



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 02:11 PM UTC

PDB ID : 2MF2 / pdb_00002mf2
BMRB ID : 17288
Title : Structural and biophysical characterization of the mRNA interferase SaMazF from *Staphylococcus aureus*.
Authors : Zorzini, V.; Cheung, A.; Loris, R.; van Nuland, N.A.J.
Deposited on : 2013-10-03

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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

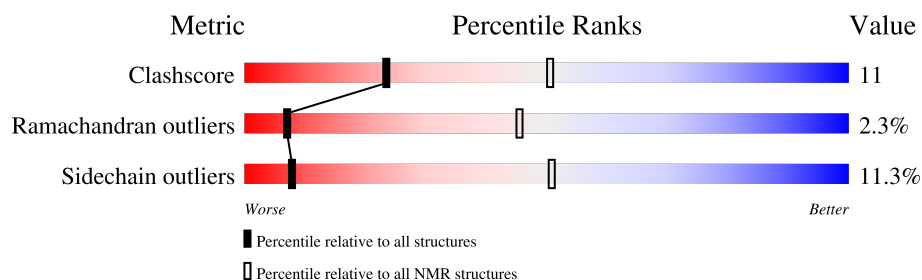
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 46%.

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	132	
1	B	132	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:14-A:60, A:67-A:125, B:14-B:60, B:67-B:125 (212)	0.83	1

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4238 atoms, of which 2156 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called mRNA interferase MazF.

Mol	Chain	Residues	Atoms						Trace
1	A	132	Total	C	H	N	O	S	0
			2119	650	1078	193	196	2	
1	B	132	Total	C	H	N	O	S	0
			2119	650	1078	193	196	2	

There are 26 discrepancies between the modelled and reference sequences:

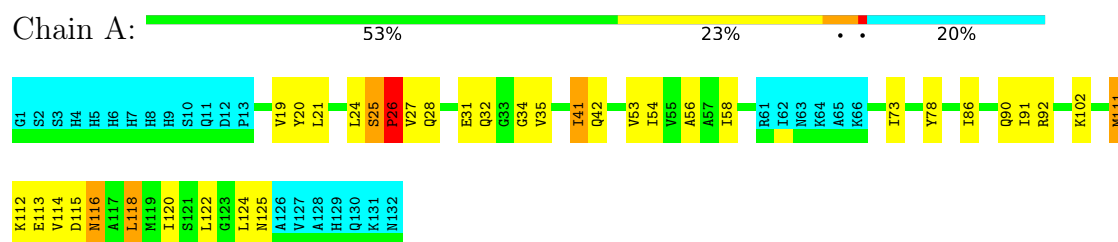
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q7A0D7
A	2	SER	-	expression tag	UNP Q7A0D7
A	3	SER	-	expression tag	UNP Q7A0D7
A	4	HIS	-	expression tag	UNP Q7A0D7
A	5	HIS	-	expression tag	UNP Q7A0D7
A	6	HIS	-	expression tag	UNP Q7A0D7
A	7	HIS	-	expression tag	UNP Q7A0D7
A	8	HIS	-	expression tag	UNP Q7A0D7
A	9	HIS	-	expression tag	UNP Q7A0D7
A	10	SER	-	expression tag	UNP Q7A0D7
A	11	GLN	-	expression tag	UNP Q7A0D7
A	12	ASP	-	expression tag	UNP Q7A0D7
A	13	PRO	-	expression tag	UNP Q7A0D7
B	1	GLY	-	expression tag	UNP Q7A0D7
B	2	SER	-	expression tag	UNP Q7A0D7
B	3	SER	-	expression tag	UNP Q7A0D7
B	4	HIS	-	expression tag	UNP Q7A0D7
B	5	HIS	-	expression tag	UNP Q7A0D7
B	6	HIS	-	expression tag	UNP Q7A0D7
B	7	HIS	-	expression tag	UNP Q7A0D7
B	8	HIS	-	expression tag	UNP Q7A0D7
B	9	HIS	-	expression tag	UNP Q7A0D7
B	10	SER	-	expression tag	UNP Q7A0D7
B	11	GLN	-	expression tag	UNP Q7A0D7
B	12	ASP	-	expression tag	UNP Q7A0D7
B	13	PRO	-	expression tag	UNP Q7A0D7

4 Residue-property plots [i](#)

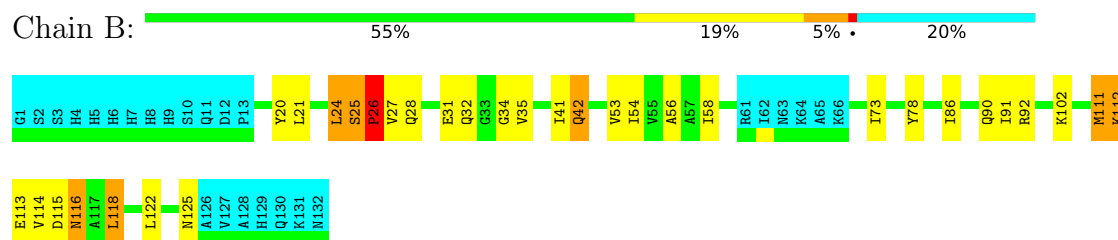
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: mRNA interferase MazF



