.67
(1,40)	1:35:A:GLN:N	1:35:A:GLN:CA	1:35:A:GLN:C	1:36:A:TYR:N	18	1.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,17)	1:12:A:LYS:C	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	20	1.65
(1,59)	1:53:A:GLU:C	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	17	1.64
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	19	1.64
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	8	1.63
(1,89)	1:80:A:LEU:C	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	19	1.62
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	5	1.62
(1,85)	1:78:A:PRO:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	16	1.6
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	12	1.6
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	7	1.6
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	19	1.59
(1,44)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:ASN:N	10	1.59
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	17	1.58
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	6	1.56
(1,86)	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	1:80:A:LEU:N	7	1.56
(1,95)	1:85:A:CYS:C	1:86:A:GLY:N	1:86:A:GLY:CA	1:86:A:GLY:C	20	1.55
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	20	1.55
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	11	1.55
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	18	1.55
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	8	1.54
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	14	1.52
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	4	1.52
(1,48)	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	1:43:A:ARG:N	7	1.51
(1,59)	1:53:A:GLU:C	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	16	1.5
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	5	1.49
(1,21)	1:20:A:ILE:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	5	1.48
(1,36)	1:30:A:THR:N	1:30:A:THR:CA	1:30:A:THR:C	1:31:A:ASN:N	3	1.45
(1,1)	1:4:A:CYS:C	1:5:A:LYS:N	1:5:A:LYS:CA	1:5:A:LYS:C	11	1.45
(1,47)	1:41:A:GLY:C	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	17	1.43
(1,101)	1:88:A:ARG:C	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	11	1.42
(1,93)	1:82:A:HIS:C	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	6	1.39
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	15	1.39
(1,69)	1:61:A:PHE:C	1:62:A:ARG:N	1:62:A:ARG:CA	1:62:A:ARG:C	9	1.39
(1,107)	1:91:A:LEU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	17	1.38
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	4	1.37
(1,71)	1:65:A:ILE:C	1:66:A:ASN:N	1:66:A:ASN:CA	1:66:A:ASN:C	8	1.37
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	4	1.37
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	2	1.36
(1,65)	1:58:A:ASN:C	1:59:A:CYS:N	1:59:A:CYS:CA	1:59:A:CYS:C	20	1.36
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	7	1.35
(1,100)	1:88:A:ARG:N	1:88:A:ARG:CA	1:88:A:ARG:C	1:89:A:TYR:N	16	1.35
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	3	1.35
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	11	1.35
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	17	1.33
(1,19)	1:19:A:ARG:C	1:20:A:ILE:N	1:20:A:ILE:CA	1:20:A:ILE:C	8	1.33
(1,84)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:PRO:N	10	1.32
(1,85)	1:78:A:PRO:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	3	1.31