- Molecule 1: mRNA interferase MazF

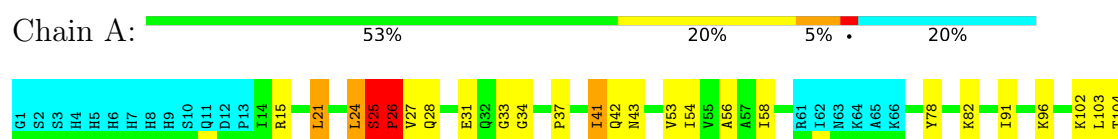


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

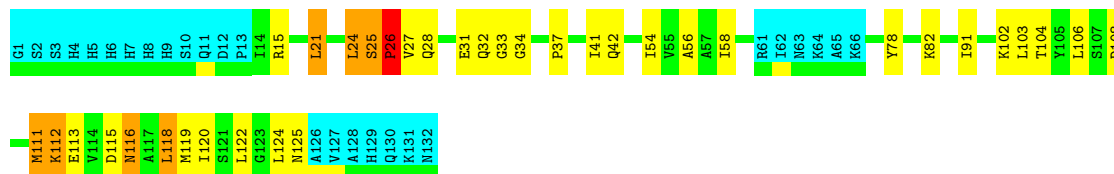
- Molecule 1: mRNA interferase MazF





- Molecule 1: mRNA interferase MazF

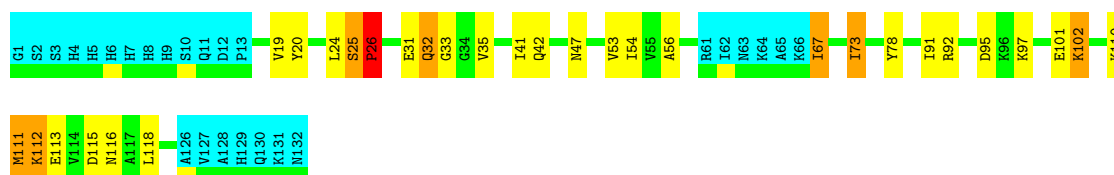
Chain B: 53% 21% 5% • 20%



4.2.2 Score per residue for model 2

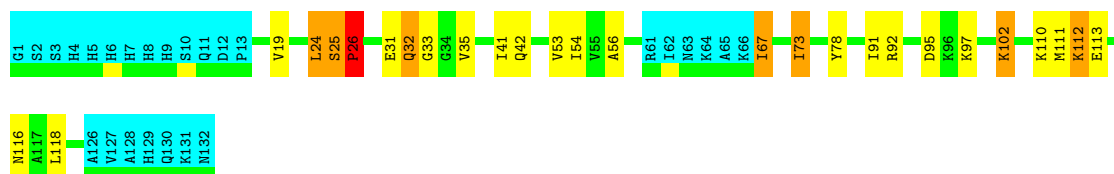
- Molecule 1: mRNA interferase MazF

Chain A: 57% 17% 5% • 20%



- Molecule 1: mRNA interferase MazF

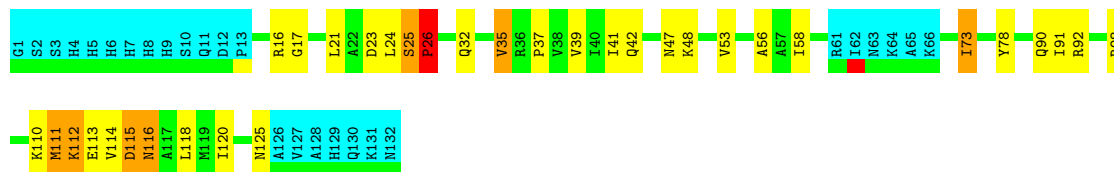
Chain B: 60% 14% 5% • 20%



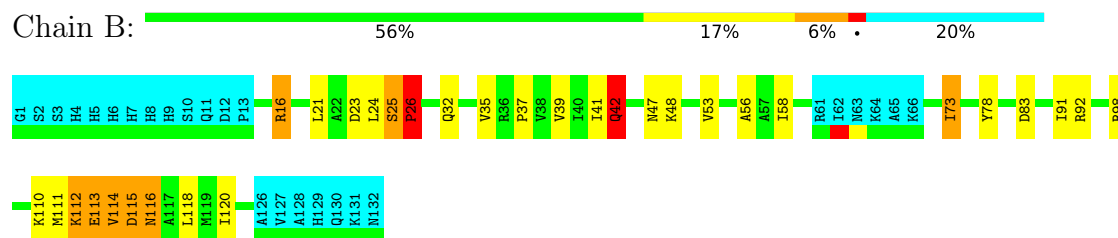
4.2.3 Score per residue for model 3

- Molecule 1: mRNA interferase MazF

Chain A: 55% 20% 5% • 20%

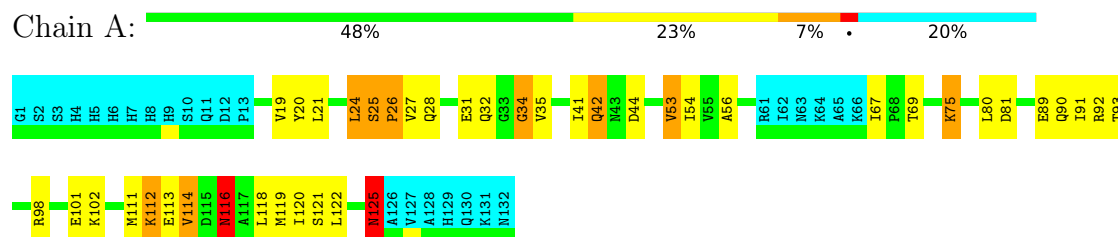


- Molecule 1: mRNA interferase MazF

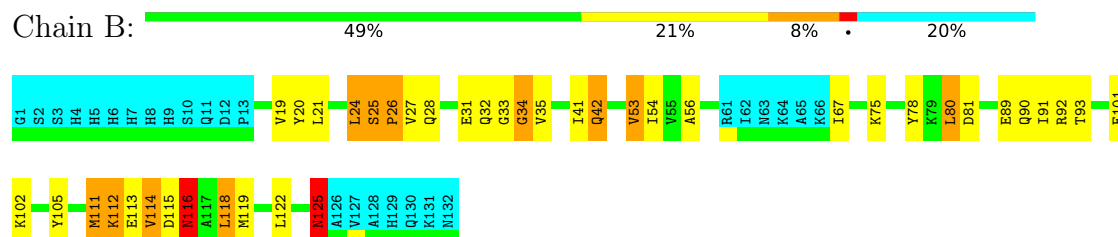


4.2.4 Score per residue for model 4

- Molecule 1: mRNA interferase MazF

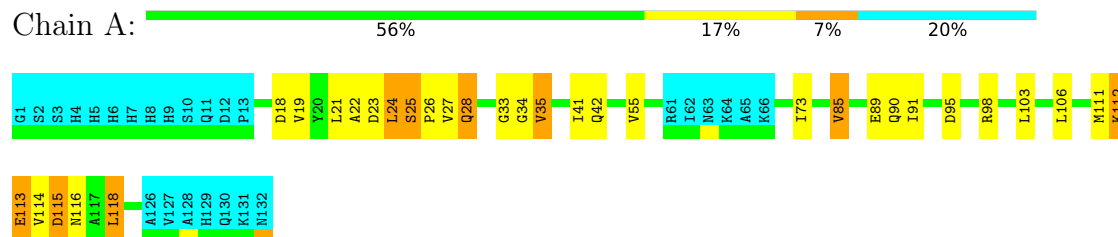


- Molecule 1: mRNA interferase MazF



4.2.5 Score per residue for model 5

- Molecule 1: mRNA interferase MazF



- Molecule 1: mRNA interferase MazF

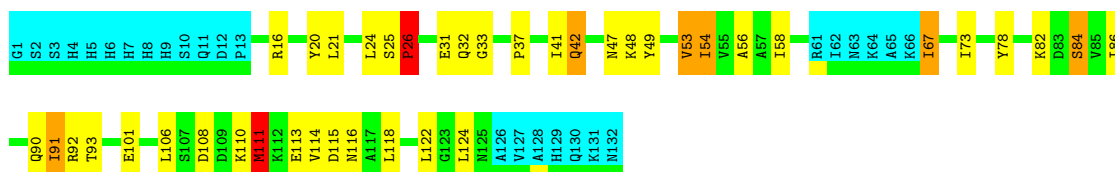




4.2.6 Score per residue for model 6

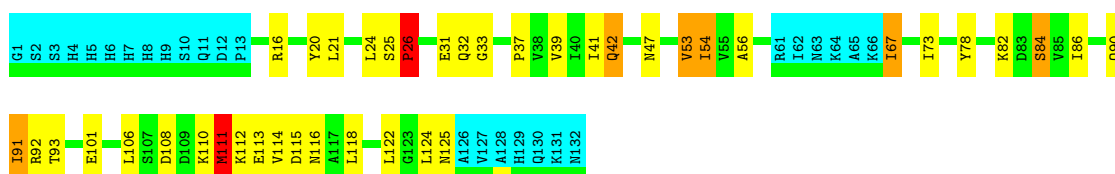
- Molecule 1: mRNA interferase MazF

Chain A: 49% 25% 5% • 20%



- Molecule 1: mRNA interferase MazF

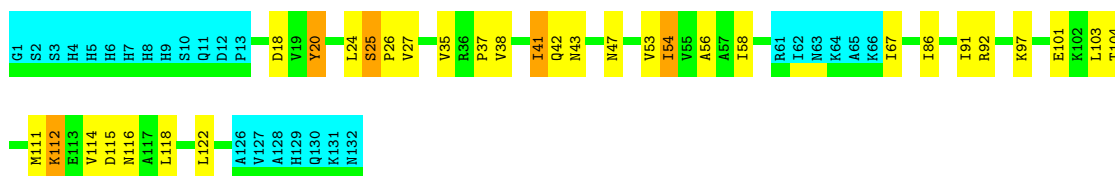
Chain B: 49% 25% 5% • 20%



4.2.7 Score per residue for model 7

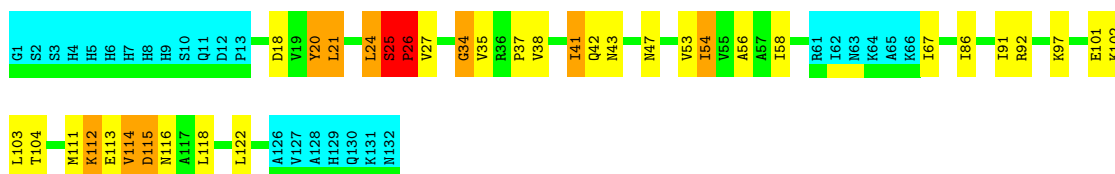
- Molecule 1: mRNA interferase MazF

Chain A: 56% 20% • 20%



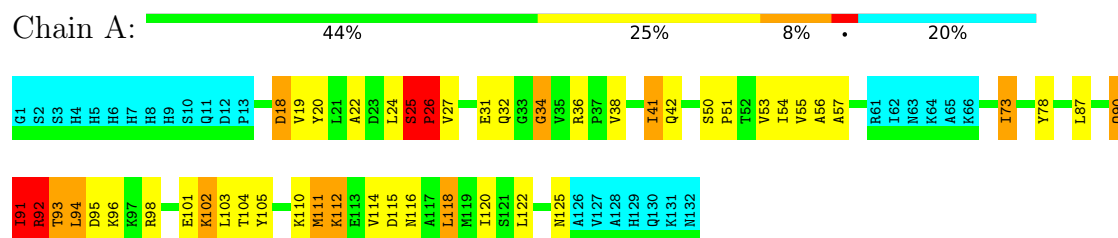
- Molecule 1: mRNA interferase MazF

Chain B: 53% 19% 7% • 20%

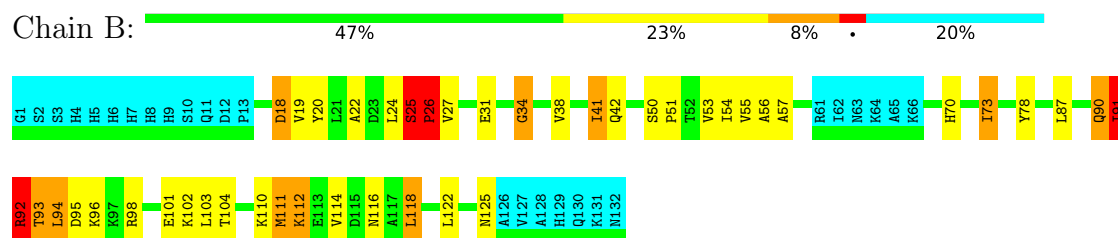


4.2.8 Score per residue for model 8

- Molecule 1: mRNA interferase MazF

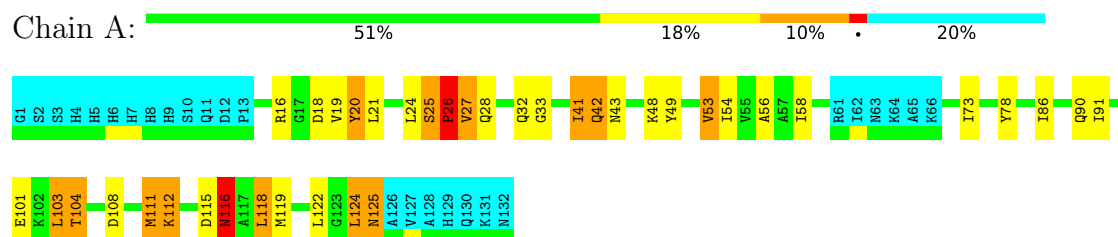


- Molecule 1: mRNA interferase MazF

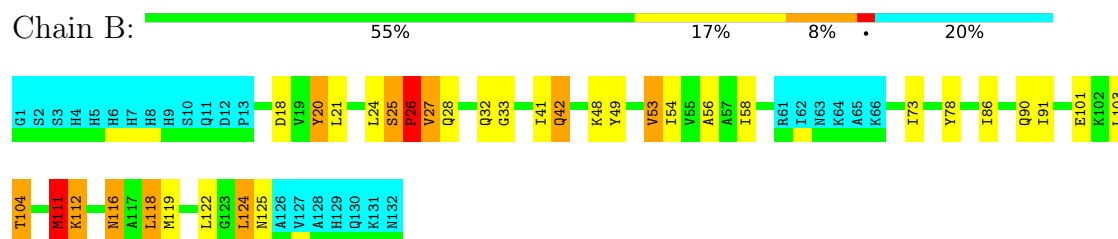


4.2.9 Score per residue for model 9

- Molecule 1: mRNA interferase MazF



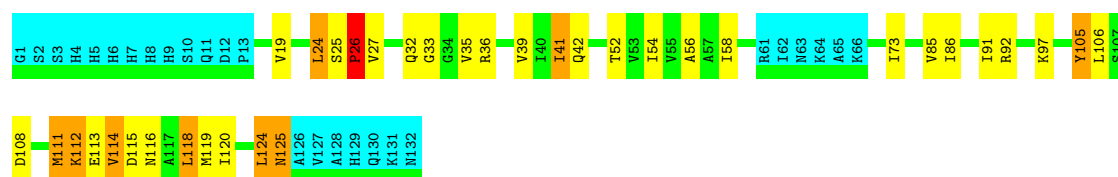
- Molecule 1: mRNA interferase MazF



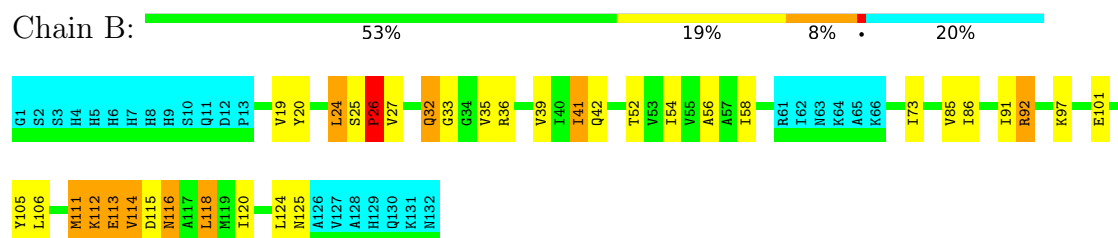
4.2.10 Score per residue for model 10

- Molecule 1: mRNA interferase MazF



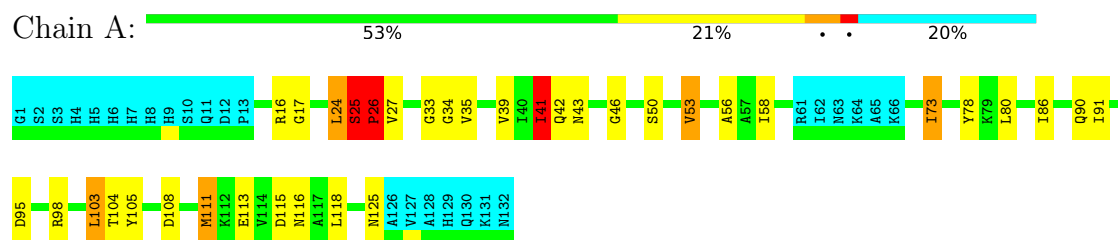


- Molecule 1: mRNA interferase MazF

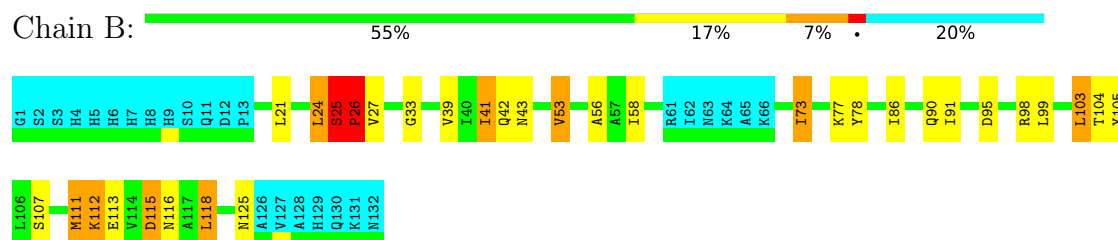


4.2.11 Score per residue for model 11

- Molecule 1: mRNA interferase MazF

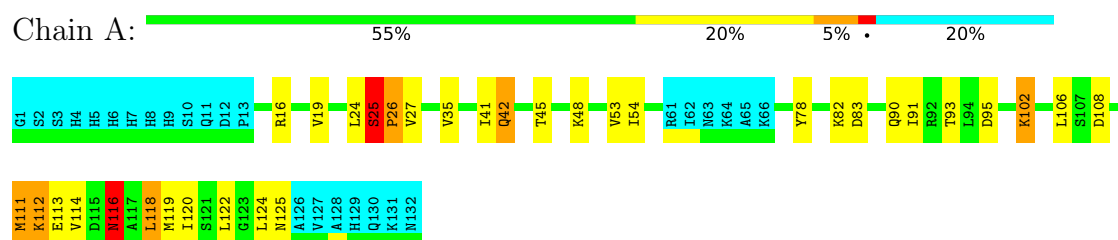


- Molecule 1: mRNA interferase MazF

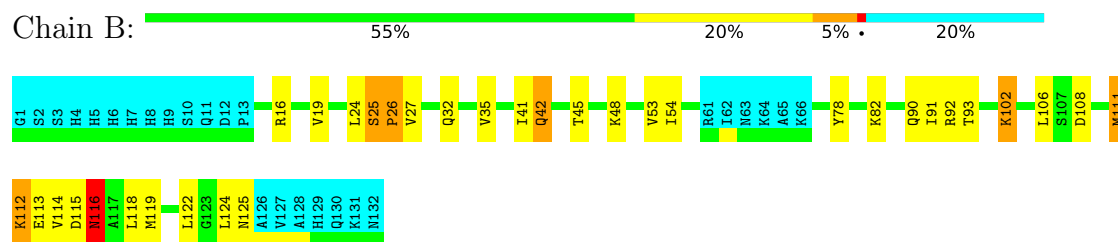


4.2.12 Score per residue for model 12

- Molecule 1: mRNA interferase MazF

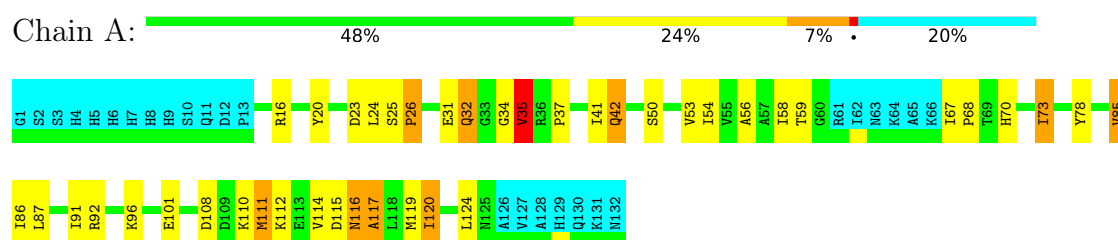


- Molecule 1: mRNA interferase MazF

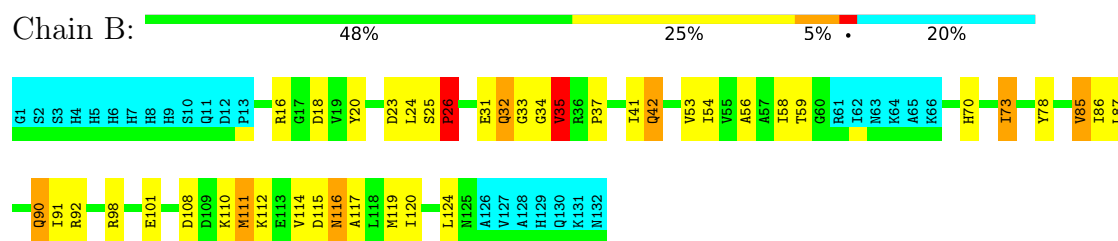


4.2.13 Score per residue for model 13

- Molecule 1: mRNA interferase MazF

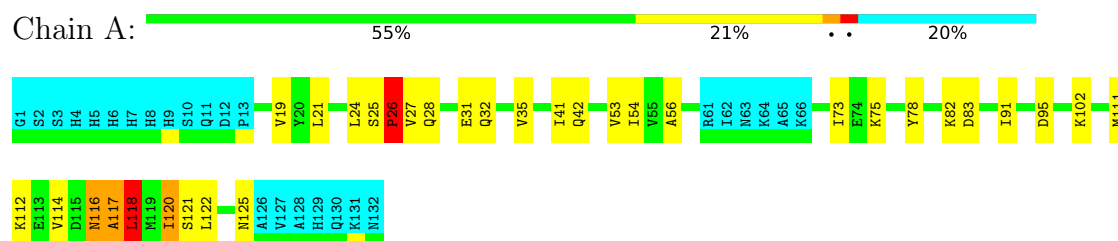


- Molecule 1: mRNA interferase MazF



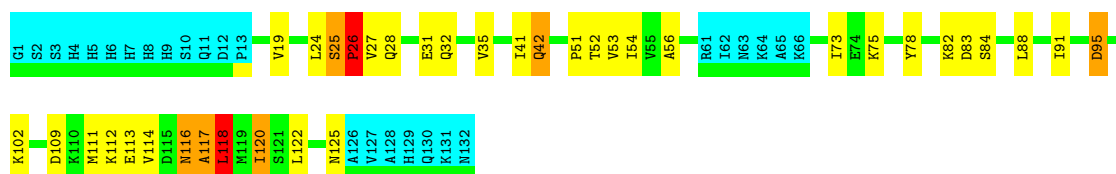
4.2.14 Score per residue for model 14

- Molecule 1: mRNA interferase MazF



- Molecule 1: mRNA interferase MazF

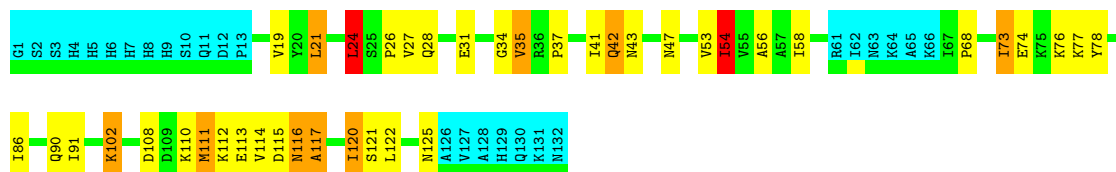




4.2.15 Score per residue for model 15

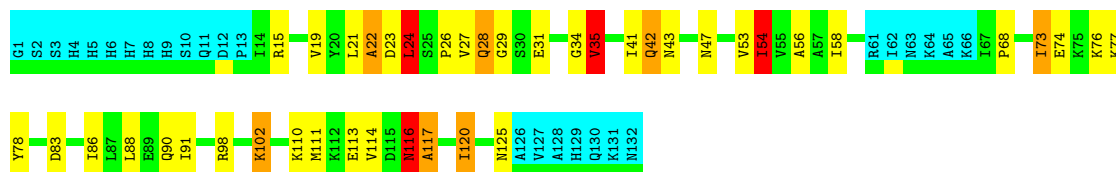
- Molecule 1: mRNA interferase MazF

Chain A: 49% 23% 7% 20%



- Molecule 1: mRNA interferase MazF

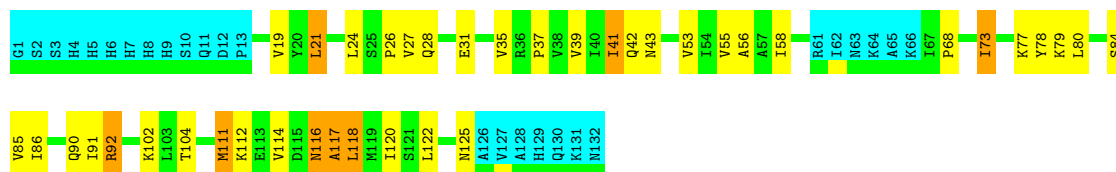
Chain B: 48% 23% 5% 20%



4.2.16 Score per residue for model 16

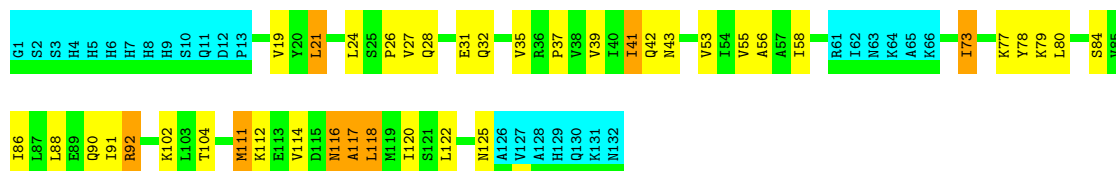
- Molecule 1: mRNA interferase MazF

Chain A: 50% 24% 6% 20%



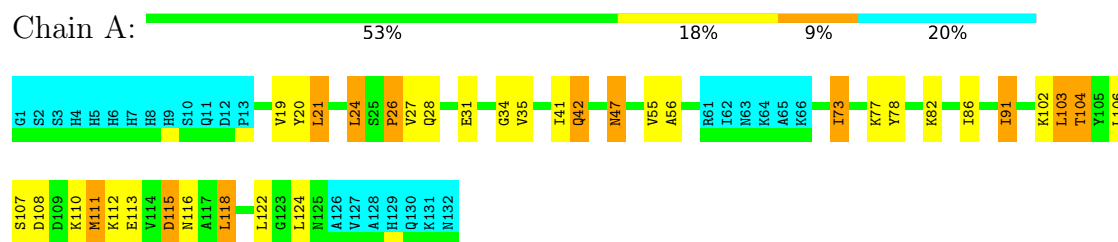
- Molecule 1: mRNA interferase MazF

Chain B: 50% 24% 6% 20%

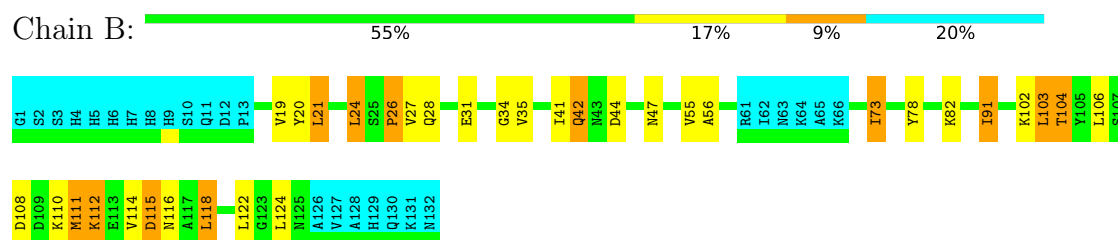


4.2.17 Score per residue for model 17

- Molecule 1: mRNA interferase MazF

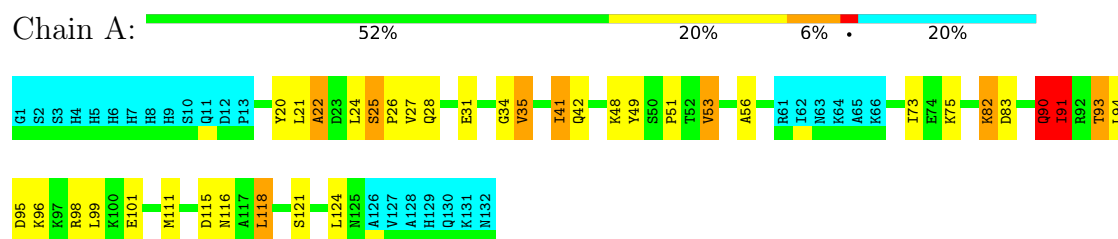


- Molecule 1: mRNA interferase MazF

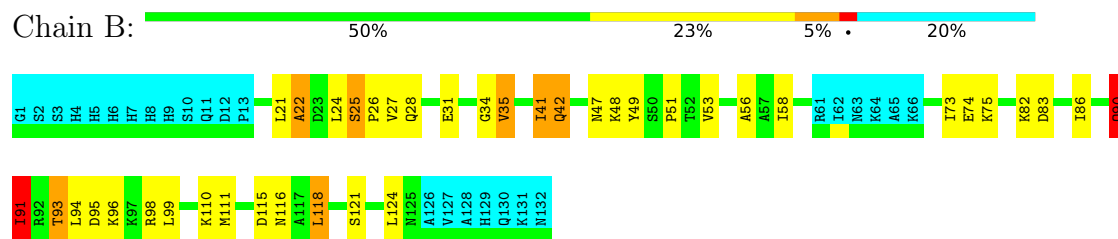


4.2.18 Score per residue for model 18

- Molecule 1: mRNA interferase MazF



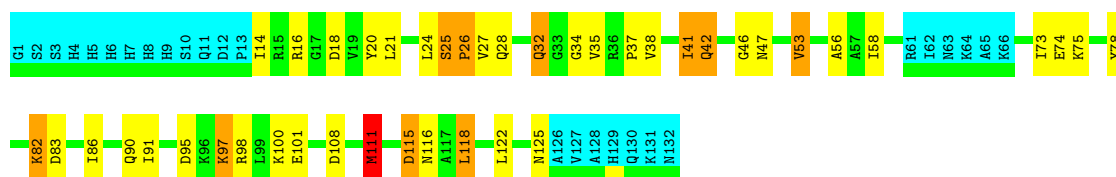
- Molecule 1: mRNA interferase MazF



4.2.19 Score per residue for model 19

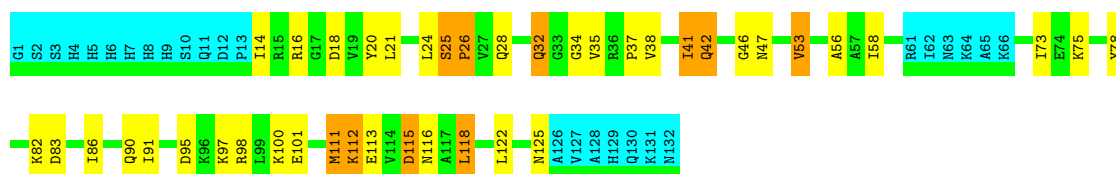
- Molecule 1: mRNA interferase MazF





• Molecule 1: mRNA interferase MazF

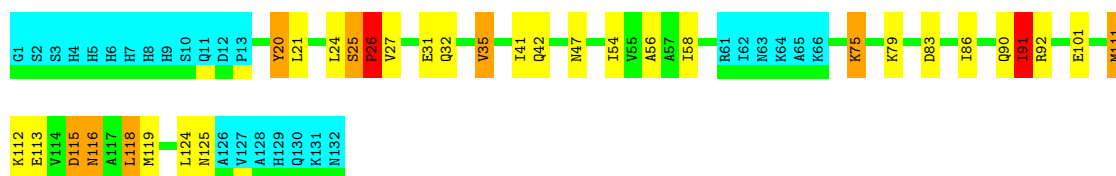
Chain B: 48% 24% 8% 20%



4.2.20 Score per residue for model 20

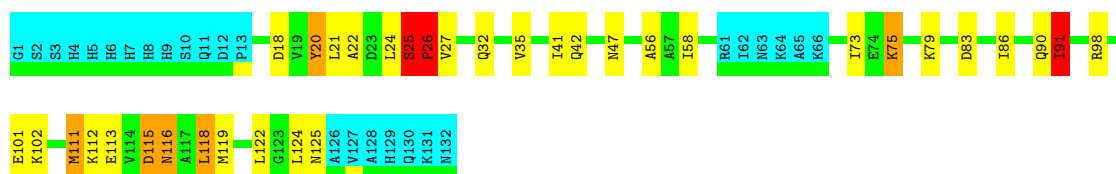
• Molecule 1: mRNA interferase MazF

Chain A: 56% 17% 6% 20%



• Molecule 1: mRNA interferase MazF

Chain B: 54% 20% 5% 20%



5 Refinement protocol and experimental data overview

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

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
RECOORD, CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1520
Number of shifts mapped to atoms	1520
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	46%

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	1.52±0.06	7±3/840 (0.9± 0.3%)	1.30±0.05	4±2/1133 (0.3± 0.2%)
1	B	1.52±0.06	8±2/840 (1.0± 0.3%)	1.29±0.06	4±2/1133 (0.4± 0.2%)
All	All	1.52	311/33600 (0.9%)	1.30	164/45320 (0.4%)

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	0.3±0.6
1	B	0.0±0.0	0.2±0.5
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	116	ASN	C-N	-10.07	1.20	1.33	15	4
1	A	117	ALA	N-CA	-9.94	1.34	1.46	15	4
1	A	116	ASN	N-CA	8.57	1.57	1.46	13	2
1	B	91	ILE	CA-C	-8.53	1.42	1.52	8	2
1	B	118	LEU	N-CA	-8.42	1.36	1.46	8	16
1	A	91	ILE	CA-C	-8.33	1.42	1.52	8	2
1	A	118	LEU	N-CA	-8.08	1.36	1.46	8	15
1	B	116	ASN	CA-CB	-8.07	1.40	1.53	17	9
1	A	125	ASN	N-CA	-7.68	1.36	1.47	4	1
1	B	112	LYS	N-CA	-7.51	1.37	1.46	9	9
1	B	117	ALA	N-CA	-7.50	1.37	1.46	16	4
1	B	113	GLU	CA-C	-7.48	1.43	1.53	5	9
1	B	116	ASN	C-N	-7.45	1.23	1.33	16	4
1	B	125	ASN	N-CA	-7.39	1.37	1.47	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	24	LEU	C-N	-7.33	1.22	1.33	10	3
1	A	116	ASN	CA-C	-7.29	1.42	1.52	13	4
1	A	113	GLU	CA-C	-7.29	1.43	1.53	5	7
1	A	113	GLU	C-O	-7.05	1.15	1.23	5	4
1	B	113	GLU	N-CA	-6.99	1.37	1.46	3	8
1	B	33	GLY	C-N	-6.96	1.25	1.33	1	2
1	A	112	LYS	N-CA	-6.88	1.38	1.46	8	3
1	B	35	VAL	C-N	-6.84	1.25	1.33	19	12
1	A	15	ARG	N-CA	-6.66	1.37	1.46	1	1
1	A	114	VAL	N-CA	-6.63	1.38	1.46	4	3
1	B	15	ARG	N-CA	-6.62	1.38	1.45	1	1
1	B	111	MET	C-N	-6.50	1.25	1.33	5	3
1	A	35	VAL	C-N	-6.50	1.25	1.33	19	14
1	A	111	MET	C-N	-6.49	1.25	1.33	5	1
1	B	34	GLY	C-N	-6.46	1.27	1.33	15	5
1	B	114	VAL	N-CA	-6.42	1.39	1.46	4	5
1	B	24	LEU	N-CA	-6.35	1.38	1.46	15	2
1	B	90	GLN	C-O	-6.31	1.16	1.24	18	1
1	A	34	GLY	C-N	-6.26	1.26	1.33	17	5
1	B	41	ILE	CA-CB	6.25	1.61	1.54	8	4
1	A	100	LYS	N-CA	-6.23	1.39	1.47	19	1
1	A	41	ILE	CA-CB	6.20	1.61	1.54	8	6
1	A	33	GLY	CA-C	-6.15	1.48	1.52	2	1
1	B	18	ASP	C-N	-6.15	1.25	1.33	9	7
1	A	25	SER	CA-C	6.15	1.60	1.52	1	3
1	A	90	GLN	C-O	-6.15	1.16	1.24	18	1
1	B	25	SER	CA-C	6.12	1.60	1.52	1	3
1	A	103	LEU	CA-C	-6.10	1.47	1.52	17	2
1	B	21	LEU	C-N	-6.07	1.25	1.33	5	10
1	B	111	MET	CA-C	-5.96	1.45	1.52	6	3
1	A	18	ASP	C-N	-5.96	1.25	1.33	9	5
1	A	24	LEU	N-CA	-5.92	1.38	1.46	5	2
1	B	33	GLY	N-CA	-5.92	1.39	1.45	1	1
1	B	115	ASP	C-N	-5.89	1.25	1.33	1	6
1	B	54	ILE	CA-CB	5.85	1.60	1.54	15	1
1	B	116	ASN	CG-ND2	-5.82	1.21	1.33	9	2
1	A	113	GLU	N-CA	-5.81	1.39	1.46	2	5
1	A	21	LEU	C-N	-5.80	1.25	1.33	5	9
1	B	22	ALA	CA-C	-5.80	1.45	1.52	18	2
1	B	112	LYS	C-N	-5.79	1.26	1.33	2	4
1	A	103	LEU	C-N	-5.77	1.28	1.33	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	113	GLU	C-O	-5.75	1.16	1.23	5	1
1	A	24	LEU	C-N	-5.71	1.21	1.33	10	3
1	B	100	LYS	N-CA	-5.70	1.40	1.47	19	1
1	A	115	ASP	C-N	-5.69	1.25	1.33	1	7
1	A	33	GLY	C-N	-5.68	1.27	1.33	1	1
1	B	20	TYR	CA-C	-5.68	1.46	1.52	17	4
1	A	54	ILE	CA-CB	5.67	1.60	1.54	15	1
1	B	112	LYS	CA-C	-5.66	1.45	1.52	8	4
1	B	103	LEU	CA-C	-5.65	1.48	1.52	17	2
1	A	20	TYR	CA-C	-5.60	1.45	1.52	9	4
1	B	33	GLY	CA-C	-5.59	1.47	1.52	13	1
1	A	91	ILE	N-CA	5.56	1.53	1.46	18	1
1	A	21	LEU	N-CA	-5.51	1.38	1.45	9	1
1	B	91	ILE	CA-CB	-5.51	1.47	1.55	8	1
1	B	103	LEU	C-N	-5.51	1.28	1.33	11	1
1	B	91	ILE	N-CA	5.50	1.53	1.46	18	1
1	A	116	ASN	CA-CB	-5.49	1.44	1.53	17	1
1	B	113	GLU	CA-CB	-5.47	1.44	1.53	3	1
1	A	22	ALA	CA-C	-5.46	1.45	1.52	18	1
1	A	91	ILE	CA-CB	-5.42	1.47	1.55	8	1
1	A	93	THR	N-CA	5.41	1.53	1.46	8	1
1	B	93	THR	N-CA	5.40	1.53	1.46	8	1
1	A	75	LYS	C-N	-5.37	1.27	1.33	4	1
1	A	111	MET	CA-C	-5.34	1.45	1.52	19	2
1	A	25	SER	N-CA	-5.33	1.40	1.46	5	1
1	A	85	VAL	C-N	-5.30	1.25	1.33	10	2
1	A	80	LEU	C-N	-5.25	1.26	1.33	11	1
1	A	112	LYS	C-N	-5.23	1.27	1.33	17	2
1	A	25	SER	CA-CB	-5.22	1.46	1.53	5	1
1	A	20	TYR	C-N	-5.19	1.26	1.33	9	1
1	A	104	THR	N-CA	-5.15	1.38	1.46	9	1
1	A	43	ASN	C-N	-5.12	1.26	1.34	9	1
1	B	86	ILE	CA-CB	5.11	1.60	1.54	5	1
1	B	25	SER	CA-CB	-5.11	1.46	1.53	5	1
1	B	99	LEU	C-N	-5.10	1.27	1.33	11	1
1	A	19	VAL	C-N	-5.10	1.25	1.33	9	1
1	B	98	ARG	N-CA	-5.10	1.39	1.46	13	1
1	A	86	ILE	CA-CB	5.09	1.60	1.54	17	1
1	B	23	ASP	C-N	-5.08	1.26	1.33	5	1
1	B	21	LEU	N-CA	-5.08	1.39	1.45	9	1
1	B	85	VAL	C-N	-5.08	1.25	1.33	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	35	VAL	N-CA	-5.08	1.40	1.46	11	1
1	B	104	THR	N-CA	-5.07	1.38	1.46	9	1
1	B	116	ASN	N-CA	-5.06	1.40	1.46	6	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	B	116	ASN	CA-CB-CG	12.01	124.61	112.60	8	16
1	A	116	ASN	CA-CB-CG	10.36	122.96	112.60	8	15
1	B	116	ASN	CB-CA-C	-8.76	97.12	110.88	8	2
1	B	116	ASN	N-CA-CB	-8.36	97.76	110.13	1	9
1	A	116	ASN	CB-CA-C	-8.04	98.25	110.88	8	1
1	B	115	ASP	CA-CB-CG	7.93	120.53	112.60	3	5
1	B	80	LEU	CB-CA-C	-7.43	108.01	116.63	4	1
1	B	43	ASN	CA-CB-CG	7.16	119.75	112.60	15	1
1	A	117	ALA	N-CA-C	-7.09	103.24	112.68	13	1
1	A	125	ASN	CA-CB-CG	7.01	119.61	112.60	4	2
1	B	125	ASN	CA-CB-CG	6.98	119.58	112.60	4	1
1	B	33	GLY	N-CA-C	6.90	120.33	110.46	9	1
1	A	33	GLY	CA-C-N	6.75	129.86	121.83	9	2
1	A	33	GLY	C-N-CA	6.75	129.86	121.83	9	2
1	A	33	GLY	N-CA-C	6.74	120.09	110.46	9	1
1	B	25	SER	CA-C-N	6.63	128.13	119.84	2	4
1	B	25	SER	C-N-CA	6.63	128.13	119.84	2	4
1	A	25	SER	CA-C-N	6.50	127.97	119.84	2	4
1	A	25	SER	C-N-CA	6.50	127.97	119.84	2	4
1	B	33	GLY	CA-C-N	6.47	129.53	121.83	9	2
1	B	33	GLY	C-N-CA	6.47	129.53	121.83	9	2
1	A	116	ASN	N-CA-CB	-6.46	100.58	110.13	1	8
1	B	24	LEU	N-CA-C	-6.41	105.75	112.93	7	2
1	B	26	PRO	CA-N-CD	-6.22	103.29	112.00	11	10
1	A	115	ASP	CA-CB-CG	6.19	118.79	112.60	3	7
1	B	25	SER	N-CA-C	6.16	122.23	109.11	5	1
1	A	79	LYS	N-CA-C	6.14	119.82	111.17	20	1
1	B	79	LYS	N-CA-C	6.14	119.82	111.17	20	1
1	A	43	ASN	CA-CB-CG	6.13	118.73	112.60	15	1
1	A	26	PRO	CA-N-CD	-6.12	103.44	112.00	11	8
1	A	117	ALA	N-CA-CB	-6.08	100.77	110.19	16	1
1	A	103	LEU	CB-CA-C	-6.00	100.26	110.88	8	1
1	B	34	GLY	N-CA-C	-5.99	102.66	110.45	4	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	115	ASP	CB-CA-C	-5.98	101.75	110.96	3	2
1	A	25	SER	N-CA-C	5.96	121.81	109.11	5	1
1	B	112	LYS	CB-CA-C	-5.94	100.58	110.68	4	1
1	B	25	SER	CB-CA-C	5.89	121.78	110.17	7	1
1	A	95	ASP	CA-CB-CG	5.87	118.47	112.60	14	1
1	A	125	ASN	CB-CA-C	5.87	119.92	111.82	4	1
1	B	125	ASN	CB-CA-C	5.81	119.84	111.82	4	1
1	B	103	LEU	CB-CA-C	-5.77	100.67	110.88	8	1
1	A	42	GLN	N-CA-C	5.76	117.76	110.33	8	2
1	B	95	ASP	CA-CB-CG	5.67	118.27	112.60	14	1
1	B	42	GLN	N-CA-C	5.67	117.64	110.33	8	3
1	A	34	GLY	N-CA-C	-5.62	101.97	111.08	1	3
1	B	32	GLN	CB-CG-CD	5.46	121.88	112.60	19	1
1	A	113	GLU	N-CA-C	-5.42	104.92	112.45	15	1
1	B	116	ASN	CB-CG-ND2	-5.41	108.28	116.40	1	4
1	A	120	ILE	CB-CA-C	-5.37	105.10	111.97	8	1
1	A	112	LYS	CB-CA-C	-5.33	101.62	110.68	4	1
1	B	113	GLU	N-CA-C	-5.28	105.11	112.45	15	1
1	B	67	ILE	N-CA-C	5.26	120.24	108.88	6	1
1	A	24	LEU	N-CA-CB	-5.26	101.66	110.39	1	1
1	A	92	ARG	N-CA-C	5.23	121.93	110.80	8	1
1	B	92	ARG	N-CA-C	5.22	121.93	110.80	8	1
1	A	121	SER	N-CA-CB	-5.22	102.44	110.01	15	1
1	A	24	LEU	N-CA-C	-5.21	106.92	113.28	11	1
1	B	24	LEU	N-CA-CB	-5.18	101.80	110.39	1	1
1	A	47	ASN	CA-CB-CG	5.17	117.77	112.60	17	1
1	B	104	THR	N-CA-CB	-5.16	103.07	111.22	8	1
1	A	67	ILE	N-CA-C	5.16	120.02	108.88	6	1
1	A	105	TYR	CA-C-N	5.14	131.36	121.54	10	1
1	A	105	TYR	C-N-CA	5.14	131.36	121.54	10	1
1	A	67	ILE	N-CA-CB	5.09	118.34	111.21	6	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	16	ARG	Sidechain	2
1	A	92	ARG	Sidechain	2
1	B	92	ARG	Sidechain	2
1	A	25	SER	Peptide	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	16	ARG	Sidechain	1
1	B	25	SER	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	831	883	883	20±6
1	B	831	883	883	20±6
All	All	33240	35320	35320	755