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	2	1.3
(1,25)	1:22:A:GLN:C	1:23:A:TYR:N	1:23:A:TYR:CA	1:23:A:TYR:C	12	1.3
(1,21)	1:20:A:ILE:C	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1	1.3
(1,23)	1:21:A:LEU:C	1:22:A:GLN:N	1:22:A:GLN:CA	1:22:A:GLN:C	16	1.29
(1,87)	1:79:A:ASP:C	1:80:A:LEU:N	1:80:A:LEU:CA	1:80:A:LEU:C	3	1.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	9	1.27
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	18	1.26
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	16	1.26
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	14	1.25
(1,5)	1:6:A:GLU:C	1:7:A:ILE:N	1:7:A:ILE:CA	1:7:A:ILE:C	12	1.24
(1,126)	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	1:114:A:ARG:N	12	1.22
(1,113)	1:101:A:LYS:C	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	2	1.22
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	20	1.21
(1,44)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:ASN:N	20	1.21
(1,63)	1:57:A:TRP:C	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	18	1.2
(1,34)	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	1:28:A:GLY:N	8	1.2
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	2	1.2
(1,65)	1:58:A:ASN:C	1:59:A:CYS:N	1:59:A:CYS:CA	1:59:A:CYS:C	11	1.19
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	8	1.19
(1,10)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:VAL:N	9	1.19
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	13	1.18
(1,85)	1:78:A:PRO:C	1:79:A:ASP:N	1:79:A:ASP:CA	1:79:A:ASP:C	2	1.17
(1,68)	1:61:A:PHE:N	1:61:A:PHE:CA	1:61:A:PHE:C	1:62:A:ARG:N	14	1.17
(1,17)	1:12:A:LYS:C	1:13:A:ASN:N	1:13:A:ASN:CA	1:13:A:ASN:C	9	1.17
(1,112)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:MET:N	16	1.16
(1,77)	1:72:A:GLU:C	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	17	1.16
(1,11)	1:9:A:ILE:C	1:10:A:VAL:N	1:10:A:VAL:CA	1:10:A:VAL:C	10	1.15
(1,102)	1:89:A:TYR:N	1:89:A:TYR:CA	1:89:A:TYR:C	1:90:A:GLU:N	5	1.14
(1,84)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:PRO:N	17	1.14
(1,50)	1:43:A:ARG:N	1:43:A:ARG:CA	1:43:A:ARG:C	1:44:A:ILE:N	14	1.13
(1,111)	1:100:A:PHE:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	16	1.12
(1,63)	1:57:A:TRP:C	1:58:A:ASN:N	1:58:A:ASN:CA	1:58:A:ASN:C	3	1.12
(1,33)	1:26:A:ARG:C	1:27:A:SER:N	1:27:A:SER:CA	1:27:A:SER:C	7	1.12
(1,92)	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	1:83:A:PRO:N	18	1.11
(1,78)	1:73:A:VAL:N	1:73:A:VAL:CA	1:73:A:VAL:C	1:74:A:GLU:N	20	1.1
(1,125)	1:112:A:LYS:C	1:113:A:TRP:N	1:113:A:TRP:CA	1:113:A:TRP:C	2	1.09
(1,58)	1:47:A:PHE:N	1:47:A:PHE:CA	1:47:A:PHE:C	1:48:A:LYS:N	14	1.07
(1,31)	1:25:A:CYS:C	1:26:A:ARG:N	1:26:A:ARG:CA	1:26:A:ARG:C	9	1.07
(1,91)	1:81:A:LYS:C	1:82:A:HIS:N	1:82:A:HIS:CA	1:82:A:HIS:C	3	1.06
(1,48)	1:42:A:THR:N	1:42:A:THR:CA	1:42:A:THR:C	1:43:A:ARG:N	3	1.06
(1,28)	1:24:A:HIS:N	1:24:A:HIS:CA	1:24:A:HIS:C	1:25:A:CYS:N	13	1.04
(1,89)	1:80:A:LEU:C	1:81:A:LYS:N	1:81:A:LYS:CA	1:81:A:LYS:C	4	1.03
(1,22)	1:21:A:LEU:N	1:21:A:LEU:CA	1:21:A:LEU:C	1:22:A:GLN:N	2	1.03
(1,60)	1:54:A:ARG:N	1:54:A:ARG:CA	1:54:A:ARG:C	1:55:A:SER:N	10	1.02
(1,38)	1:31:A:ASN:N	1:31:A:ASN:CA	1:31:A:ASN:C	1:32:A:VAL:N	17	1.02
(1,114)	1:102:A:MET:N	1:102:A:MET:CA	1:102:A:MET:C	1:103:A:ASP:N	17	1.01
(1,122)	1:108:A:GLN:N	1:108:A:GLN:CA	1:108:A:GLN:C	1:109:A:PRO:N	12	1.0
(1,94)	1:83:A:PRO:N	1:83:A:PRO:CA	1:83:A:PRO:C	1:84:A:LEU:N	2	1.0