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:ILE:HG21	1:A:78:TYR:CE1	0.78	2.14	9	9
1:A:92:ARG:HB3	1:B:92:ARG:HB3	0.78	1.56	8	1
1:B:73:ILE:HG21	1:B:78:TYR:CE1	0.76	2.15	9	9
1:A:24:LEU:O	1:A:27:VAL:HG13	0.70	1.86	7	10
1:B:119:MET:SD	1:B:125:ASN:HA	0.68	2.28	20	3
1:A:90:GLN:HB3	1:A:91:ILE:HD13	0.67	1.66	8	1
1:A:119:MET:SD	1:A:125:ASN:HA	0.66	2.30	20	3
1:B:24:LEU:O	1:B:27:VAL:HG13	0.66	1.90	7	9
1:B:90:GLN:HB3	1:B:91:ILE:HD13	0.65	1.67	8	1
1:B:112:LYS:HE3	1:B:113:GLU:N	0.64	2.07	5	1
1:A:42:GLN:HG3	1:A:54:ILE:HG22	0.64	1.69	6	4
1:A:112:LYS:O	1:A:116:ASN:HB3	0.64	1.92	9	5
1:A:91:ILE:O	1:A:92:ARG:HG3	0.64	1.92	8	1
1:B:91:ILE:O	1:B:92:ARG:HG3	0.64	1.92	8	1
1:B:116:ASN:O	1:B:120:ILE:HD13	0.63	1.93	13	4
1:A:112:LYS:HE3	1:A:113:GLU:N	0.62	2.09	5	1
1:B:112:LYS:O	1:B:116:ASN:HB3	0.62	1.94	4	3
1:B:42:GLN:HG3	1:B:54:ILE:HG22	0.62	1.69	6	5
1:A:55:VAL:O	1:A:91:ILE:HB	0.62	1.94	17	3
1:A:92:ARG:HB3	1:B:92:ARG:CB	0.62	2.24	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:54:ILE:HA	1:B:92:ARG:O	0.62	1.94	8	1
1:B:118:LEU:O	1:B:122:LEU:HG	0.62	1.94	14	8
1:A:54:ILE:HA	1:A:92:ARG:O	0.62	1.94	8	1
1:A:92:ARG:CB	1:B:92:ARG:HB3	0.62	2.25	8	1
1:B:55:VAL:O	1:B:91:ILE:HB	0.61	1.95	17	3
1:A:124:LEU:HD11	1:B:124:LEU:HD11	0.61	1.73	1	2
1:A:112:LYS:N	1:A:112:LYS:HE2	0.61	2.11	9	6
1:B:112:LYS:HE2	1:B:112:LYS:N	0.61	2.11	3	6
1:A:73:ILE:HG23	1:A:110:LYS:HG2	0.61	1.72	3	1
1:A:93:THR:OG1	1:B:92:ARG:HB2	0.61	1.95	8	1
1:A:92:ARG:HB2	1:B:93:THR:OG1	0.61	1.96	8	1
1:A:116:ASN:O	1:A:120:ILE:HD13	0.61	1.94	13	4
1:A:54:ILE:HG21	1:B:122:LEU:HG	0.61	1.72	6	1
1:B:56:ALA:HA	1:B:91:ILE:HG13	0.60	1.73	8	1
1:B:103:LEU:HG	1:B:104:THR:OG1	0.60	1.96	1	4
1:A:122:LEU:HG	1:B:54:ILE:HG21	0.60	1.73	6	2
1:A:56:ALA:HA	1:A:91:ILE:HG13	0.60	1.73	8	1
1:A:118:LEU:O	1:A:122:LEU:HG	0.60	1.97	14	9
1:A:103:LEU:HG	1:A:104:THR:OG1	0.59	1.97	1	5
1:A:28:GLN:HE21	1:A:28:GLN:N	0.58	1.96	5	1
1:A:112:LYS:NZ	1:A:113:GLU:HG3	0.58	2.13	5	1
1:B:104:THR:HG22	1:B:105:TYR:H	0.58	1.59	11	1
1:A:54:ILE:HG21	1:B:122:LEU:HD22	0.58	1.76	14	5
1:A:51:PRO:O	1:A:95:ASP:HA	0.58	1.98	18	2
1:B:51:PRO:O	1:B:95:ASP:HA	0.57	1.99	18	3
1:A:112:LYS:HA	1:A:115:ASP:OD2	0.57	1.99	3	1
1:A:27:VAL:HB	1:A:31:GLU:HB2	0.57	1.75	1	9
1:A:104:THR:HG22	1:A:105:TYR:H	0.57	1.58	11	1
1:A:75:LYS:HG2	1:A:83:ASP:N	0.57	2.13	14	3
1:A:27:VAL:C	1:A:28:GLN:HE21	0.57	2.08	5	1
1:B:24:LEU:O	1:B:33:GLY:HA2	0.56	2.00	10	3
1:A:73:ILE:HG21	1:A:78:TYR:CZ	0.56	2.33	11	6
1:A:122:LEU:HD22	1:B:54:ILE:HG21	0.56	1.76	14	4
1:B:73:ILE:HG23	1:B:110:LYS:HG2	0.56	1.75	3	1
1:B:112:LYS:NZ	1:B:113:GLU:HG3	0.56	2.14	5	1
1:B:57:ALA:N	1:B:91:ILE:HG21	0.56	2.15	8	1
1:A:57:ALA:N	1:A:91:ILE:HG21	0.56	2.16	8	1
1:B:75:LYS:HG2	1:B:83:ASP:N	0.56	2.15	14	3
1:B:42:GLN:OE1	1:B:53:VAL:HA	0.56	2.01	11	7
1:A:42:GLN:OE1	1:A:53:VAL:HA	0.56	2.01	1	8
1:A:42:GLN:HG2	1:A:43:ASN:N	0.56	2.16	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:125:ASN:HD22	1:B:125:ASN:C	0.56	2.09	4	1
1:A:25:SER:HB3	1:A:26:PRO:HD2	0.55	1.78	10	8
1:A:57:ALA:H	1:A:91:ILE:HG21	0.55	1.62	8	1
1:A:54:ILE:HD13	1:B:91:ILE:HD11	0.55	1.79	7	2
1:A:91:ILE:HD11	1:B:54:ILE:HD13	0.55	1.78	7	2
1:A:55:VAL:HG22	1:A:94:LEU:CD2	0.55	2.31	8	1
1:B:55:VAL:HG22	1:B:94:LEU:CD2	0.55	2.31	8	1
1:B:73:ILE:HG21	1:B:78:TYR:CZ	0.55	2.36	19	6
1:A:125:ASN:C	1:A:125:ASN:HD22	0.54	2.10	4	1
1:B:27:VAL:HB	1:B:31:GLU:HB2	0.54	1.79	1	8
1:B:48:LYS:HB2	1:B:49:TYR:CD1	0.54	2.37	18	2
1:B:42:GLN:HG2	1:B:43:ASN:N	0.54	2.16	11	3
1:B:57:ALA:H	1:B:91:ILE:HG21	0.54	1.61	8	1
1:B:25:SER:HB3	1:B:26:PRO:HD2	0.54	1.80	10	8
1:A:119:MET:CG	1:A:125:ASN:HA	0.54	2.33	9	1
1:B:42:GLN:OE1	1:B:53:VAL:HB	0.54	2.03	19	1
1:A:42:GLN:OE1	1:A:53:VAL:HB	0.53	2.03	19	2
1:B:113:GLU:HA	1:B:116:ASN:ND2	0.53	2.18	10	2
1:B:73:ILE:HD12	1:B:78:TYR:CD2	0.53	2.38	14	2
1:A:48:LYS:HB2	1:A:49:TYR:CD1	0.53	2.38	18	2
1:A:56:ALA:CA	1:A:91:ILE:HG13	0.53	2.34	8	1
1:A:19:VAL:O	1:A:102:LYS:HA	0.53	2.04	8	7
1:B:111:MET:HE3	1:B:111:MET:HA	0.53	1.81	8	4
1:A:73:ILE:HD12	1:A:78:TYR:CD2	0.52	2.38	14	2
1:B:24:LEU:HB2	1:B:34:GLY:O	0.52	2.05	13	3
1:B:56:ALA:CA	1:B:91:ILE:HG13	0.52	2.33	8	1
1:A:117:ALA:O	1:A:121:SER:HB2	0.52	2.04	14	1
1:B:112:LYS:HA	1:B:115:ASP:OD2	0.52	2.04	3	2
1:B:90:GLN:HE22	1:B:92:ARG:NH2	0.52	2.03	13	1
1:A:19:VAL:HG23	1:A:105:TYR:O	0.52	2.04	10	1
1:B:25:SER:HB2	1:B:26:PRO:HD2	0.52	1.81	7	1
1:A:111:MET:HE3	1:A:111:MET:HA	0.52	1.81	8	4
1:B:42:GLN:HE22	1:B:47:ASN:N	0.52	2.03	15	5
1:B:119:MET:CG	1:B:125:ASN:HA	0.52	2.35	9	1
1:B:19:VAL:HG12	1:B:103:LEU:HB2	0.51	1.80	5	1
1:A:95:ASP:O	1:A:98:ARG:HG2	0.51	2.05	11	1
1:A:73:ILE:CG2	1:A:110:LYS:HD3	0.51	2.35	13	1
1:B:27:VAL:HB	1:B:31:GLU:CB	0.51	2.35	17	3
1:B:20:TYR:O	1:B:38:VAL:HG22	0.51	2.06	8	3
1:B:98:ARG:NE	1:B:98:ARG:HA	0.51	2.20	3	2
1:B:19:VAL:O	1:B:102:LYS:HA	0.51	2.05	2	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:VAL:HG12	1:A:103:LEU:HB2	0.51	1.81	5	1
1:B:112:LYS:CE	1:B:113:GLU:HG3	0.51	2.35	5	1
1:B:95:ASP:O	1:B:98:ARG:HG2	0.51	2.05	11	1
1:A:93:THR:HB	1:B:91:ILE:O	0.51	2.06	4	3
1:B:112:LYS:HA	1:B:112:LYS:HE2	0.51	1.82	8	6
1:A:28:GLN:NE2	1:B:26:PRO:HB2	0.51	2.21	9	3
1:B:54:ILE:HD11	1:B:91:ILE:HD13	0.51	1.81	10	3
1:A:112:LYS:HA	1:A:112:LYS:HE2	0.51	1.83	8	1
1:A:24:LEU:HB2	1:A:34:GLY:O	0.50	2.06	8	2
1:B:59:THR:HB	1:B:85:VAL:HG23	0.50	1.83	13	1
1:A:27:VAL:HB	1:A:31:GLU:CB	0.50	2.36	1	3
1:A:91:ILE:O	1:B:93:THR:HB	0.50	2.06	4	3
1:A:24:LEU:O	1:A:33:GLY:HA2	0.50	2.06	10	2
1:A:25:SER:CB	1:A:34:GLY:H	0.50	2.18	5	1
1:B:110:LYS:O	1:B:114:VAL:HG22	0.50	2.06	6	2
1:B:25:SER:CB	1:B:34:GLY:H	0.50	2.19	5	1
1:B:119:MET:HB2	1:B:124:LEU:HB2	0.50	1.84	12	1
1:A:54:ILE:HD11	1:A:91:ILE:HD13	0.50	1.83	10	3
1:A:32:GLN:HB3	1:A:92:ARG:NH2	0.50	2.22	13	2
1:A:24:LEU:HD22	1:A:33:GLY:HA3	0.50	1.84	5	1
1:A:58:ILE:HG12	1:A:86:ILE:CD1	0.50	2.37	19	6
1:A:32:GLN:NE2	1:A:36:ARG:HG3	0.50	2.22	10	1
1:B:25:SER:HB3	1:B:34:GLY:HA2	0.49	1.84	4	1
1:A:50:SER:O	1:A:96:LYS:HE2	0.49	2.07	8	1
1:A:68:PRO:O	1:A:117:ALA:HA	0.49	2.07	13	3
1:A:37:PRO:HB2	1:A:58:ILE:HD12	0.49	1.83	7	7
1:B:16:ARG:HB3	1:B:42:GLN:O	0.49	2.07	6	3
1:B:58:ILE:HG12	1:B:86:ILE:CD1	0.49	2.38	19	7
1:B:32:GLN:HB3	1:B:92:ARG:NH2	0.49	2.23	13	2
1:A:116:ASN:O	1:A:120:ILE:HG13	0.49	2.07	10	4
1:A:112:LYS:CE	1:A:113:GLU:HG3	0.49	2.38	5	1
1:B:23:ASP:O	1:B:98:ARG:HD2	0.49	2.07	5	2
1:B:56:ALA:CB	1:B:91:ILE:HG22	0.49	2.37	15	15
1:A:42:GLN:HG2	1:A:43:ASN:H	0.49	1.68	11	1
1:A:119:MET:HE2	1:A:120:ILE:HD12	0.49	1.84	13	1
1:B:73:ILE:HD12	1:B:78:TYR:CE2	0.49	2.43	14	1
1:B:112:LYS:HE3	1:B:113:GLU:HG3	0.49	1.84	5	1
1:A:113:GLU:HA	1:A:116:ASN:ND2	0.49	2.22	10	1
1:A:25:SER:HB3	1:A:34:GLY:HA2	0.49	1.84	4	1
1:B:24:LEU:HD22	1:B:24:LEU:O	0.49	2.08	15	2
1:A:56:ALA:CB	1:A:91:ILE:HG22	0.49	2.38	15	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:LEU:C	1:A:26:PRO:HD3	0.49	2.33	19	3
1:B:24:LEU:HD11	1:B:92:ARG:NE	0.49	2.23	13	1
1:A:20:TYR:O	1:A:38:VAL:HG22	0.49	2.07	8	3
1:B:50:SER:O	1:B:96:LYS:HE2	0.49	2.08	8	1
1:B:32:GLN:NE2	1:B:36:ARG:HG3	0.49	2.23	10	1
1:B:115:ASP:O	1:B:118:LEU:HB3	0.48	2.07	19	6
1:A:111:MET:HA	1:A:111:MET:HE2	0.48	1.85	11	2
1:B:28:GLN:HE21	1:B:28:GLN:N	0.48	2.06	15	1
1:A:95:ASP:OD1	1:A:97:LYS:HB3	0.48	2.08	19	1
1:B:116:ASN:O	1:B:120:ILE:HD12	0.48	2.08	1	1
1:A:42:GLN:HE22	1:A:47:ASN:N	0.48	2.07	15	6
1:A:16:ARG:HB3	1:A:42:GLN:O	0.48	2.08	6	2
1:A:110:LYS:O	1:A:114:VAL:HG22	0.48	2.08	6	2
1:B:70:HIS:CD2	1:B:87:LEU:HD22	0.48	2.43	8	2
1:A:26:PRO:HB2	1:B:28:GLN:HE22	0.48	1.67	9	1
1:B:37:PRO:HB2	1:B:58:ILE:HD12	0.48	1.83	7	5
1:A:20:TYR:HA	1:A:101:GLU:O	0.48	2.07	20	10
1:A:119:MET:HB2	1:A:124:LEU:HB2	0.48	1.86	12	1
1:A:24:LEU:HD22	1:A:24:LEU:O	0.48	2.07	15	3
1:B:20:TYR:HA	1:B:101:GLU:O	0.48	2.08	20	9
1:A:23:ASP:HA	1:A:35:VAL:HB	0.48	1.86	13	1
1:A:24:LEU:HD22	1:A:92:ARG:NH1	0.48	2.23	6	1
1:A:73:ILE:HD12	1:A:78:TYR:CE2	0.48	2.43	14	1
1:B:78:TYR:O	1:B:79:LYS:HG2	0.48	2.09	16	1
1:A:78:TYR:CE2	1:A:106:LEU:HA	0.48	2.43	12	2
1:B:24:LEU:C	1:B:26:PRO:HD3	0.48	2.34	19	3
1:B:14:ILE:HB	1:B:47:ASN:OD1	0.48	2.08	19	1
1:A:45:THR:HA	1:A:48:LYS:CD	0.47	2.39	12	1
1:B:44:ASP:HA	1:B:47:ASN:ND2	0.47	2.24	17	1
1:A:26:PRO:HB2	1:B:28:GLN:NE2	0.47	2.24	14	3
1:B:73:ILE:CG2	1:B:110:LYS:HD3	0.47	2.39	13	1
1:B:68:PRO:O	1:B:117:ALA:HA	0.47	2.10	15	1
1:A:32:GLN:C	1:A:32:GLN:HE21	0.47	2.17	19	1
1:A:39:VAL:CG2	1:A:56:ALA:HB3	0.47	2.39	10	4
1:A:108:ASP:O	1:A:111:MET:HB2	0.47	2.10	19	4
1:B:58:ILE:HG12	1:B:86:ILE:HD12	0.47	1.87	15	5
1:B:39:VAL:CG2	1:B:56:ALA:HB3	0.47	2.40	10	5
1:A:98:ARG:NE	1:A:98:ARG:HA	0.47	2.24	4	3
1:A:59:THR:HB	1:A:85:VAL:HG23	0.47	1.85	13	1
1:A:67:ILE:HD12	1:A:67:ILE:H	0.46	1.69	2	1
1:B:24:LEU:HD22	1:B:92:ARG:NH1	0.46	2.25	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:90:GLN:O	1:B:91:ILE:HG13	0.46	2.11	20	1
1:B:42:GLN:HG2	1:B:43:ASN:H	0.46	1.69	11	1
1:A:78:TYR:O	1:A:79:LYS:HG2	0.46	2.10	16	1
1:B:112:LYS:HA	1:B:112:LYS:CE	0.46	2.39	8	2
1:B:116:ASN:HD22	1:B:116:ASN:N	0.46	2.07	15	2
1:A:58:ILE:HG12	1:A:86:ILE:HD12	0.46	1.87	10	5
1:B:19:VAL:HG23	1:B:105:TYR:O	0.46	2.10	10	1
1:B:25:SER:HB3	1:B:34:GLY:N	0.46	2.24	19	1
1:A:108:ASP:O	1:A:111:MET:HB3	0.46	2.11	13	4
1:B:74:GLU:OE1	1:B:110:LYS:HE3	0.46	2.11	15	2
1:A:90:GLN:C	1:A:91:ILE:HD13	0.46	2.35	8	1
1:B:104:THR:CG2	1:B:105:TYR:H	0.46	2.24	11	1
1:B:42:GLN:OE1	1:B:47:ASN:HB3	0.46	2.11	18	1
1:B:22:ALA:HA	1:B:98:ARG:O	0.46	2.11	8	2
1:B:16:ARG:HD2	1:B:41:ILE:O	0.46	2.10	19	1
1:B:42:GLN:OE1	1:B:53:VAL:HG13	0.45	2.11	2	1
1:A:75:LYS:HG2	1:A:82:LYS:C	0.45	2.36	14	1
1:A:93:THR:HG21	1:B:89:GLU:O	0.45	2.11	4	1
1:A:57:ALA:H	1:A:91:ILE:CG1	0.45	2.24	8	1
1:B:94:LEU:HD22	1:B:94:LEU:N	0.45	2.27	8	1
1:B:47:ASN:OD1	1:B:48:LYS:HD2	0.45	2.11	3	1
1:B:116:ASN:O	1:B:120:ILE:HG13	0.45	2.11	3	2
1:B:111:MET:HA	1:B:111:MET:HE2	0.45	1.87	6	4
1:A:94:LEU:HD22	1:A:94:LEU:N	0.45	2.26	8	1
1:B:57:ALA:H	1:B:91:ILE:CG1	0.45	2.25	8	1
1:A:90:GLN:O	1:A:91:ILE:HG13	0.45	2.10	20	1
1:B:111:MET:HA	1:B:111:MET:CE	0.45	2.42	6	1
1:A:91:ILE:O	1:A:92:ARG:HD2	0.45	2.12	16	1
1:A:87:LEU:O	1:A:91:ILE:HD11	0.45	2.11	8	1
1:B:24:LEU:HB3	1:B:34:GLY:O	0.45	2.11	5	1
1:B:23:ASP:HA	1:B:35:VAL:HB	0.45	1.89	13	1
1:B:67:ILE:HD12	1:B:67:ILE:H	0.45	1.72	2	1
1:A:115:ASP:OD1	1:B:124:LEU:HG	0.45	2.12	13	1
1:A:22:ALA:HA	1:A:98:ARG:O	0.44	2.12	8	1
1:A:28:GLN:HE22	1:B:26:PRO:HB2	0.44	1.72	9	1
1:A:75:LYS:HA	1:A:75:LYS:HE3	0.44	1.89	20	1
1:A:89:GLU:O	1:B:93:THR:HG21	0.44	2.12	4	1
1:B:25:SER:HB2	1:B:34:GLY:H	0.44	1.73	5	1
1:A:90:GLN:HB3	1:A:91:ILE:CD1	0.44	2.41	8	1
1:A:24:LEU:HB3	1:A:32:GLN:O	0.44	2.13	13	1
1:B:108:ASP:O	1:B:111:MET:HB3	0.44	2.12	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ASN:OD1	1:A:48:LYS:HD2	0.44	2.13	3	1
1:A:111:MET:HA	1:A:111:MET:CE	0.44	2.42	6	1
1:B:87:LEU:O	1:B:91:ILE:HD11	0.44	2.12	8	1
1:B:90:GLN:C	1:B:91:ILE:HD13	0.44	2.36	8	1
1:B:75:LYS:HE3	1:B:75:LYS:HA	0.44	1.89	20	1
1:A:112:LYS:HE3	1:A:113:GLU:HG3	0.44	1.89	5	1
1:B:56:ALA:HA	1:B:91:ILE:HB	0.44	1.88	8	1
1:B:91:ILE:O	1:B:92:ARG:HD2	0.44	2.12	16	1
1:A:111:MET:C	1:A:112:LYS:HE2	0.44	2.38	12	4
1:A:104:THR:CG2	1:A:105:TYR:H	0.44	2.25	11	1
1:B:78:TYR:CE2	1:B:106:LEU:HA	0.44	2.48	12	2
1:A:25:SER:HB3	1:A:34:GLY:H	0.44	1.73	19	1
1:A:75:LYS:HD2	1:A:81:ASP:C	0.44	2.37	4	1
1:B:73:ILE:HD13	1:B:86:ILE:HD11	0.44	1.90	6	1
1:A:95:ASP:OD2	1:A:97:LYS:HB3	0.44	2.13	2	1
1:A:21:LEU:HA	1:A:37:PRO:HA	0.44	1.88	3	3
1:A:23:ASP:O	1:A:98:ARG:HD2	0.44	2.13	5	1
1:A:115:ASP:O	1:A:118:LEU:HB3	0.44	2.12	5	5
1:B:19:VAL:HB	1:B:104:THR:O	0.44	2.13	16	1
1:A:50:SER:O	1:A:96:LYS:HE3	0.44	2.13	13	1
1:B:16:ARG:HG2	1:B:111:MET:SD	0.44	2.53	13	1
1:A:24:LEU:HD22	1:A:92:ARG:CZ	0.43	2.43	6	1
1:A:112:LYS:HA	1:A:112:LYS:CE	0.43	2.42	8	1
1:A:119:MET:CB	1:A:124:LEU:HG	0.43	2.43	20	2
1:A:22:ALA:O	1:A:35:VAL:HA	0.43	2.13	18	2
1:B:24:LEU:HD22	1:B:33:GLY:HA3	0.43	1.89	5	1
1:B:73:ILE:HG12	1:B:84:SER:O	0.43	2.13	6	2
1:B:88:LEU:HG	1:B:117:ALA:HB3	0.43	1.88	14	3
1:A:93:THR:HB	1:B:90:GLN:O	0.43	2.13	18	1
1:A:56:ALA:HA	1:A:91:ILE:HB	0.43	1.88	8	1
1:B:108:ASP:O	1:B:111:MET:HB2	0.43	2.14	6	1
1:A:16:ARG:HD3	1:A:41:ILE:O	0.43	2.13	11	1
1:A:32:GLN:HB3	1:A:92:ARG:HH22	0.43	1.74	13	1
1:B:19:VAL:CG1	1:B:103:LEU:HB2	0.43	2.43	5	1
1:A:73:ILE:HG12	1:A:84:SER:O	0.43	2.13	6	1
1:B:25:SER:CB	1:B:26:PRO:HD2	0.43	2.42	8	3
1:A:91:ILE:HD11	1:B:54:ILE:CD1	0.43	2.43	10	1
1:B:32:GLN:HB3	1:B:92:ARG:HH22	0.43	1.71	13	1
1:B:22:ALA:O	1:B:35:VAL:HA	0.43	2.14	15	2
1:A:90:GLN:O	1:B:93:THR:HB	0.43	2.13	18	1
1:A:42:GLN:OE1	1:A:53:VAL:HG13	0.43	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:SER:CB	1:A:26:PRO:HD2	0.43	2.42	8	3
1:B:119:MET:CB	1:B:124:LEU:HG	0.43	2.43	20	2
1:A:25:SER:HB2	1:A:34:GLY:H	0.43	1.74	5	1
1:A:70:HIS:CD2	1:A:87:LEU:HD22	0.43	2.48	13	1
1:A:42:GLN:HG3	1:A:54:ILE:H	0.43	1.74	15	1
1:B:21:LEU:HA	1:B:37:PRO:HA	0.43	1.90	6	4
1:A:69:THR:HA	1:A:121:SER:OG	0.43	2.14	4	1
1:A:19:VAL:CG1	1:A:103:LEU:HB2	0.43	2.43	5	1
1:B:111:MET:C	1:B:112:LYS:HE2	0.43	2.39	12	2
1:B:75:LYS:HG2	1:B:82:LYS:C	0.43	2.38	14	1
1:B:109:ASP:O	1:B:113:GLU:HG3	0.43	2.13	14	1
1:A:16:ARG:HD2	1:A:41:ILE:O	0.43	2.13	19	1
1:A:25:SER:HB3	1:A:34:GLY:N	0.43	2.29	19	1
1:B:25:SER:HB3	1:B:34:GLY:H	0.43	1.74	19	1
1:B:73:ILE:HG21	1:B:78:TYR:CD1	0.43	2.49	19	1
1:A:57:ALA:HB3	1:A:91:ILE:HD12	0.42	1.91	8	1
1:B:24:LEU:HB3	1:B:92:ARG:NH1	0.42	2.29	12	1
1:A:82:LYS:NZ	1:A:82:LYS:HB3	0.42	2.29	18	2
1:A:91:ILE:HD11	1:B:91:ILE:HD11	0.42	1.91	16	1
1:B:24:LEU:HD13	1:B:24:LEU:O	0.42	2.14	16	1
1:B:27:VAL:HG12	1:B:92:ARG:NH1	0.42	2.30	4	1
1:B:19:VAL:HB	1:B:104:THR:H	0.42	1.75	17	1
1:A:14:ILE:HB	1:A:47:ASN:OD1	0.42	2.14	19	1
1:A:48:LYS:HB3	1:A:49:TYR:CD1	0.42	2.50	6	1
1:A:56:ALA:HA	1:A:91:ILE:CG1	0.42	2.43	8	1
1:A:110:LYS:N	1:A:110:LYS:HD2	0.42	2.29	17	1
1:B:56:ALA:HA	1:B:91:ILE:CG1	0.42	2.43	8	1
1:B:90:GLN:HB3	1:B:91:ILE:CD1	0.42	2.43	8	1
1:B:24:LEU:HB3	1:B:32:GLN:O	0.42	2.13	13	1
1:B:42:GLN:HG3	1:B:54:ILE:H	0.42	1.75	15	1
1:A:19:VAL:HB	1:A:104:THR:H	0.42	1.74	17	1
1:B:124:LEU:HD12	1:B:124:LEU:H	0.42	1.73	13	1
1:A:19:VAL:HB	1:A:104:THR:O	0.42	2.14	16	1
1:A:77:LYS:HE2	1:A:107:SER:OG	0.42	2.15	17	1
1:B:118:LEU:HA	1:B:121:SER:OG	0.42	2.15	18	1
1:B:95:ASP:OD1	1:B:97:LYS:HB3	0.42	2.15	19	1
1:B:95:ASP:OD2	1:B:97:LYS:HB3	0.42	2.15	2	1
1:A:124:LEU:HG	1:B:115:ASP:OD1	0.42	2.14	13	1
1:A:27:VAL:HG12	1:A:92:ARG:NH1	0.42	2.30	4	1
1:A:73:ILE:HD13	1:A:86:ILE:HD11	0.42	1.92	6	1
1:A:112:LYS:HE2	1:A:112:LYS:CA	0.42	2.45	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:ILE:HD12	1:A:91:ILE:C	0.42	2.40	10	2
1:A:119:MET:O	1:A:124:LEU:HB2	0.42	2.15	10	1
1:B:91:ILE:C	1:B:91:ILE:HD12	0.42	2.40	10	2
1:B:119:MET:HE2	1:B:120:ILE:HD12	0.42	1.92	13	1
1:B:96:LYS:O	1:B:99:LEU:HB2	0.42	2.15	18	1
1:A:41:ILE:CD1	1:B:122:LEU:HB3	0.42	2.44	7	1
1:B:24:LEU:HD22	1:B:92:ARG:CZ	0.42	2.45	10	1
1:A:124:LEU:H	1:A:124:LEU:HD12	0.42	1.74	13	1
1:A:94:LEU:HB2	1:A:98:ARG:CZ	0.41	2.45	18	1
1:B:42:GLN:HE22	1:B:46:GLY:C	0.41	2.23	19	1
1:A:17:GLY:HA2	1:A:111:MET:SD	0.41	2.54	3	1
1:B:78:TYR:HD1	1:B:105:TYR:O	0.41	1.98	4	1
1:A:122:LEU:HB3	1:B:41:ILE:CD1	0.41	2.45	7	1
1:A:16:ARG:HG2	1:A:111:MET:SD	0.41	2.55	13	1
1:A:78:TYR:C	1:A:104:THR:HG21	0.41	2.40	17	1
1:B:94:LEU:HB2	1:B:98:ARG:CZ	0.41	2.45	18	1
1:B:20:TYR:CZ	1:B:102:LYS:HB3	0.41	2.51	7	1
1:A:56:ALA:HA	1:A:91:ILE:HG22	0.41	1.91	17	1
1:A:54:ILE:HG21	1:B:122:LEU:CD2	0.41	2.46	7	1
1:B:23:ASP:C	1:B:25:SER:H	0.41	2.22	3	1
1:A:25:SER:HB3	1:A:34:GLY:CA	0.41	2.45	4	1
1:B:75:LYS:HD2	1:B:81:ASP:C	0.41	2.40	4	1
1:A:46:GLY:O	1:A:50:SER:HB3	0.41	2.15	11	1
1:A:73:ILE:HB	1:A:78:TYR:CE1	0.41	2.51	14	1
1:B:56:ALA:HA	1:B:91:ILE:HG22	0.41	1.91	17	1
1:A:32:GLN:HG3	1:A:36:ARG:NH2	0.41	2.31	8	1
1:B:57:ALA:HB3	1:B:91:ILE:HD12	0.41	1.92	8	1
1:A:54:ILE:CD1	1:B:91:ILE:HD11	0.41	2.44	10	1
1:A:17:GLY:O	1:A:105:TYR:HA	0.41	2.16	11	1
1:B:73:ILE:HD11	1:B:86:ILE:HG12	0.41	1.93	20	1
1:A:104:THR:CG2	1:A:105:TYR:N	0.41	2.84	8	1
1:B:45:THR:HA	1:B:48:LYS:CD	0.41	2.46	12	1
1:A:124:LEU:HD12	1:A:124:LEU:N	0.41	2.31	13	1
1:A:118:LEU:HA	1:A:121:SER:OG	0.41	2.16	18	1
1:A:73:ILE:HG22	1:A:74:GLU:H	0.41	1.74	19	1
1:B:20:TYR:CZ	1:B:102:LYS:HG2	0.41	2.51	20	1
1:A:23:ASP:C	1:A:25:SER:H	0.41	2.24	3	1
1:B:41:ILE:HD13	1:B:41:ILE:C	0.41	2.41	7	1
1:A:57:ALA:H	1:A:91:ILE:CG2	0.41	2.28	8	1
1:A:108:ASP:O	1:A:112:LYS:HD2	0.41	2.16	10	1
1:A:24:LEU:HD11	1:A:92:ARG:NE	0.41	2.31	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:ASN:C	1:A:125:ASN:ND2	0.40	2.78	4	1
1:A:122:LEU:CD2	1:B:54:ILE:HG21	0.40	2.45	7	1
1:A:24:LEU:HD13	1:A:24:LEU:O	0.40	2.15	16	1
1:A:27:VAL:HA	1:A:92:ARG:NH2	0.40	2.31	20	1
1:A:41:ILE:C	1:A:41:ILE:HD13	0.40	2.41	7	1
1:B:57:ALA:H	1:B:91:ILE:CG2	0.40	2.28	8	1
1:B:116:ASN:O	1:B:119:MET:HB3	0.40	2.16	9	1
1:B:77:LYS:HD3	1:B:107:SER:OG	0.40	2.16	11	1
1:B:110:LYS:N	1:B:110:LYS:HD2	0.40	2.30	17	1
1:A:96:LYS:O	1:A:99:LEU:HB2	0.40	2.16	18	1
1:A:112:LYS:HE2	1:A:112:LYS:N	0.40	2.32	2	1
1:A:41:ILE:HD13	1:A:42:GLN:N	0.40	2.31	16	1
1:B:41:ILE:HD13	1:B:42:GLN:N	0.40	2.31	16	1
1:A:24:LEU:HB3	1:A:34:GLY:O	0.40	2.16	5	1
1:A:42:GLN:HE22	1:A:46:GLY:C	0.40	2.24	19	1
1:A:112:LYS:HE2	1:A:112:LYS:HA	0.40	1.94	1	1
1:A:74:GLU:OE1	1:A:110:LYS:HE3	0.40	2.16	15	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	106/132 (80%)	94±2 (89±2%)	9±2 (9±2%)	2±1 (2±1%)	7	44
1	B	106/132 (80%)	94±2 (89±2%)	10±2 (9±2%)	2±1 (2±1%)	7	45
All	All	4240/5280 (80%)	3765 (89%)	377 (9%)	98 (2%)	7	45

All 24 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	26	PRO	20
1	B	26	PRO	19
1	A	25	SER	11
1	B	25	SER	11

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Mol	Chain	Res	Type	Models (Total)
1	A	125	ASN	9
1	B	125	ASN	8
1	A	91	ILE	2
1	B	91	ILE	2
1	A	96	LYS	1
1	A	89	GLU	1
1	B	89	GLU	1
1	A	67	ILE	1
1	B	67	ILE	1
1	A	92	ARG	1
1	B	92	ARG	1
1	A	106	LEU	1
1	B	106	LEU	1
1	A	33	GLY	1
1	B	33	GLY	1
1	B	29	GLY	1
1	A	42	GLN	1
1	B	42	GLN	1
1	A	83	ASP	1
1	B	83	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/117 (81%)	84±3 (89±3%)	11±3 (11±3%)	8	50
1	B	95/117 (81%)	84±3 (89±3%)	11±3 (11±3%)	8	51
All	All	3800/4680 (81%)	3371 (89%)	429 (11%)	8	51

All 91 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	41	ILE	20
1	B	41	ILE	20
1	A	111	MET	19
1	B	111	MET	19

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Mol	Chain	Res	Type	Models (Total)
1	B	32	GLN	13
1	A	26	PRO	12
1	A	90	GLN	12
1	B	26	PRO	11
1	B	42	GLN	11
1	A	73	ILE	11
1	B	73	ILE	11
1	A	53	VAL	11
1	B	53	VAL	11
1	B	90	GLN	11
1	A	42	GLN	10
1	B	114	VAL	10
1	A	32	GLN	9
1	A	114	VAL	9
1	A	28	GLN	7
1	B	28	GLN	7
1	A	82	LYS	6
1	A	102	LYS	6
1	A	124	LEU	6
1	B	82	LYS	6
1	A	112	LYS	6
1	A	21	LEU	5
1	B	102	LYS	5
1	A	35	VAL	5
1	B	35	VAL	5
1	B	112	LYS	5
1	B	124	LEU	5
1	B	21	LEU	4
1	A	67	ILE	4
1	A	24	LEU	4
1	A	116	ASN	4
1	B	24	LEU	4
1	B	116	ASN	4
1	A	54	ILE	4
1	B	54	ILE	4
1	A	91	ILE	4
1	B	91	ILE	4
1	A	31	GLU	3
1	A	118	LEU	3
1	B	31	GLU	3
1	B	67	ILE	3
1	B	118	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	106	LEU	3
1	B	106	LEU	3
1	A	97	LYS	3
1	A	120	ILE	3
1	A	80	LEU	2
1	A	125	ASN	2
1	B	80	LEU	2
1	B	125	ASN	2
1	A	95	ASP	2
1	A	84	SER	2
1	B	84	SER	2
1	A	92	ARG	2
1	B	92	ARG	2
1	B	97	LYS	2
1	B	104	THR	2
1	B	52	THR	2
1	A	25	SER	2
1	B	25	SER	2
1	B	120	ILE	2
1	A	77	LYS	2
1	B	77	LYS	2
1	A	110	LYS	1
1	B	110	LYS	1
1	A	44	ASP	1
1	A	119	MET	1
1	B	119	MET	1
1	B	95	ASP	1
1	A	18	ASP	1
1	A	94	LEU	1
1	B	18	ASP	1
1	B	94	LEU	1
1	A	27	VAL	1
1	B	27	VAL	1
1	A	52	THR	1
1	A	85	VAL	1
1	B	85	VAL	1
1	A	76	LYS	1
1	A	115	ASP	1
1	B	76	LYS	1
1	B	83	ASP	1
1	A	104	THR	1
1	A	93	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	B	93	THR	1
1	A	75	LYS	1
1	B	75	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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 46% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1520
Number of shifts mapped to atoms	1520
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	119	-0.06 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	113	-0.10 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	117	0.08 ± 0.13	None needed (< 0.5 ppm)
^{15}N	110	0.40 ± 0.75	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 46%, i.e. 1362 atoms were assigned a chemical shift out of a possible 2982. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	522/1058 (49%)	212/430 (49%)	210/424 (50%)	100/204 (49%)
Sidechain	807/1838 (44%)	554/1194 (46%)	245/574 (43%)	8/70 (11%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	33/86 (38%)	17/40 (42%)	16/44 (36%)	0/2 (0%)
Overall	1362/2982 (46%)	783/1664 (47%)	471/1042 (45%)	108/276 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 1519 atoms were assigned a chemical shift out of a possible 3676. 0 out of 46 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	582/1316 (44%)	236/534 (44%)	236/528 (45%)	110/254 (43%)
Sidechain	903/2176 (41%)	621/1410 (44%)	271/676 (40%)	11/90 (12%)
Aromatic	34/184 (18%)	18/96 (19%)	16/72 (22%)	0/16 (0%)
Overall	1519/3676 (41%)	875/2040 (43%)	523/1276 (41%)	121/360 (34%)

7.1.4 Statistically unusual chemical shifts ⓘ

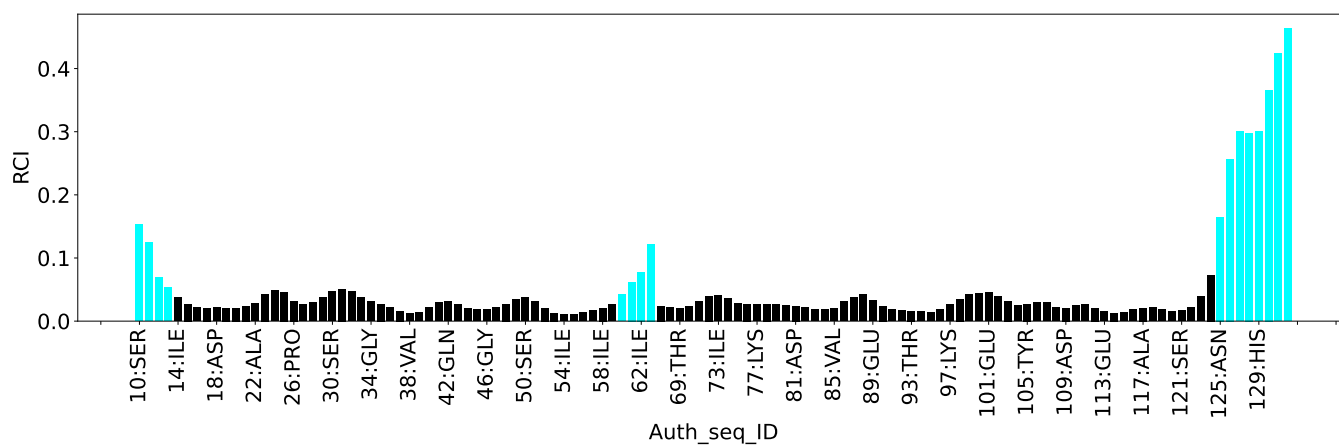
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	93	THR	HG1	5.63	0.08 – 2.19	21.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3268
Intra-residue ($ i-j =0$)	826
Sequential ($ i-j =1$)	908
Medium range ($ i-j >1$ and $ i-j <5$)	451
Long range ($ i-j \geq 5$)	1011
Inter-chain	72
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	303
Number of unmapped restraints	0
Number of restraints per residue	13.5
Number of long range restraints per residue ¹	3.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	138.6	0.2
0.2-0.5 (Medium)	50.0	0.5
>0.5 (Large)	7.0	5.21

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	15.6	8.47
10.0-20.0 (Medium)	0.2	16.27
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

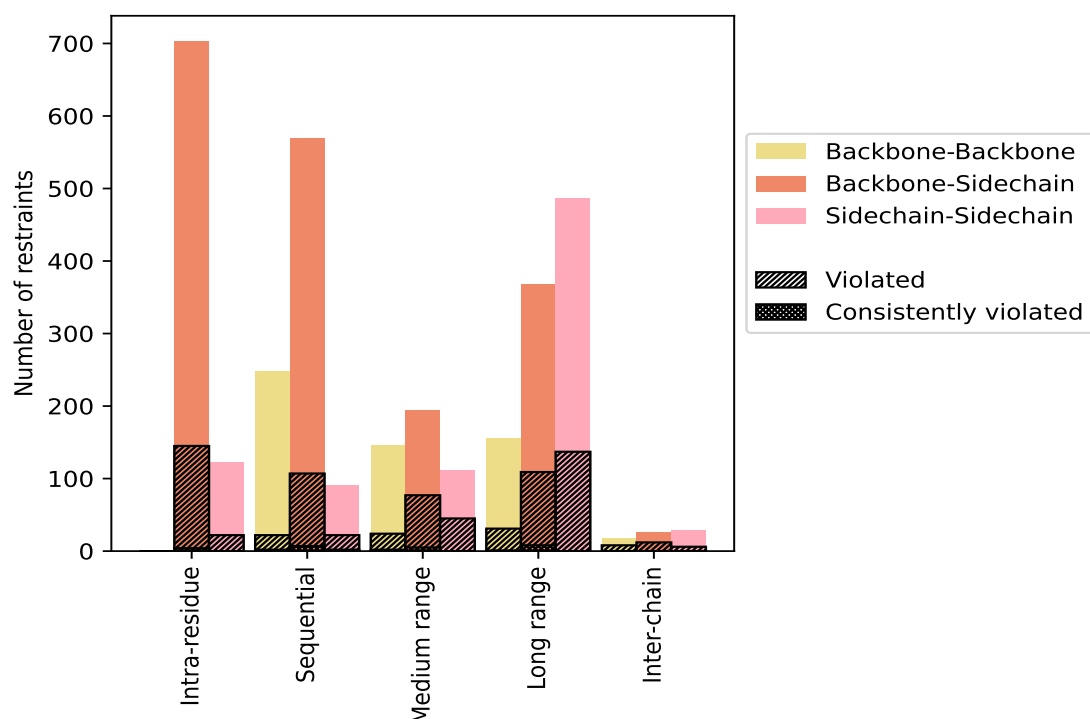
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	826	25.3	167	20.2	5.1	4	0.5	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	703	21.5	145	20.6	4.4	4	0.6	0.1
Sidechain-Sidechain	123	3.8	22	17.9	0.7	0	0.0	0.0
Sequential (i-j =1)	908	27.8	151	16.6	4.6	11	1.2	0.3
Backbone-Backbone	248	7.6	22	8.9	0.7	2	0.8	0.1
Backbone-Sidechain	569	17.4	107	18.8	3.3	7	1.2	0.2
Sidechain-Sidechain	91	2.8	22	24.2	0.7	2	2.2	0.1
Medium range (i-j >1 & i-j <5)	451	13.8	146	32.4	4.5	7	1.6	0.2
Backbone-Backbone	146	4.5	24	16.4	0.7	2	1.4	0.1
Backbone-Sidechain	194	5.9	77	39.7	2.4	5	2.6	0.2
Sidechain-Sidechain	111	3.4	45	40.5	1.4	0	0.0	0.0
Long range (i-j ≥5)	1011	30.9	277	27.4	8.5	9	0.9	0.3
Backbone-Backbone	156	4.8	31	19.9	0.9	1	0.6	0.0
Backbone-Sidechain	368	11.3	109	29.6	3.3	8	2.2	0.2
Sidechain-Sidechain	487	14.9	137	28.1	4.2	0	0.0	0.0
Inter-chain	72	2.2	26	36.1	0.8	0	0.0	0.0
Backbone-Backbone	18	0.6	8	44.4	0.2	0	0.0	0.0
Backbone-Sidechain	26	0.8	12	46.2	0.4	0	0.0	0.0
Sidechain-Sidechain	28	0.9	6	21.4	0.2	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3268	100.0	767	23.5	23.5	31	0.9	0.9
Backbone-Backbone	568	17.4	85	15.0	2.6	5	0.9	0.2
Backbone-Sidechain	1860	56.9	450	24.2	13.8	24	1.3	0.7
Sidechain-Sidechain	840	25.7	232	27.6	7.1	2	0.2	0.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	50	45	29	64	9	197	0.2	1.46	0.18	0.16
2	29	51	36	66	5	187	0.2	1.36	0.17	0.15
3	46	56	51	68	0	221	0.22	3.05	0.28	0.15
4	46	59	38	83	6	232	0.28	5.06	0.62	0.16
5	56	51	49	57	9	222	0.2	1.16	0.15	0.16
6	38	48	40	74	5	205	0.19	1.18	0.15	0.15
7	50	52	38	70	9	219	0.21	2.83	0.27	0.15
8	39	49	44	89	14	235	0.22	2.05	0.23	0.16
9	35	44	48	68	8	203	0.21	2.28	0.24	0.15
10	58	46	42	59	7	212	0.21	2.82	0.27	0.15

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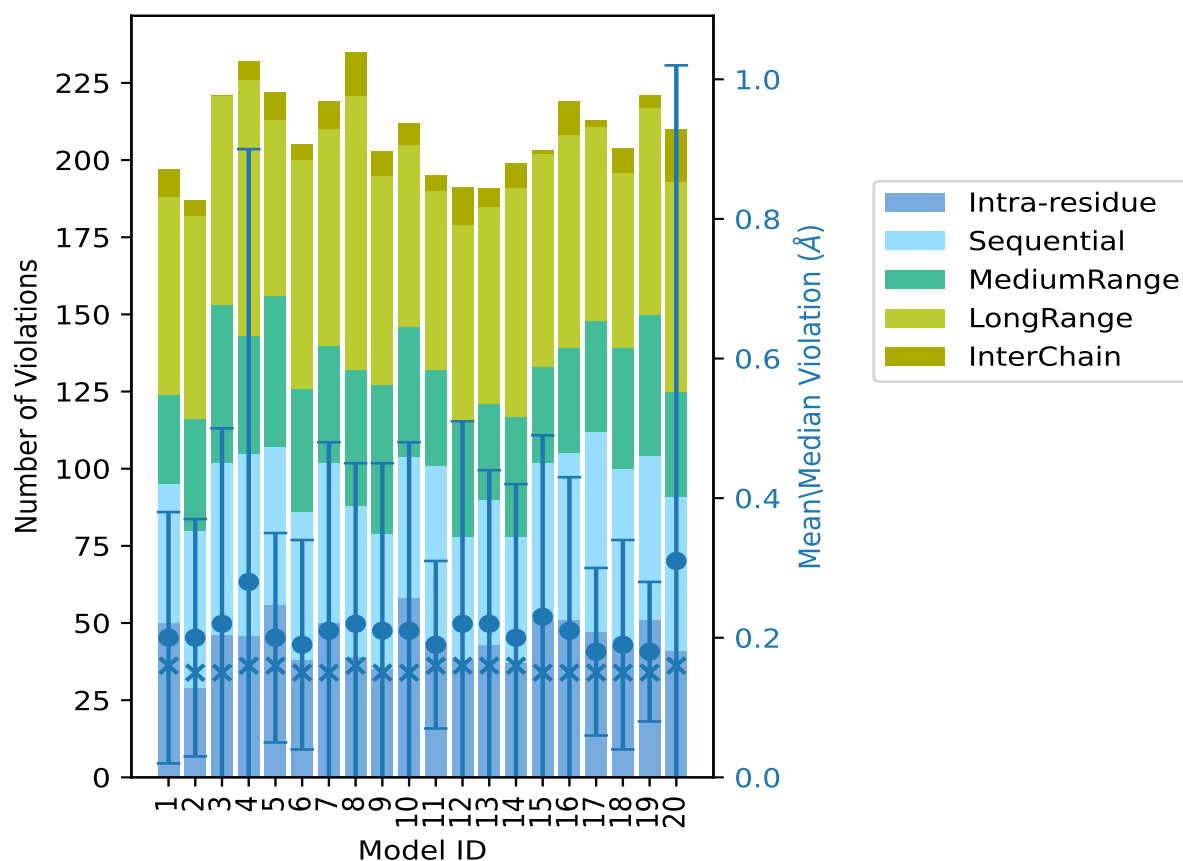
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	44	57	31	58	5	195	0.19	1.13	0.12	0.16
12	38	40	37	64	12	191	0.22	3.05	0.29	0.16
13	43	47	31	64	6	191	0.22	1.75	0.22	0.16
14	37	41	39	74	8	199	0.2	2.3	0.22	0.16
15	51	51	31	69	1	203	0.23	2.3	0.26	0.15
16	51	54	34	69	11	219	0.21	1.81	0.22	0.15
17	47	65	36	63	2	213	0.18	1.06	0.12	0.15
18	43	57	39	57	8	204	0.19	1.26	0.15	0.15
19	51	53	46	67	4	221	0.18	0.97	0.1	0.15
20	41	50	34	68	17	210	0.31	5.21	0.71	0.16

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

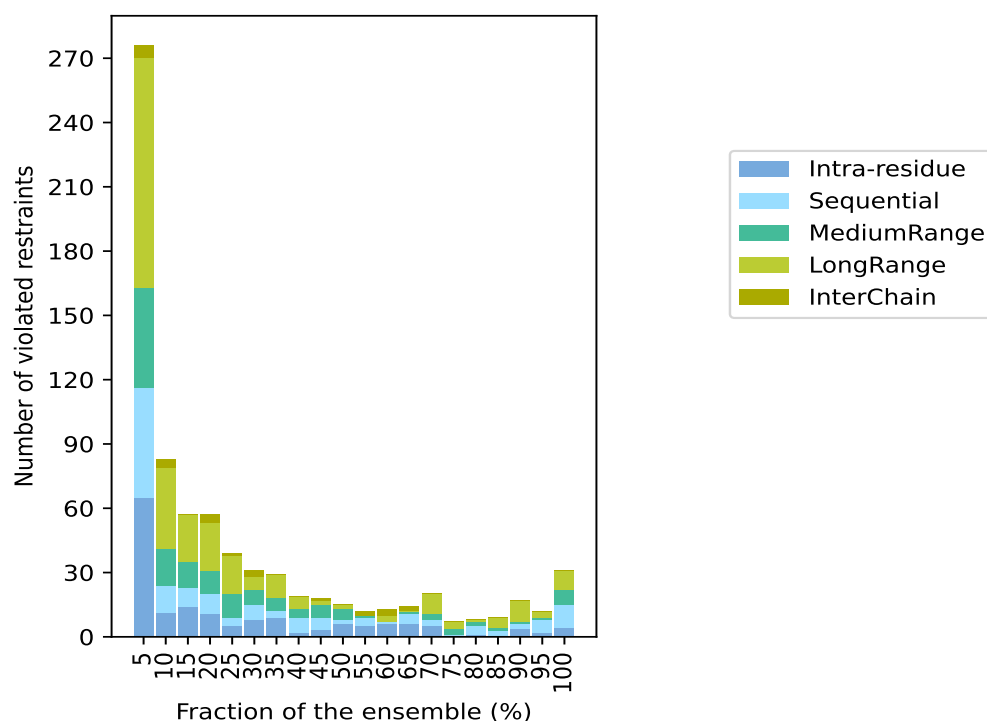
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2501(IR:659, SQ:757, MR:305, LR:734, IC:46) restraints are 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	%
65	51	47	107	6	276	1	5.0
11	13	17	38	4	83	2	10.0
14	9	12	22	0	57	3	15.0
11	9	11	22	4	57	4	20.0
5	4	11	18	1	39	5	25.0
8	7	7	6	3	31	6	30.0
9	3	6	11	0	29	7	35.0
2	7	4	6	0	19	8	40.0
3	6	6	2	1	18	9	45.0
6	2	5	2	0	15	10	50.0
5	4	1	0	2	12	11	55.0
6	1	0	3	3	13	12	60.0
6	5	1	0	2	14	13	65.0
5	3	3	9	0	20	14	70.0
0	1	3	3	0	7	15	75.0
1	4	2	1	0	8	16	80.0
0	3	1	5	0	9	17	85.0
4	2	1	10	0	17	18	90.0
2	6	1	3	0	12	19	95.0
4	11	7	9	0	31	20	100.0

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

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

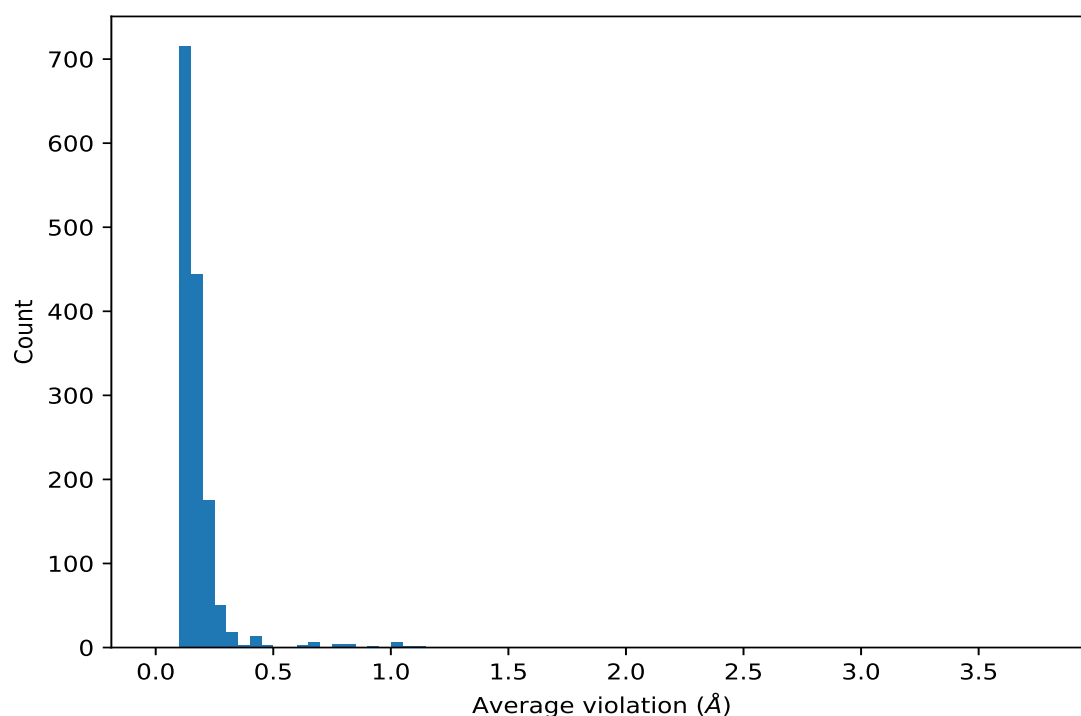
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	20	1.48	1.22	1.1
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	20	1.44	1.18	1.06
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	20	1.12	0.53	1.01
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	20	1.12	0.53	1.01
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	20	0.66	1.06	0.31
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	20	0.66	1.06	0.31
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	20	0.63	1.01	0.3
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	20	0.63	1.01	0.3
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	20	0.29	0.04	0.3
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	20	0.29	0.04	0.3
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	20	0.29	0.04	0.3
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	20	0.29	0.04	0.29
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	20	0.29	0.04	0.29
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	20	0.29	0.04	0.29
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	20	0.27	0.03	0.26
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	20	0.27	0.03	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	20	0.26	0.08	0.3
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	20	0.26	0.08	0.3
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	20	0.26	0.05	0.27
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	20	0.26	0.05	0.27
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	20	0.26	0.05	0.27
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	20	0.26	0.04	0.27
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	20	0.26	0.04	0.27
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	20	0.26	0.04	0.27
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	20	0.26	0.08	0.26
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	20	0.26	0.08	0.26
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	20	0.26	0.08	0.26
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	20	0.26	0.08	0.26
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	20	0.22	0.05	0.24
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	20	0.22	0.05	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	20	0.21	0.02	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	20	0.21	0.02	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	20	0.21	0.02	0.22
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	20	0.21	0.01	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	20	0.21	0.01	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	20	0.21	0.01	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	20	0.21	0.02	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	20	0.21	0.02	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	20	0.21	0.02	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	20	0.21	0.01	0.21
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	20	0.21	0.01	0.21
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	20	0.21	0.01	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	20	0.2	0.03	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	20	0.2	0.03	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	20	0.2	0.03	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	20	0.2	0.03	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	20	0.2	0.03	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	20	0.2	0.03	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	20	0.2	0.03	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	20	0.2	0.03	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	20	0.2	0.03	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	20	0.2	0.03	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	20	0.2	0.03	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	20	0.2	0.03	0.2
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	20	0.18	0.04	0.18
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	20	0.18	0.04	0.18
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	20	0.18	0.04	0.18
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	20	0.18	0.02	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	20	0.18	0.04	0.18
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	20	0.18	0.04	0.18
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	20	0.18	0.04	0.18
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	20	0.18	0.02	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	20	0.18	0.02	0.18
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	20	0.18	0.02	0.18
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	20	0.18	0.03	0.18
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	20	0.18	0.03	0.18
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	20	0.18	0.03	0.18
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	20	0.18	0.03	0.18
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	20	0.18	0.03	0.18
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	20	0.18	0.03	0.18
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	20	0.17	0.02	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	20	0.17	0.02	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	20	0.17	0.02	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	20	0.17	0.02	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	20	0.17	0.02	0.17
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	20	0.17	0.02	0.17
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	20	0.16	0.06	0.14
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	20	0.16	0.06	0.14
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	20	0.16	0.06	0.14
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	20	0.15	0.03	0.14
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	19	0.42	0.14	0.43
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	19	0.23	0.07	0.2
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	19	0.23	0.07	0.2
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	19	0.23	0.06	0.2
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	19	0.23	0.06	0.2
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	19	0.18	0.04	0.19
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	19	0.17	0.06	0.15
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	19	0.17	0.06	0.15
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	19	0.17	0.06	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	19	0.16	0.02	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	19	0.16	0.02	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	19	0.16	0.02	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	19	0.16	0.02	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	19	0.16	0.02	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	19	0.16	0.02	0.17
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	19	0.16	0.02	0.16
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	19	0.16	0.02	0.16
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	19	0.16	0.02	0.16
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	19	0.15	0.02	0.15
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	19	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	19	0.13	0.02	0.13
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	19	0.12	0.02	0.12
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	19	0.12	0.02	0.12
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	18	0.44	0.12	0.44
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	18	0.26	0.12	0.24
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	18	0.26	0.12	0.24
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	18	0.26	0.12	0.24
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	18	0.26	0.12	0.24
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	18	0.26	0.12	0.24
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	18	0.26	0.12	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	18	0.24	0.09	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	18	0.24	0.09	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	18	0.24	0.09	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	18	0.24	0.09	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	18	0.24	0.09	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	18	0.24	0.09	0.24
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	18	0.22	0.06	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	18	0.22	0.06	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	18	0.22	0.06	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	18	0.22	0.06	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	18	0.22	0.06	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	18	0.22	0.06	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	18	0.21	0.01	0.22
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	18	0.21	0.01	0.21
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	18	0.2	0.02	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	18	0.2	0.02	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	18	0.2	0.02	0.19
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	18	0.2	0.02	0.19
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	18	0.2	0.02	0.19
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	18	0.2	0.02	0.19
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	18	0.19	0.05	0.19
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	18	0.18	0.03	0.19
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	18	0.18	0.05	0.18
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	18	0.16	0.03	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	18	0.16	0.03	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	18	0.16	0.03	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	18	0.16	0.01	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	18	0.16	0.01	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	18	0.16	0.01	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	18	0.16	0.01	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	18	0.16	0.01	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	18	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	18	0.16	0.03	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	18	0.16	0.03	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	18	0.16	0.03	0.15
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	18	0.15	0.03	0.14
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	18	0.13	0.02	0.13
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	17	0.93	1.14	0.31
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	17	0.93	1.14	0.31
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	17	0.22	0.03	0.22
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	17	0.22	0.03	0.22
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	17	0.22	0.03	0.22
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	17	0.21	0.03	0.22
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	17	0.21	0.03	0.22
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	17	0.21	0.03	0.22
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	17	0.2	0.04	0.21
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	17	0.2	0.04	0.21
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	17	0.2	0.04	0.21
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	17	0.2	0.04	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	17	0.2	0.04	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	17	0.2	0.04	0.21
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	17	0.19	0.04	0.2
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	17	0.19	0.04	0.2
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	17	0.19	0.04	0.2
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	17	0.19	0.04	0.2
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	17	0.19	0.04	0.2
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	17	0.19	0.04	0.2
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	17	0.14	0.04	0.13
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	17	0.12	0.01	0.12
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	16	0.78	0.89	0.21
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	16	0.78	0.89	0.21
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	16	0.78	0.89	0.21
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	16	0.78	0.89	0.21
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	16	0.3	0.03	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	16	0.3	0.03	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	16	0.3	0.03	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	16	0.3	0.03	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	16	0.3	0.03	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	16	0.3	0.03	0.3
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	16	0.23	0.06	0.26
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	16	0.19	0.06	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	16	0.19	0.06	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	16	0.19	0.06	0.2
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	16	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	16	0.13	0.02	0.12
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	16	0.13	0.02	0.12
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	16	0.13	0.02	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	16	0.13	0.02	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	16	0.13	0.02	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	16	0.13	0.02	0.12
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	15	0.21	0.07	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	15	0.21	0.07	0.2
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	15	0.18	0.09	0.14
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	15	0.18	0.09	0.14
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	15	0.18	0.09	0.14
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	15	0.18	0.09	0.14
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	15	0.17	0.05	0.15
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	15	0.14	0.04	0.14
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	15	0.14	0.02	0.14
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	15	0.13	0.02	0.13
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	15	0.13	0.02	0.13
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	15	0.13	0.02	0.13
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	15	0.13	0.02	0.13
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	15	0.13	0.02	0.13
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	15	0.13	0.02	0.13
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	15	0.12	0.02	0.11
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	14	0.26	0.22	0.15
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	14	0.26	0.22	0.15
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	14	0.26	0.22	0.15
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	14	0.26	0.22	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	14	0.24	0.03	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	14	0.24	0.03	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	14	0.24	0.03	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	14	0.23	0.03	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	14	0.23	0.03	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	14	0.23	0.03	0.24
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	14	0.23	0.08	0.23
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	14	0.23	0.08	0.23
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	14	0.22	0.05	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	14	0.22	0.05	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	14	0.22	0.05	0.22
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	14	0.21	0.06	0.22
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	14	0.21	0.07	0.19
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	14	0.21	0.07	0.19
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	14	0.2	0.06	0.2
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	14	0.17	0.04	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	14	0.17	0.04	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	14	0.17	0.04	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	14	0.17	0.03	0.16
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	14	0.17	0.03	0.16
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	14	0.17	0.03	0.16
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	14	0.14	0.03	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	14	0.14	0.03	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	14	0.14	0.03	0.13
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	14	0.14	0.03	0.12
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	14	0.14	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	14	0.14	0.03	0.12
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	14	0.14	0.02	0.14
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	14	0.14	0.02	0.14
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	14	0.14	0.02	0.14
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	14	0.14	0.02	0.14
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	14	0.14	0.02	0.14
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	14	0.14	0.02	0.14
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	14	0.14	0.02	0.13
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	14	0.14	0.02	0.13
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	14	0.14	0.02	0.13
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	14	0.14	0.02	0.13
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	14	0.14	0.02	0.13
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	14	0.14	0.02	0.13
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	14	0.13	0.03	0.12
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	14	0.13	0.03	0.12
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	14	0.13	0.03	0.12
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	14	0.13	0.01	0.13
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	14	0.12	0.01	0.12
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	14	0.12	0.01	0.12
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	14	0.12	0.01	0.12
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	14	0.12	0.01	0.12
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	14	0.12	0.01	0.12
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	14	0.12	0.01	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	14	0.12	0.01	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	14	0.12	0.01	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	14	0.12	0.01	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	14	0.12	0.01	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	14	0.12	0.01	0.12
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	14	0.12	0.01	0.12
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	13	0.25	0.09	0.29
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	13	0.25	0.09	0.29
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	13	0.21	0.04	0.19
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	13	0.19	0.04	0.2
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	13	0.19	0.04	0.2
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	13	0.19	0.04	0.2
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	13	0.19	0.04	0.2
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	13	0.19	0.04	0.2
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	13	0.19	0.04	0.2
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	13	0.17	0.05	0.17
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	13	0.17	0.05	0.15
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	13	0.15	0.03	0.14
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	13	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	13	0.14	0.02	0.14
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	13	0.14	0.02	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	13	0.14	0.03	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	13	0.14	0.03	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	13	0.14	0.03	0.14
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	13	0.14	0.02	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	13	0.14	0.02	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	13	0.14	0.02	0.15
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	13	0.14	0.02	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	13	0.14	0.02	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	13	0.12	0.01	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	13	0.12	0.01	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	13	0.12	0.01	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	13	0.12	0.02	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	13	0.12	0.02	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	13	0.12	0.02	0.12
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	13	0.12	0.02	0.12
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	12	0.32	0.1	0.28
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	12	0.29	0.11	0.29
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	12	0.21	0.05	0.21
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	12	0.21	0.05	0.21
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	12	0.19	0.04	0.2
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	12	0.19	0.04	0.2
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	12	0.19	0.05	0.18
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	12	0.15	0.02	0.15
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	12	0.14	0.03	0.15
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	12	0.14	0.04	0.14
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	12	0.14	0.02	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	12	0.14	0.02	0.14
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	12	0.13	0.02	0.13
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	12	0.13	0.02	0.13
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	12	0.13	0.02	0.13
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	12	0.13	0.03	0.12
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	12	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	12	0.13	0.02	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	12	0.13	0.02	0.13
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	11	0.65	0.66	0.18
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	11	0.65	0.66	0.18
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	11	0.65	0.66	0.18
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	11	0.24	0.08	0.26
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	11	0.24	0.08	0.26
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	11	0.19	0.09	0.14
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	11	0.19	0.09	0.14
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	11	0.19	0.09	0.14
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	11	0.19	0.09	0.13
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	11	0.19	0.09	0.13
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	11	0.19	0.09	0.13
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	11	0.16	0.03	0.17
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	11	0.16	0.03	0.17
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	11	0.16	0.03	0.17
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	11	0.16	0.03	0.16
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	11	0.16	0.03	0.16
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	11	0.16	0.03	0.16
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	11	0.15	0.04	0.13
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	11	0.15	0.06	0.13
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	11	0.14	0.03	0.14
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	11	0.14	0.04	0.12
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	11	0.14	0.02	0.14
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	11	0.12	0.02	0.12
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	10	0.4	0.3	0.3
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	10	0.4	0.3	0.24
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	10	0.25	0.08	0.26
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	10	0.25	0.08	0.26
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	10	0.19	0.04	0.18
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	10	0.16	0.03	0.14
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	10	0.16	0.03	0.14
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	10	0.16	0.03	0.14
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	10	0.15	0.03	0.15
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	10	0.15	0.03	0.15
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	10	0.15	0.03	0.15
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	10	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	10	0.15	0.04	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	10	0.15	0.04	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	10	0.13	0.03	0.13
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	10	0.13	0.03	0.13
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	10	0.13	0.03	0.13
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	10	0.13	0.03	0.13
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	10	0.13	0.03	0.13
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	10	0.13	0.03	0.13
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	10	0.13	0.02	0.13
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	10	0.13	0.02	0.13
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	10	0.13	0.02	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	10	0.13	0.01	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	10	0.13	0.01	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	10	0.13	0.01	0.12
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	10	0.13	0.02	0.12
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	10	0.12	0.01	0.11
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	10	0.11	0.01	0.11
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	9	0.17	0.05	0.15
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	9	0.17	0.03	0.16
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	9	0.17	0.02	0.16
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	9	0.16	0.02	0.16
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	9	0.16	0.05	0.15
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	9	0.16	0.04	0.17
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	9	0.15	0.03	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	9	0.15	0.03	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	9	0.15	0.03	0.15
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	9	0.15	0.04	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	9	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	9	0.15	0.03	0.16
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	9	0.14	0.02	0.14
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	9	0.14	0.03	0.14
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	9	0.14	0.03	0.14
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	9	0.13	0.02	0.12
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	9	0.13	0.02	0.12
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	9	0.13	0.02	0.12
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	9	0.13	0.02	0.12
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	9	0.13	0.02	0.12
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	9	0.13	0.03	0.11
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	9	0.13	0.03	0.11
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	9	0.13	0.01	0.13
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	8	0.4	0.17	0.38
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	8	0.27	0.18	0.24
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	8	0.27	0.18	0.24
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	8	0.27	0.18	0.24
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	8	0.21	0.04	0.19
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	8	0.21	0.04	0.19
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	8	0.21	0.04	0.19
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	8	0.21	0.04	0.2
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	8	0.21	0.04	0.2
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	8	0.21	0.04	0.2
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	8	0.17	0.03	0.18
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	8	0.16	0.01	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	8	0.16	0.03	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	8	0.16	0.03	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	8	0.16	0.03	0.16
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	8	0.16	0.02	0.16
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	8	0.15	0.03	0.14
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	8	0.15	0.03	0.14
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	8	0.15	0.03	0.14
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	8	0.15	0.02	0.15
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	8	0.14	0.03	0.12
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	8	0.14	0.03	0.12
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	8	0.14	0.03	0.12
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	8	0.14	0.03	0.12
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	8	0.13	0.01	0.13
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	8	0.13	0.01	0.13
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	8	0.13	0.01	0.13
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	8	0.13	0.01	0.13
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	8	0.13	0.01	0.13
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	8	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	8	0.13	0.02	0.12
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	8	0.13	0.02	0.12
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	8	0.13	0.02	0.12
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	8	0.13	0.02	0.12
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	8	0.12	0.01	0.12
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	8	0.12	0.01	0.12
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	8	0.12	0.01	0.12
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	8	0.12	0.01	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	8	0.12	0.01	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	8	0.12	0.01	0.12
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	7	1.06	0.73	1.5
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	7	1.06	0.73	1.5
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	7	0.88	0.44	0.92
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	7	0.67	0.38	0.89
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	7	0.47	0.39	0.34
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	7	0.47	0.39	0.34
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	7	0.47	0.39	0.34
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	7	0.44	0.15	0.39
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	7	0.41	0.67	0.13
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	7	0.41	0.66	0.14
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	7	0.23	0.02	0.23
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	7	0.23	0.06	0.22
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	7	0.23	0.06	0.22
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	7	0.23	0.06	0.22
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	7	0.23	0.04	0.23
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	7	0.17	0.02	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	7	0.17	0.02	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	7	0.17	0.02	0.17
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	7	0.16	0.01	0.15
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	7	0.15	0.01	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	7	0.15	0.02	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	7	0.15	0.02	0.15
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	7	0.15	0.02	0.14
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	7	0.15	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	7	0.15	0.02	0.14
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	7	0.15	0.03	0.15
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	7	0.15	0.03	0.15
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	7	0.15	0.03	0.15
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	7	0.15	0.02	0.15
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	7	0.15	0.02	0.15
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	7	0.15	0.02	0.15
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	7	0.15	0.02	0.15
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	7	0.15	0.02	0.15
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	7	0.15	0.02	0.15
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	7	0.15	0.02	0.14
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	7	0.15	0.02	0.14
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	7	0.15	0.04	0.15
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	7	0.15	0.04	0.15
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	7	0.15	0.04	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	7	0.15	0.04	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	7	0.15	0.04	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	7	0.15	0.04	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	7	0.15	0.04	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	7	0.15	0.04	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	7	0.15	0.04	0.15
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	7	0.14	0.03	0.12
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	7	0.14	0.03	0.12
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	7	0.14	0.05	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	7	0.14	0.05	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	7	0.14	0.05	0.13
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	7	0.14	0.03	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	7	0.14	0.03	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	7	0.14	0.03	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	7	0.14	0.03	0.13
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	7	0.13	0.02	0.13
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	7	0.13	0.02	0.13
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	7	0.13	0.02	0.13
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	7	0.13	0.03	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	7	0.13	0.03	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	7	0.13	0.03	0.11
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	7	0.12	0.02	0.13
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	7	0.12	0.02	0.13
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	7	0.12	0.02	0.13
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	7	0.12	0.01	0.11
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	7	0.11	0.01	0.11
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	7	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	7	0.11	0.01	0.11
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	7	0.11	0.01	0.11
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	7	0.11	0.01	0.11
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	7	0.11	0.01	0.11
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	6	0.82	0.48	1.11
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	6	0.82	0.48	1.11
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	6	0.82	0.48	1.11
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	6	0.32	0.32	0.15
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	6	0.32	0.32	0.15
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	6	0.32	0.32	0.15
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD21	6	0.28	0.01	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD22	6	0.28	0.01	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD23	6	0.28	0.01	0.28
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD21	6	0.28	0.01	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD22	6	0.28	0.01	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD23	6	0.28	0.01	0.29
(1,2157)	1:113:B:GLU:HA	1:116:B:ASN:HD21	6	0.24	0.04	0.24
(1,942)	1:103:A:LEU:HD11	1:104:A:THR:H	6	0.2	0.09	0.18
(1,942)	1:103:A:LEU:HD12	1:104:A:THR:H	6	0.2	0.09	0.18
(1,942)	1:103:A:LEU:HD13	1:104:A:THR:H	6	0.2	0.09	0.18
(1,1011)	1:113:A:GLU:HA	1:116:A:ASN:HD21	6	0.2	0.05	0.21
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD11	6	0.18	0.1	0.12
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD12	6	0.18	0.1	0.12
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD13	6	0.18	0.1	0.12
(1,1710)	1:127:B:VAL:HA	1:128:B:ALA:H	6	0.18	0.06	0.16
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	6	0.17	0.05	0.17
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	6	0.17	0.05	0.17
(1,567)	1:127:A:VAL:HA	1:128:A:ALA:H	6	0.17	0.07	0.14
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD21	6	0.17	0.01	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD22	6	0.17	0.01	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD23	6	0.17	0.01	0.16
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD11	6	0.16	0.07	0.14
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD12	6	0.16	0.07	0.14
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD13	6	0.16	0.07	0.14
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	6	0.16	0.03	0.15
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	6	0.16	0.03	0.15
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	6	0.16	0.03	0.15
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	6	0.15	0.03	0.15
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE3	6	0.15	0.03	0.15
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	6	0.15	0.03	0.15
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE3	6	0.15	0.03	0.15
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD11	6	0.15	0.05	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD12	6	0.15	0.05	0.13
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD13	6	0.15	0.05	0.13
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE2	6	0.14	0.02	0.15
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE3	6	0.14	0.02	0.15
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE2	6	0.14	0.02	0.15
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE3	6	0.14	0.02	0.15
(1,2548)	1:74:A:GLU:HB2	1:77:A:LYS:H	6	0.14	0.02	0.12
(1,2548)	1:74:A:GLU:HB3	1:77:A:LYS:H	6	0.14	0.02	0.12
(1,2111)	1:111:B:MET:HG3	1:112:B:LYS:H	6	0.14	0.02	0.14
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD2	6	0.14	0.02	0.14
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD3	6	0.14	0.02	0.14
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG21	6	0.13	0.02	0.12
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG22	6	0.13	0.02	0.12
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG23	6	0.13	0.02	0.12
(1,1342)	1:91:A:ILE:HG21	1:93:B:THR:HB	6	0.13	0.02	0.12
(1,1342)	1:91:A:ILE:HG22	1:93:B:THR:HB	6	0.13	0.02	0.12
(1,1342)	1:91:A:ILE:HG23	1:93:B:THR:HB	6	0.13	0.02	0.12
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD1	6	0.13	0.02	0.12
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD2	6	0.13	0.02	0.12
(1,169)	1:27:A:VAL:HG11	1:33:A:GLY:HA2	6	0.13	0.01	0.12
(1,169)	1:27:A:VAL:HG12	1:33:A:GLY:HA2	6	0.13	0.01	0.12
(1,169)	1:27:A:VAL:HG13	1:33:A:GLY:HA2	6	0.13	0.01	0.12
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB2	6	0.13	0.02	0.12
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB3	6	0.13	0.02	0.12
(1,455)	1:105:A:TYR:H	1:106:A:LEU:H	6	0.12	0.01	0.12
(1,1900)	1:27:B:VAL:HG11	1:33:B:GLY:H	6	0.12	0.02	0.12
(1,1900)	1:27:B:VAL:HG12	1:33:B:GLY:H	6	0.12	0.02	0.12
(1,1900)	1:27:B:VAL:HG13	1:33:B:GLY:H	6	0.12	0.02	0.12
(1,371)	1:20:A:TYR:H	1:21:A:LEU:H	6	0.12	0.01	0.12
(1,2982)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	6	0.12	0.02	0.11
(1,2982)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	6	0.12	0.02	0.11
(1,2982)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	6	0.12	0.02	0.11
(1,2982)	1:53:B:VAL:HG21	1:94:B:LEU:HB2	6	0.12	0.02	0.11
(1,2982)	1:53:B:VAL:HG22	1:94:B:LEU:HB2	6	0.12	0.02	0.11
(1,2982)	1:53:B:VAL:HG23	1:94:B:LEU:HB2	6	0.12	0.02	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD21	6	0.12	0.02	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD22	6	0.12	0.02	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD23	6	0.12	0.02	0.11
(1,1083)	1:76:A:LYS:H	1:80:A:LEU:H	6	0.11	0.01	0.11
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG21	5	1.04	0.44	1.18
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG22	5	1.04	0.44	1.18
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG23	5	1.04	0.44	1.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG21	5	1.01	0.43	1.14
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG22	5	1.01	0.43	1.14
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG23	5	1.01	0.43	1.14
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD11	5	0.41	0.02	0.42
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD12	5	0.41	0.02	0.42
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD13	5	0.41	0.02	0.42
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	5	0.23	0.01	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	5	0.23	0.01	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	5	0.23	0.01	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	5	0.23	0.01	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	5	0.23	0.01	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	5	0.23	0.01	0.24
(1,2088)	1:103:B:LEU:HD11	1:104:B:THR:H	5	0.22	0.08	0.17
(1,2088)	1:103:B:LEU:HD12	1:104:B:THR:H	5	0.22	0.08	0.17
(1,2088)	1:103:B:LEU:HD13	1:104:B:THR:H	5	0.22	0.08	0.17
(1,1499)	1:48:B:LYS:H	1:48:B:LYS:HD3	5	0.2	0.07	0.2
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD1	5	0.18	0.05	0.17
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD2	5	0.18	0.05	0.17
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	5	0.17	0.03	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	5	0.17	0.03	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	5	0.17	0.03	0.15
(1,1145)	1:27:A:VAL:HG21	1:33:A:GLY:HA3	5	0.17	0.03	0.18
(1,1145)	1:27:A:VAL:HG22	1:33:A:GLY:HA3	5	0.17	0.03	0.18
(1,1145)	1:27:A:VAL:HG23	1:33:A:GLY:HA3	5	0.17	0.03	0.18
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE1	5	0.16	0.04	0.16
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE2	5	0.16	0.04	0.16
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE1	5	0.16	0.04	0.16
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE2	5	0.16	0.04	0.16
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE1	5	0.16	0.04	0.16
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE2	5	0.16	0.04	0.16
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE1	5	0.16	0.04	0.14
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE2	5	0.16	0.04	0.14
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE1	5	0.16	0.04	0.14
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE2	5	0.16	0.04	0.14
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE1	5	0.16	0.04	0.14
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE2	5	0.16	0.04	0.14
(1,19)	1:27:B:VAL:HG21	1:33:B:GLY:HA3	5	0.15	0.03	0.15
(1,19)	1:27:B:VAL:HG22	1:33:B:GLY:HA3	5	0.15	0.03	0.15
(1,19)	1:27:B:VAL:HG23	1:33:B:GLY:HA3	5	0.15	0.03	0.15
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD21	5	0.15	0.03	0.15
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD22	5	0.15	0.03	0.15
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD23	5	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2866)	1:24:B:LEU:HB2	1:25:B:SER:H	5	0.15	0.03	0.14
(1,2866)	1:24:B:LEU:HB3	1:25:B:SER:H	5	0.15	0.03	0.14
(1,2039)	1:87:B:LEU:H	1:90:B:GLN:H	5	0.15	0.05	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG21	5	0.14	0.02	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG22	5	0.14	0.02	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG23	5	0.14	0.02	0.14
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB2	5	0.14	0.04	0.12
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB3	5	0.14	0.04	0.12
(1,2874)	1:24:B:LEU:HD11	1:32:B:GLN:HE22	5	0.14	0.02	0.14
(1,2874)	1:24:B:LEU:HD12	1:32:B:GLN:HE22	5	0.14	0.02	0.14
(1,2874)	1:24:B:LEU:HD13	1:32:B:GLN:HE22	5	0.14	0.02	0.14
(1,2874)	1:24:B:LEU:HD21	1:32:B:GLN:HE22	5	0.14	0.02	0.14
(1,2874)	1:24:B:LEU:HD22	1:32:B:GLN:HE22	5	0.14	0.02	0.14
(1,2874)	1:24:B:LEU:HD23	1:32:B:GLN:HE22	5	0.14	0.02	0.14
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD11	5	0.14	0.03	0.13
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD12	5	0.14	0.03	0.13
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD13	5	0.14	0.03	0.13
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD2	5	0.14	0.01	0.14
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD3	5	0.14	0.01	0.14
(1,2152)	1:123:B:GLY:H	1:125:B:ASN:H	5	0.14	0.02	0.13
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD2	5	0.13	0.03	0.12
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD3	5	0.13	0.03	0.12
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD2	5	0.13	0.03	0.12
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD3	5	0.13	0.03	0.12
(1,1006)	1:123:A:GLY:H	1:125:A:ASN:H	5	0.13	0.02	0.13
(1,1498)	1:48:B:LYS:H	1:48:B:LYS:HD2	5	0.13	0.03	0.13
(1,3048)	1:74:B:GLU:HB2	1:77:B:LYS:H	5	0.13	0.02	0.13
(1,3048)	1:74:B:GLU:HB3	1:77:B:LYS:H	5	0.13	0.02	0.13
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD11	5	0.13	0.03	0.12
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD12	5	0.13	0.03	0.12
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD13	5	0.13	0.03	0.12
(1,1295)	1:27:B:VAL:HG11	1:33:B:GLY:HA2	5	0.13	0.01	0.13
(1,1295)	1:27:B:VAL:HG12	1:33:B:GLY:HA2	5	0.13	0.01	0.13
(1,1295)	1:27:B:VAL:HG13	1:33:B:GLY:HA2	5	0.13	0.01	0.13
(1,1767)	1:96:A:LYS:HB2	1:97:A:LYS:H	5	0.13	0.02	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD21	5	0.13	0.02	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD22	5	0.13	0.02	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD23	5	0.13	0.02	0.12
(1,2200)	1:119:B:MET:HE1	1:125:B:ASN:HD22	5	0.13	0.02	0.13
(1,2200)	1:119:B:MET:HE2	1:125:B:ASN:HD22	5	0.13	0.02	0.13
(1,2200)	1:119:B:MET:HE3	1:125:B:ASN:HD22	5	0.13	0.02	0.13
(1,2150)	1:119:B:MET:HE1	1:124:B:LEU:H	5	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2150)	1:119:B:MET:HE2	1:124:B:LEU:H	5	0.12	0.0	0.12
(1,2150)	1:119:B:MET:HE3	1:124:B:LEU:H	5	0.12	0.0	0.12
(1,1506)	1:20:B:TYR:H	1:21:B:LEU:H	5	0.12	0.01	0.12
(1,754)	1:27:A:VAL:HG11	1:33:A:GLY:H	5	0.12	0.02	0.11
(1,754)	1:27:A:VAL:HG12	1:33:A:GLY:H	5	0.12	0.02	0.11
(1,754)	1:27:A:VAL:HG13	1:33:A:GLY:H	5	0.12	0.02	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG12	5	0.12	0.02	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	5	0.12	0.02	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG12	5	0.12	0.02	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	5	0.12	0.02	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG12	5	0.12	0.02	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	5	0.12	0.02	0.11
(1,2236)	1:76:B:LYS:H	1:80:B:LEU:H	5	0.12	0.02	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG11	5	0.11	0.01	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG12	5	0.11	0.01	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG13	5	0.11	0.01	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG11	5	0.11	0.01	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG12	5	0.11	0.01	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG13	5	0.11	0.01	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG21	5	0.11	0.01	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG22	5	0.11	0.01	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG23	5	0.11	0.01	0.11
(1,3110)	1:87:B:LEU:HD11	1:90:B:GLN:HB3	5	0.11	0.01	0.11
(1,3110)	1:87:B:LEU:HD12	1:90:B:GLN:HB3	5	0.11	0.01	0.11
(1,3110)	1:87:B:LEU:HD13	1:90:B:GLN:HB3	5	0.11	0.01	0.11
(1,3110)	1:87:B:LEU:HD21	1:90:B:GLN:HB3	5	0.11	0.01	0.11
(1,3110)	1:87:B:LEU:HD22	1:90:B:GLN:HB3	5	0.11	0.01	0.11
(1,3110)	1:87:B:LEU:HD23	1:90:B:GLN:HB3	5	0.11	0.01	0.11
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG11	5	0.11	0.01	0.11
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG12	5	0.11	0.01	0.11
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG13	5	0.11	0.01	0.11
(1,2199)	1:120:B:ILE:HG13	1:125:B:ASN:HD21	4	0.84	0.57	0.84
(1,1047)	1:120:A:ILE:HG13	1:125:A:ASN:HD21	4	0.62	0.36	0.61
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD11	4	0.42	0.01	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD12	4	0.42	0.01	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD13	4	0.42	0.01	0.42
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB1	4	0.3	0.07	0.3
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB2	4	0.3	0.07	0.3
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB3	4	0.3	0.07	0.3
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	4	0.3	0.07	0.3
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	4	0.3	0.07	0.3
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	4	0.3	0.07	0.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD21	4	0.26	0.01	0.26
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD22	4	0.26	0.01	0.26
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD11	4	0.22	0.06	0.24
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD12	4	0.22	0.06	0.24
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD13	4	0.22	0.06	0.24
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD21	4	0.22	0.06	0.24
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD22	4	0.22	0.06	0.24
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD23	4	0.22	0.06	0.24
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD11	4	0.21	0.05	0.23
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD12	4	0.21	0.05	0.23
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD13	4	0.21	0.05	0.23
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD21	4	0.21	0.05	0.23
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD22	4	0.21	0.05	0.23
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD23	4	0.21	0.05	0.23
(1,364)	1:48:A:LYS:H	1:48:A:LYS:HD3	4	0.2	0.07	0.2
(1,2876)	1:24:B:LEU:HD11	1:90:B:GLN:HE21	4	0.19	0.06	0.2
(1,2876)	1:24:B:LEU:HD12	1:90:B:GLN:HE21	4	0.19	0.06	0.2
(1,2876)	1:24:B:LEU:HD13	1:90:B:GLN:HE21	4	0.19	0.06	0.2
(1,2876)	1:24:B:LEU:HD21	1:90:B:GLN:HE21	4	0.19	0.06	0.2
(1,2876)	1:24:B:LEU:HD22	1:90:B:GLN:HE21	4	0.19	0.06	0.2
(1,2876)	1:24:B:LEU:HD23	1:90:B:GLN:HE21	4	0.19	0.06	0.2
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD11	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD12	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD13	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD21	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD22	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD23	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD11	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD12	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD13	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD21	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD22	4	0.19	0.1	0.14
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD23	4	0.19	0.1	0.14
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD11	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD12	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD13	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD21	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD22	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD23	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD11	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD12	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD13	4	0.19	0.1	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD21	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD22	4	0.19	0.1	0.15
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD23	4	0.19	0.1	0.15
(1,2869)	1:24:B:LEU:HD11	1:32:B:GLN:H	4	0.19	0.04	0.18
(1,2869)	1:24:B:LEU:HD12	1:32:B:GLN:H	4	0.19	0.04	0.18
(1,2869)	1:24:B:LEU:HD13	1:32:B:GLN:H	4	0.19	0.04	0.18
(1,2869)	1:24:B:LEU:HD21	1:32:B:GLN:H	4	0.19	0.04	0.18
(1,2869)	1:24:B:LEU:HD22	1:32:B:GLN:H	4	0.19	0.04	0.18
(1,2869)	1:24:B:LEU:HD23	1:32:B:GLN:H	4	0.19	0.04	0.18
(1,2362)	1:24:A:LEU:HD11	1:32:A:GLN:H	4	0.18	0.03	0.18
(1,2362)	1:24:A:LEU:HD12	1:32:A:GLN:H	4	0.18	0.03	0.18
(1,2362)	1:24:A:LEU:HD13	1:32:A:GLN:H	4	0.18	0.03	0.18
(1,2362)	1:24:A:LEU:HD21	1:32:A:GLN:H	4	0.18	0.03	0.18
(1,2362)	1:24:A:LEU:HD22	1:32:A:GLN:H	4	0.18	0.03	0.18
(1,2362)	1:24:A:LEU:HD23	1:32:A:GLN:H	4	0.18	0.03	0.18
(1,1141)	1:111:B:MET:HE1	1:114:B:VAL:HB	4	0.18	0.03	0.17
(1,1141)	1:111:B:MET:HE2	1:114:B:VAL:HB	4	0.18	0.03	0.17
(1,1141)	1:111:B:MET:HE3	1:114:B:VAL:HB	4	0.18	0.03	0.17
(1,14)	1:111:A:MET:HE1	1:114:A:VAL:HB	4	0.17	0.03	0.16
(1,14)	1:111:A:MET:HE2	1:114:A:VAL:HB	4	0.17	0.03	0.16
(1,14)	1:111:A:MET:HE3	1:114:A:VAL:HB	4	0.17	0.03	0.16
(1,751)	1:24:A:LEU:HD21	1:32:A:GLN:H	4	0.17	0.03	0.17
(1,751)	1:24:A:LEU:HD22	1:32:A:GLN:H	4	0.17	0.03	0.17
(1,751)	1:24:A:LEU:HD23	1:32:A:GLN:H	4	0.17	0.03	0.17
(1,1897)	1:24:B:LEU:HD21	1:32:B:GLN:H	4	0.16	0.04	0.16
(1,1897)	1:24:B:LEU:HD22	1:32:B:GLN:H	4	0.16	0.04	0.16
(1,1897)	1:24:B:LEU:HD23	1:32:B:GLN:H	4	0.16	0.04	0.16
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD21	4	0.16	0.02	0.16
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD22	4	0.16	0.02	0.16
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD23	4	0.16	0.02	0.16
(1,893)	1:87:A:LEU:H	1:90:A:GLN:H	4	0.16	0.04	0.15
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD11	4	0.16	0.04	0.15
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD12	4	0.16	0.04	0.15
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD13	4	0.16	0.04	0.15
(1,2359)	1:24:A:LEU:HB2	1:25:A:SER:H	4	0.16	0.02	0.16
(1,2359)	1:24:A:LEU:HB3	1:25:A:SER:H	4	0.16	0.02	0.16
(1,471)	1:90:A:GLN:H	1:90:A:GLN:HE21	4	0.16	0.03	0.16
(1,1610)	1:90:B:GLN:H	1:90:B:GLN:HE21	4	0.16	0.03	0.16
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD1	4	0.15	0.05	0.12
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD2	4	0.15	0.05	0.12
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB2	4	0.15	0.03	0.15
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB3	4	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,478)	1:111:A:MET:H	1:111:A:MET:HE1	4	0.14	0.06	0.12
(1,478)	1:111:A:MET:H	1:111:A:MET:HE2	4	0.14	0.06	0.12
(1,478)	1:111:A:MET:H	1:111:A:MET:HE3	4	0.14	0.06	0.12
(1,625)	1:96:B:LYS:HB2	1:97:B:LYS:H	4	0.14	0.02	0.13
(1,1888)	1:95:A:ASP:H	1:31:B:GLU:H	4	0.14	0.01	0.14
(1,2107)	1:112:B:LYS:H	1:115:B:ASP:H	4	0.14	0.03	0.14
(1,2633)	1:95:A:ASP:HB2	1:30:B:SER:H	4	0.14	0.03	0.13
(1,2633)	1:95:A:ASP:HB3	1:30:B:SER:H	4	0.14	0.03	0.13
(1,742)	1:31:A:GLU:H	1:95:B:ASP:H	4	0.14	0.02	0.14
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE21	4	0.13	0.04	0.12
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE22	4	0.13	0.04	0.12
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE21	4	0.13	0.04	0.12
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE22	4	0.13	0.04	0.12
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD21	4	0.13	0.04	0.12
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD22	4	0.13	0.04	0.12
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD23	4	0.13	0.04	0.12
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	4	0.13	0.02	0.13
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	4	0.13	0.02	0.13
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	4	0.13	0.02	0.13
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	4	0.13	0.02	0.13
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	4	0.13	0.02	0.13
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	4	0.13	0.02	0.13
(1,961)	1:112:A:LYS:H	1:115:A:ASP:H	4	0.13	0.02	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD21	4	0.13	0.02	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD22	4	0.13	0.02	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD23	4	0.13	0.02	0.12
(1,1742)	1:42:B:GLN:HE22	1:43:B:ASN:H	4	0.13	0.01	0.12
(1,1116)	1:18:A:ASP:HA	1:105:A:TYR:HA	4	0.12	0.02	0.12
(1,2269)	1:18:B:ASP:HA	1:105:B:TYR:HA	4	0.12	0.01	0.12
(1,600)	1:42:A:GLN:HE22	1:43:A:ASN:H	4	0.12	0.01	0.12
(1,1042)	1:119:B:MET:HG3	1:124:B:LEU:H	4	0.12	0.03	0.11
(1,1489)	1:115:B:ASP:HB3	1:116:B:ASN:H	4	0.12	0.01	0.12
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG12	4	0.12	0.02	0.11
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	4	0.12	0.02	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG12	4	0.12	0.02	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	4	0.12	0.02	0.11
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG12	4	0.12	0.02	0.11
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	4	0.12	0.02	0.11
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG11	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG12	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG13	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG11	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG12	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG13	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG21	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG22	4	0.12	0.01	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG23	4	0.12	0.01	0.12
(1,418)	1:126:A:ALA:HB1	1:127:A:VAL:H	4	0.12	0.02	0.12
(1,418)	1:126:A:ALA:HB2	1:127:A:VAL:H	4	0.12	0.02	0.12
(1,418)	1:126:A:ALA:HB3	1:127:A:VAL:H	4	0.12	0.02	0.12
(1,1675)	1:124:B:LEU:H	1:124:B:LEU:HG	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB2	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB3	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB2	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB3	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB2	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB3	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB2	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB3	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB2	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB3	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB2	4	0.12	0.01	0.12
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB3	4	0.12	0.01	0.12
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG11	4	0.12	0.01	0.12
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG12	4	0.12	0.01	0.12
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG13	4	0.12	0.01	0.12
(1,865)	1:80:A:LEU:HD11	1:82:A:LYS:H	4	0.12	0.02	0.11
(1,865)	1:80:A:LEU:HD12	1:82:A:LYS:H	4	0.12	0.02	0.11
(1,865)	1:80:A:LEU:HD13	1:82:A:LYS:H	4	0.12	0.02	0.11
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG21	4	0.12	0.02	0.12
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG22	4	0.12	0.02	0.12
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG23	4	0.12	0.02	0.12
(1,534)	1:124:A:LEU:H	1:124:A:LEU:HG	4	0.12	0.0	0.12
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD11	4	0.12	0.01	0.12
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD12	4	0.12	0.01	0.12
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD13	4	0.12	0.01	0.12
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD21	4	0.12	0.01	0.12
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD22	4	0.12	0.01	0.12
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD23	4	0.12	0.01	0.12
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG11	4	0.11	0.0	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG12	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG13	4	0.11	0.0	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG21	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG22	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG23	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG21	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG22	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG23	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG21	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG22	4	0.11	0.01	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG23	4	0.11	0.01	0.11
(1,1004)	1:119:A:MET:HE1	1:124:A:LEU:H	4	0.11	0.01	0.11
(1,1004)	1:119:A:MET:HE2	1:124:A:LEU:H	4	0.11	0.01	0.11
(1,1004)	1:119:A:MET:HE3	1:124:A:LEU:H	4	0.11	0.01	0.11
(1,2149)	1:119:B:MET:HA	1:124:B:LEU:H	4	0.11	0.01	0.1
(1,1121)	1:20:A:TYR:HE1	1:40:A:ILE:HG13	3	0.25	0.07	0.29
(1,1121)	1:20:A:TYR:HE2	1:40:A:ILE:HG13	3	0.25	0.07	0.29
(1,2274)	1:20:B:TYR:HE1	1:40:B:ILE:HG13	3	0.25	0.09	0.31
(1,2274)	1:20:B:TYR:HE2	1:40:B:ILE:HG13	3	0.25	0.09	0.31
(1,766)	1:35:A:VAL:HG21	1:36:A:ARG:H	3	0.22	0.02	0.22
(1,766)	1:35:A:VAL:HG22	1:36:A:ARG:H	3	0.22	0.02	0.22
(1,766)	1:35:A:VAL:HG23	1:36:A:ARG:H	3	0.22	0.02	0.22
(1,1912)	1:35:B:VAL:HG21	1:36:B:ARG:H	3	0.21	0.01	0.21
(1,1912)	1:35:B:VAL:HG22	1:36:B:ARG:H	3	0.21	0.01	0.21
(1,1912)	1:35:B:VAL:HG23	1:36:B:ARG:H	3	0.21	0.01	0.21
(1,1234)	1:22:B:ALA:HB1	1:24:B:LEU:HG	3	0.19	0.03	0.19
(1,1234)	1:22:B:ALA:HB2	1:24:B:LEU:HG	3	0.19	0.03	0.19
(1,1234)	1:22:B:ALA:HB3	1:24:B:LEU:HG	3	0.19	0.03	0.19
(1,109)	1:22:A:ALA:HB1	1:24:A:LEU:HG	3	0.18	0.02	0.19
(1,109)	1:22:A:ALA:HB2	1:24:A:LEU:HG	3	0.18	0.02	0.19
(1,109)	1:22:A:ALA:HB3	1:24:A:LEU:HG	3	0.18	0.02	0.19
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD11	3	0.18	0.02	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD12	3	0.18	0.02	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD13	3	0.18	0.02	0.2
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD11	3	0.17	0.02	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD12	3	0.17	0.02	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD13	3	0.17	0.02	0.19
(1,582)	1:116:A:ASN:HA	1:116:A:ASN:HD21	3	0.17	0.05	0.15
(1,472)	1:90:A:GLN:HB3	1:90:A:GLN:HE21	3	0.16	0.03	0.15
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB2	3	0.16	0.04	0.14
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB3	3	0.16	0.04	0.14
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB2	3	0.16	0.04	0.14
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB3	3	0.16	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB2	3	0.16	0.04	0.14
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB3	3	0.16	0.04	0.14
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB2	3	0.16	0.04	0.14
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB3	3	0.16	0.04	0.14
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE1	3	0.15	0.06	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE2	3	0.15	0.06	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE3	3	0.15	0.06	0.11
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD21	3	0.15	0.02	0.15
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD22	3	0.15	0.02	0.15
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD21	3	0.15	0.02	0.15
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD22	3	0.15	0.02	0.15
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD1	3	0.15	0.03	0.14
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD2	3	0.15	0.03	0.14
(1,363)	1:48:A:LYS:H	1:48:A:LYS:HD2	3	0.15	0.02	0.14
(1,857)	1:73:A:ILE:HG21	1:74:A:GLU:H	3	0.15	0.04	0.13
(1,857)	1:73:A:ILE:HG22	1:74:A:GLU:H	3	0.15	0.04	0.13
(1,857)	1:73:A:ILE:HG23	1:74:A:GLU:H	3	0.15	0.04	0.13
(1,1071)	1:24:A:LEU:HD11	1:32:A:GLN:H	3	0.14	0.03	0.14
(1,1071)	1:24:A:LEU:HD12	1:32:A:GLN:H	3	0.14	0.03	0.14
(1,1071)	1:24:A:LEU:HD13	1:32:A:GLN:H	3	0.14	0.03	0.14
(1,2163)	1:113:B:GLU:HA	1:116:B:ASN:HD22	3	0.14	0.0	0.14
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG11	3	0.14	0.01	0.14
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG12	3	0.14	0.01	0.14
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG13	3	0.14	0.01	0.14
(1,2194)	1:119:A:MET:HG3	1:124:A:LEU:H	3	0.14	0.04	0.11
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD11	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD12	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD13	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD21	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD22	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD23	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD11	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD12	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD13	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD21	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD22	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD23	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD11	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD12	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD13	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD21	3	0.14	0.03	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD22	3	0.14	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD23	3	0.14	0.03	0.15
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB2	3	0.14	0.01	0.14
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB3	3	0.14	0.01	0.14
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB2	3	0.14	0.01	0.14
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB3	3	0.14	0.01	0.14
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB2	3	0.14	0.01	0.14
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB3	3	0.14	0.01	0.14
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD11	3	0.14	0.04	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD12	3	0.14	0.04	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD13	3	0.14	0.04	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD21	3	0.14	0.04	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD22	3	0.14	0.04	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD23	3	0.14	0.04	0.11
(1,1048)	1:119:A:MET:HE1	1:125:A:ASN:HD22	3	0.13	0.02	0.13
(1,1048)	1:119:A:MET:HE2	1:125:A:ASN:HD22	3	0.13	0.02	0.13
(1,1048)	1:119:A:MET:HE3	1:125:A:ASN:HD22	3	0.13	0.02	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	3	0.13	0.02	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	3	0.13	0.02	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	3	0.13	0.02	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG21	3	0.13	0.02	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG22	3	0.13	0.02	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG23	3	0.13	0.02	0.13
(1,214)	1:58:A:ILE:HG21	1:84:A:SER:HB3	3	0.13	0.01	0.13
(1,214)	1:58:A:ILE:HG22	1:84:A:SER:HB3	3	0.13	0.01	0.13
(1,214)	1:58:A:ILE:HG23	1:84:A:SER:HB3	3	0.13	0.01	0.13
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD21	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD22	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD23	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD21	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD22	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD23	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD21	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD22	3	0.13	0.02	0.12
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD23	3	0.13	0.02	0.12
(1,1764)	1:96:A:LYS:HB3	1:97:A:LYS:H	3	0.13	0.02	0.12
(1,2011)	1:80:B:LEU:HD11	1:82:B:LYS:H	3	0.13	0.02	0.12
(1,2011)	1:80:B:LEU:HD12	1:82:B:LYS:H	3	0.13	0.02	0.12
(1,2011)	1:80:B:LEU:HD13	1:82:B:LYS:H	3	0.13	0.02	0.12
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD11	3	0.13	0.04	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD12	3	0.13	0.04	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD13	3	0.13	0.04	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD21	3	0.13	0.04	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD22	3	0.13	0.04	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD23	3	0.13	0.04	0.11
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB2	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB3	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB2	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB3	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB2	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB3	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB2	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB3	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB2	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB3	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB2	3	0.13	0.04	0.1
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB3	3	0.13	0.04	0.1
(1,404)	1:32:A:GLN:H	1:32:A:GLN:HE21	3	0.13	0.01	0.13
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG11	3	0.13	0.01	0.13
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG12	3	0.13	0.01	0.13
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG13	3	0.13	0.01	0.13
(1,2180)	1:23:B:ASP:H	1:100:B:LYS:H	3	0.12	0.02	0.12
(1,2550)	1:74:A:GLU:HG2	1:76:A:LYS:H	3	0.12	0.01	0.12
(1,2550)	1:74:A:GLU:HG3	1:76:A:LYS:H	3	0.12	0.01	0.12
(1,43)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	3	0.12	0.02	0.12
(1,43)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	3	0.12	0.02	0.12
(1,43)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	3	0.12	0.02	0.12
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD21	3	0.12	0.01	0.11
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD22	3	0.12	0.01	0.11
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD23	3	0.12	0.01	0.11
(1,622)	1:96:B:LYS:HB3	1:97:B:LYS:H	3	0.12	0.03	0.1
(1,1003)	1:119:A:MET:HA	1:124:A:LEU:H	3	0.12	0.01	0.12
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG21	3	0.12	0.01	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG22	3	0.12	0.01	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG23	3	0.12	0.01	0.13
(1,1034)	1:23:A:ASP:H	1:100:A:LYS:H	3	0.12	0.02	0.12
(1,1169)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	3	0.12	0.02	0.12
(1,1169)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	3	0.12	0.02	0.12
(1,1169)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	3	0.12	0.02	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG11	3	0.12	0.01	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG12	3	0.12	0.01	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG13	3	0.12	0.01	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG21	3	0.12	0.01	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG22	3	0.12	0.01	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG23	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2872)	1:24:B:LEU:HD21	1:32:B:GLN:HG2	3	0.12	0.02	0.12
(1,2872)	1:24:B:LEU:HD22	1:32:B:GLN:HG2	3	0.12	0.02	0.12
(1,2872)	1:24:B:LEU:HD23	1:32:B:GLN:HG2	3	0.12	0.02	0.12
(1,926)	1:99:B:LEU:HD21	1:100:B:LYS:H	3	0.12	0.0	0.12
(1,926)	1:99:B:LEU:HD22	1:100:B:LYS:H	3	0.12	0.0	0.12
(1,926)	1:99:B:LEU:HD23	1:100:B:LYS:H	3	0.12	0.0	0.12
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG21	3	0.12	0.01	0.12
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG22	3	0.12	0.01	0.12
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG23	3	0.12	0.01	0.12
(1,2072)	1:99:A:LEU:HD21	1:100:A:LYS:H	3	0.12	0.0	0.12
(1,2072)	1:99:A:LEU:HD22	1:100:A:LYS:H	3	0.12	0.0	0.12
(1,2072)	1:99:A:LEU:HD23	1:100:A:LYS:H	3	0.12	0.0	0.12
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB2	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB3	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB2	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB3	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB2	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB3	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB2	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB3	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB2	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB3	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB2	3	0.11	0.01	0.11
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB3	3	0.11	0.01	0.11
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD11	3	0.11	0.01	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD12	3	0.11	0.01	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD13	3	0.11	0.01	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG21	3	0.11	0.01	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG22	3	0.11	0.01	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG23	3	0.11	0.01	0.12
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE1	3	0.11	0.0	0.11
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE2	3	0.11	0.0	0.11
(1,2377)	1:26:A:PRO:HD2	1:27:A:VAL:H	3	0.11	0.01	0.11
(1,2377)	1:26:A:PRO:HD3	1:27:A:VAL:H	3	0.11	0.01	0.11
(1,2610)	1:87:A:LEU:HD11	1:90:A:GLN:HB3	3	0.11	0.0	0.11
(1,2610)	1:87:A:LEU:HD12	1:90:A:GLN:HB3	3	0.11	0.0	0.11
(1,2610)	1:87:A:LEU:HD13	1:90:A:GLN:HB3	3	0.11	0.0	0.11
(1,2610)	1:87:A:LEU:HD21	1:90:A:GLN:HB3	3	0.11	0.0	0.11
(1,2610)	1:87:A:LEU:HD22	1:90:A:GLN:HB3	3	0.11	0.0	0.11
(1,2610)	1:87:A:LEU:HD23	1:90:A:GLN:HB3	3	0.11	0.0	0.11
(1,2949)	1:43:B:ASN:HB2	1:44:B:ASP:H	3	0.11	0.0	0.11
(1,2949)	1:43:B:ASN:HB3	1:44:B:ASP:H	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG21	3	0.1	0.0	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG22	3	0.1	0.0	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG23	3	0.1	0.0	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG21	3	0.1	0.0	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG22	3	0.1	0.0	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG23	3	0.1	0.0	0.1
(1,226)	1:111:B:MET:HA	1:112:B:LYS:HE2	2	3.75	0.43	3.75
(1,1353)	1:111:A:MET:HA	1:112:A:LYS:HE2	2	3.56	0.3	3.56
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE1	2	0.35	0.01	0.35
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE2	2	0.35	0.01	0.35
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE3	2	0.35	0.01	0.35
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE1	2	0.34	0.02	0.34
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE2	2	0.34	0.02	0.34
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE3	2	0.34	0.02	0.34
(1,1066)	1:32:B:GLN:HB3	1:32:B:GLN:HE21	2	0.22	0.06	0.22
(1,916)	1:95:A:ASP:HB3	1:97:A:LYS:H	2	0.22	0.04	0.22
(1,1172)	1:117:B:ALA:HB1	1:118:B:LEU:HB2	2	0.2	0.02	0.2
(1,1172)	1:117:B:ALA:HB2	1:118:B:LEU:HB2	2	0.2	0.02	0.2
(1,1172)	1:117:B:ALA:HB3	1:118:B:LEU:HB2	2	0.2	0.02	0.2
(1,2062)	1:95:B:ASP:HB3	1:97:B:LYS:H	2	0.2	0.04	0.2
(1,2161)	1:112:B:LYS:HB3	1:116:B:ASN:HD22	2	0.2	0.05	0.2
(1,2369)	1:24:A:LEU:HD11	1:90:A:GLN:HE21	2	0.2	0.06	0.2
(1,2369)	1:24:A:LEU:HD12	1:90:A:GLN:HE21	2	0.2	0.06	0.2
(1,2369)	1:24:A:LEU:HD13	1:90:A:GLN:HE21	2	0.2	0.06	0.2
(1,2369)	1:24:A:LEU:HD21	1:90:A:GLN:HE21	2	0.2	0.06	0.2
(1,2369)	1:24:A:LEU:HD22	1:90:A:GLN:HE21	2	0.2	0.06	0.2
(1,2369)	1:24:A:LEU:HD23	1:90:A:GLN:HE21	2	0.2	0.06	0.2
(1,290)	1:28:A:GLN:HG2	1:28:A:GLN:HE22	2	0.2	0.01	0.2
(1,1015)	1:112:A:LYS:HB3	1:116:A:ASN:HD22	2	0.19	0.08	0.19
(1,1419)	1:28:B:GLN:HG2	1:28:B:GLN:HE22	2	0.19	0.01	0.19
(1,1634)	1:15:B:ARG:H	1:15:B:ARG:HG3	2	0.19	0.05	0.19
(1,2218)	1:32:A:GLN:HB3	1:32:A:GLN:HE21	2	0.18	0.02	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD11	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD12	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD13	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD21	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD22	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD23	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD11	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD12	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD13	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD21	2	0.18	0.0	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD22	2	0.18	0.0	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD23	2	0.18	0.0	0.18
(1,46)	1:117:A:ALA:HB1	1:118:A:LEU:HB2	2	0.18	0.02	0.18
(1,46)	1:117:A:ALA:HB2	1:118:A:LEU:HB2	2	0.18	0.02	0.18
(1,46)	1:117:A:ALA:HB3	1:118:A:LEU:HB2	2	0.18	0.02	0.18
(1,495)	1:15:A:ARG:H	1:15:A:ARG:HG3	2	0.18	0.04	0.18
(1,356)	1:115:B:ASP:HB2	1:116:B:ASN:H	2	0.17	0.04	0.17
(1,898)	1:91:A:ILE:H	1:93:B:THR:HB	2	0.17	0.01	0.17
(1,2159)	1:112:A:LYS:HB2	1:116:A:ASN:HD21	2	0.17	0.07	0.17
(1,2019)	1:73:B:ILE:HB	1:84:B:SER:H	2	0.16	0.06	0.16
(1,2044)	1:93:A:THR:HB	1:91:B:ILE:H	2	0.16	0.02	0.16
(1,2224)	1:24:B:LEU:HD11	1:32:B:GLN:H	2	0.16	0.01	0.16
(1,2224)	1:24:B:LEU:HD12	1:32:B:GLN:H	2	0.16	0.01	0.16
(1,2224)	1:24:B:LEU:HD13	1:32:B:GLN:H	2	0.16	0.01	0.16
(1,2871)	1:24:B:LEU:HD11	1:32:B:GLN:HG2	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD11	1:32:B:GLN:HG3	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD12	1:32:B:GLN:HG2	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD12	1:32:B:GLN:HG3	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD13	1:32:B:GLN:HG2	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD13	1:32:B:GLN:HG3	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD21	1:32:B:GLN:HG2	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD21	1:32:B:GLN:HG3	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD22	1:32:B:GLN:HG2	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD22	1:32:B:GLN:HG3	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD23	1:32:B:GLN:HG2	2	0.16	0.04	0.16
(1,2871)	1:24:B:LEU:HD23	1:32:B:GLN:HG3	2	0.16	0.04	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD11	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD12	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD13	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD21	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD22	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD23	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD11	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD12	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD13	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD21	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD22	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD23	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD11	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD12	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD13	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD21	2	0.16	0.01	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD22	2	0.16	0.01	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD23	2	0.16	0.01	0.16
(1,873)	1:73:A:ILE:HB	1:84:A:SER:H	2	0.15	0.05	0.15
(1,1103)	1:73:A:ILE:HD11	1:78:A:TYR:HD1	2	0.15	0.01	0.15
(1,1103)	1:73:A:ILE:HD11	1:78:A:TYR:HD2	2	0.15	0.01	0.15
(1,1103)	1:73:A:ILE:HD12	1:78:A:TYR:HD1	2	0.15	0.01	0.15
(1,1103)	1:73:A:ILE:HD12	1:78:A:TYR:HD2	2	0.15	0.01	0.15
(1,1103)	1:73:A:ILE:HD13	1:78:A:TYR:HD1	2	0.15	0.01	0.15
(1,1103)	1:73:A:ILE:HD13	1:78:A:TYR:HD2	2	0.15	0.01	0.15
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG21	2	0.15	0.05	0.15
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG22	2	0.15	0.05	0.15
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG23	2	0.15	0.05	0.15
(1,2256)	1:73:B:ILE:HD11	1:78:B:TYR:HD1	2	0.15	0.01	0.15
(1,2256)	1:73:B:ILE:HD11	1:78:B:TYR:HD2	2	0.15	0.01	0.15
(1,2256)	1:73:B:ILE:HD12	1:78:B:TYR:HD1	2	0.15	0.01	0.15
(1,2256)	1:73:B:ILE:HD12	1:78:B:TYR:HD2	2	0.15	0.01	0.15
(1,2256)	1:73:B:ILE:HD13	1:78:B:TYR:HD1	2	0.15	0.01	0.15
(1,2256)	1:73:B:ILE:HD13	1:78:B:TYR:HD2	2	0.15	0.01	0.15
(1,1484)	1:120:B:ILE:H	1:120:B:ILE:HG13	2	0.15	0.04	0.15
(1,2587)	1:80:A:LEU:HD11	1:84:A:SER:HB2	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD11	1:84:A:SER:HB3	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD12	1:84:A:SER:HB2	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD12	1:84:A:SER:HB3	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD13	1:84:A:SER:HB2	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD13	1:84:A:SER:HB3	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD21	1:84:A:SER:HB2	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD21	1:84:A:SER:HB3	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD22	1:84:A:SER:HB2	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD22	1:84:A:SER:HB3	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD23	1:84:A:SER:HB2	2	0.15	0.03	0.15
(1,2587)	1:80:A:LEU:HD23	1:84:A:SER:HB3	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD11	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD12	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD13	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD21	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD22	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD23	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD11	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD12	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD13	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD21	2	0.15	0.03	0.15
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD22	2	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD23	2	0.15	0.03	0.15
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG11	2	0.15	0.03	0.15
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG12	2	0.15	0.03	0.15
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG13	2	0.15	0.03	0.15
(1,1938)	1:42:B:GLN:HE21	1:45:B:THR:H	2	0.14	0.03	0.14
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB1	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB2	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB3	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB1	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB2	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB3	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB1	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB2	2	0.14	0.02	0.14
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB3	2	0.14	0.02	0.14
(1,1611)	1:90:B:GLN:HB3	1:90:B:GLN:HE21	2	0.14	0.01	0.14
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	2	0.14	0.04	0.14
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	2	0.14	0.04	0.14
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	2	0.14	0.04	0.14
(1,2972)	1:48:B:LYS:HE2	1:49:B:TYR:HE1	2	0.14	0.01	0.14
(1,2972)	1:48:B:LYS:HE2	1:49:B:TYR:HE2	2	0.14	0.01	0.14
(1,2972)	1:48:B:LYS:HE3	1:49:B:TYR:HE1	2	0.14	0.01	0.14
(1,2972)	1:48:B:LYS:HE3	1:49:B:TYR:HE2	2	0.14	0.01	0.14
(1,2960)	1:45:B:THR:HG21	1:48:B:LYS:HG2	2	0.14	0.02	0.14
(1,2960)	1:45:B:THR:HG21	1:48:B:LYS:HG3	2	0.14	0.02	0.14
(1,2960)	1:45:B:THR:HG22	1:48:B:LYS:HG2	2	0.14	0.02	0.14
(1,2960)	1:45:B:THR:HG22	1:48:B:LYS:HG3	2	0.14	0.02	0.14
(1,2960)	1:45:B:THR:HG23	1:48:B:LYS:HG2	2	0.14	0.02	0.14
(1,2960)	1:45:B:THR:HG23	1:48:B:LYS:HG3	2	0.14	0.02	0.14
(1,3240)	1:119:B:MET:HE1	1:124:B:LEU:HB2	2	0.14	0.02	0.14
(1,3240)	1:119:B:MET:HE1	1:124:B:LEU:HB3	2	0.14	0.02	0.14
(1,3240)	1:119:B:MET:HE2	1:124:B:LEU:HB2	2	0.14	0.02	0.14
(1,3240)	1:119:B:MET:HE2	1:124:B:LEU:HB3	2	0.14	0.02	0.14
(1,3240)	1:119:B:MET:HE3	1:124:B:LEU:HB2	2	0.14	0.02	0.14
(1,3240)	1:119:B:MET:HE3	1:124:B:LEU:HB3	2	0.14	0.02	0.14
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB1	2	0.13	0.0	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB2	2	0.13	0.0	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB3	2	0.13	0.0	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB1	2	0.13	0.0	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB2	2	0.13	0.0	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB3	2	0.13	0.0	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB1	2	0.13	0.0	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB2	2	0.13	0.0	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB3	2	0.13	0.0	0.13
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG11	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG12	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG13	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG21	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG22	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG23	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG11	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG12	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG13	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG21	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG22	2	0.13	0.02	0.13
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG23	2	0.13	0.02	0.13
(1,41)	1:73:A:ILE:HG21	1:78:A:TYR:HB3	2	0.12	0.02	0.12
(1,41)	1:73:A:ILE:HG22	1:78:A:TYR:HB3	2	0.12	0.02	0.12
(1,41)	1:73:A:ILE:HG23	1:78:A:TYR:HB3	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD21	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD22	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD23	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD21	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD22	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD23	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD21	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD22	2	0.12	0.02	0.12
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD23	2	0.12	0.02	0.12
(1,1341)	1:58:B:ILE:HG21	1:84:B:SER:HB3	2	0.12	0.02	0.12
(1,1341)	1:58:B:ILE:HG22	1:84:B:SER:HB3	2	0.12	0.02	0.12
(1,1341)	1:58:B:ILE:HG23	1:84:B:SER:HB3	2	0.12	0.02	0.12
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG11	2	0.12	0.02	0.12
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG12	2	0.12	0.02	0.12
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG13	2	0.12	0.02	0.12
(1,2342)	1:21:A:LEU:HD11	1:103:A:LEU:H	2	0.12	0.02	0.12
(1,2342)	1:21:A:LEU:HD12	1:103:A:LEU:H	2	0.12	0.02	0.12
(1,2342)	1:21:A:LEU:HD13	1:103:A:LEU:H	2	0.12	0.02	0.12
(1,2342)	1:21:A:LEU:HD21	1:103:A:LEU:H	2	0.12	0.02	0.12
(1,2342)	1:21:A:LEU:HD22	1:103:A:LEU:H	2	0.12	0.02	0.12
(1,2342)	1:21:A:LEU:HD23	1:103:A:LEU:H	2	0.12	0.02	0.12
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG11	2	0.12	0.02	0.12
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG12	2	0.12	0.02	0.12
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG13	2	0.12	0.02	0.12
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG21	2	0.12	0.02	0.12
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG22	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)
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG23	2	0.12	0.02	0.12
(1,2884)	1:26:B:PRO:HD2	1:27:B:VAL:H	2	0.12	0.01	0.12
(1,2884)	1:26:B:PRO:HD3	1:27:B:VAL:H	2	0.12	0.01	0.12
(1,78)	1:71:A:VAL:HG21	1:113:A:GLU:HB3	2	0.12	0.02	0.12
(1,78)	1:71:A:VAL:HG22	1:113:A:GLU:HB3	2	0.12	0.02	0.12
(1,78)	1:71:A:VAL:HG23	1:113:A:GLU:HB3	2	0.12	0.02	0.12
(1,1167)	1:73:B:ILE:HG21	1:78:B:TYR:HB3	2	0.12	0.02	0.12
(1,1167)	1:73:B:ILE:HG22	1:78:B:TYR:HB3	2	0.12	0.02	0.12
(1,1167)	1:73:B:ILE:HG23	1:78:B:TYR:HB3	2	0.12	0.02	0.12
(1,1933)	1:122:A:LEU:HA	1:43:B:ASN:H	2	0.12	0.02	0.12
(1,192)	1:16:A:ARG:HA	1:40:A:ILE:HB	2	0.12	0.01	0.12
(1,261)	1:52:A:THR:HG21	1:95:A:ASP:HA	2	0.12	0.01	0.12
(1,261)	1:52:A:THR:HG22	1:95:A:ASP:HA	2	0.12	0.01	0.12
(1,261)	1:52:A:THR:HG23	1:95:A:ASP:HA	2	0.12	0.01	0.12
(1,727)	1:22:A:ALA:H	1:35:A:VAL:HB	2	0.12	0.01	0.12
(1,1118)	1:18:A:ASP:H	1:20:A:TYR:HE1	2	0.12	0.0	0.12
(1,1118)	1:18:A:ASP:H	1:20:A:TYR:HE2	2	0.12	0.0	0.12
(1,1388)	1:52:B:THR:HG21	1:95:B:ASP:HA	2	0.12	0.0	0.12
(1,1388)	1:52:B:THR:HG22	1:95:B:ASP:HA	2	0.12	0.0	0.12
(1,1388)	1:52:B:THR:HG23	1:95:B:ASP:HA	2	0.12	0.0	0.12
(1,1553)	1:126:B:ALA:HB1	1:127:B:VAL:H	2	0.12	0.0	0.12
(1,1553)	1:126:B:ALA:HB2	1:127:B:VAL:H	2	0.12	0.0	0.12
(1,1553)	1:126:B:ALA:HB3	1:127:B:VAL:H	2	0.12	0.0	0.12
(1,2365)	1:24:A:LEU:HD21	1:32:A:GLN:HG2	2	0.12	0.01	0.12
(1,2365)	1:24:A:LEU:HD22	1:32:A:GLN:HG2	2	0.12	0.01	0.12
(1,2365)	1:24:A:LEU:HD23	1:32:A:GLN:HG2	2	0.12	0.01	0.12
(1,2769)	1:123:A:GLY:HA2	1:43:B:ASN:HD21	2	0.12	0.01	0.12
(1,2769)	1:123:A:GLY:HA2	1:43:B:ASN:HD22	2	0.12	0.01	0.12
(1,2769)	1:123:A:GLY:HA3	1:43:B:ASN:HD21	2	0.12	0.01	0.12
(1,2769)	1:123:A:GLY:HA3	1:43:B:ASN:HD22	2	0.12	0.01	0.12
(1,2849)	1:21:B:LEU:HD11	1:103:B:LEU:H	2	0.12	0.01	0.12
(1,2849)	1:21:B:LEU:HD12	1:103:B:LEU:H	2	0.12	0.01	0.12
(1,2849)	1:21:B:LEU:HD13	1:103:B:LEU:H	2	0.12	0.01	0.12
(1,2849)	1:21:B:LEU:HD21	1:103:B:LEU:H	2	0.12	0.01	0.12
(1,2849)	1:21:B:LEU:HD22	1:103:B:LEU:H	2	0.12	0.01	0.12
(1,2849)	1:21:B:LEU:HD23	1:103:B:LEU:H	2	0.12	0.01	0.12
(1,2448)	1:43:A:ASN:HB2	1:44:A:ASP:H	2	0.12	0.02	0.12
(1,2448)	1:43:A:ASN:HB3	1:44:A:ASP:H	2	0.12	0.02	0.12
(1,2560)	1:75:A:LYS:HD2	1:82:A:LYS:HB2	2	0.12	0.02	0.12
(1,2560)	1:75:A:LYS:HD2	1:82:A:LYS:HB3	2	0.12	0.02	0.12
(1,2560)	1:75:A:LYS:HD3	1:82:A:LYS:HB2	2	0.12	0.02	0.12
(1,2560)	1:75:A:LYS:HD3	1:82:A:LYS:HB3	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)
(1,3049)	1:74:B:GLU:HB2	1:77:B:LYS:HB2	2	0.12	0.02	0.12
(1,3049)	1:74:B:GLU:HB2	1:77:B:LYS:HB3	2	0.12	0.02	0.12
(1,3049)	1:74:B:GLU:HB3	1:77:B:LYS:HB2	2	0.12	0.02	0.12
(1,3049)	1:74:B:GLU:HB3	1:77:B:LYS:HB3	2	0.12	0.02	0.12
(1,140)	1:19:B:VAL:HG11	1:37:B:PRO:HB3	2	0.12	0.0	0.12
(1,140)	1:19:B:VAL:HG12	1:37:B:PRO:HB3	2	0.12	0.0	0.12
(1,140)	1:19:B:VAL:HG13	1:37:B:PRO:HB3	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB1	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB2	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB3	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB1	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB2	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB3	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB1	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB2	2	0.12	0.0	0.12
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB3	2	0.12	0.0	0.12
(1,457)	1:94:A:LEU:HB3	1:95:A:ASP:H	2	0.12	0.0	0.12
(1,1266)	1:19:A:VAL:HG11	1:37:A:PRO:HB3	2	0.12	0.0	0.12
(1,1266)	1:19:A:VAL:HG12	1:37:A:PRO:HB3	2	0.12	0.0	0.12
(1,1266)	1:19:A:VAL:HG13	1:37:A:PRO:HB3	2	0.12	0.0	0.12
(1,329)	1:82:A:LYS:H	1:82:A:LYS:HB2	2	0.11	0.01	0.11
(1,1119)	1:18:A:ASP:HB3	1:20:A:TYR:HE1	2	0.11	0.01	0.11
(1,1119)	1:18:A:ASP:HB3	1:20:A:TYR:HE2	2	0.11	0.01	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG21	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG22	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG23	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG21	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG22	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG23	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG21	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG22	2	0.11	0.0	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG23	2	0.11	0.0	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD11	2	0.11	0.0	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD12	2	0.11	0.0	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD13	2	0.11	0.0	0.11
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG21	2	0.11	0.01	0.11
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG22	2	0.11	0.01	0.11
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG23	2	0.11	0.01	0.11
(1,1594)	1:94:B:LEU:HB3	1:95:B:ASP:H	2	0.11	0.01	0.11
(1,1707)	1:127:B:VAL:HB	1:128:B:ALA:H	2	0.11	0.01	0.11
(1,2271)	1:18:B:ASP:H	1:20:B:TYR:HE1	2	0.11	0.0	0.11
(1,2271)	1:18:B:ASP:H	1:20:B:TYR:HE2	2	0.11	0.0	0.11

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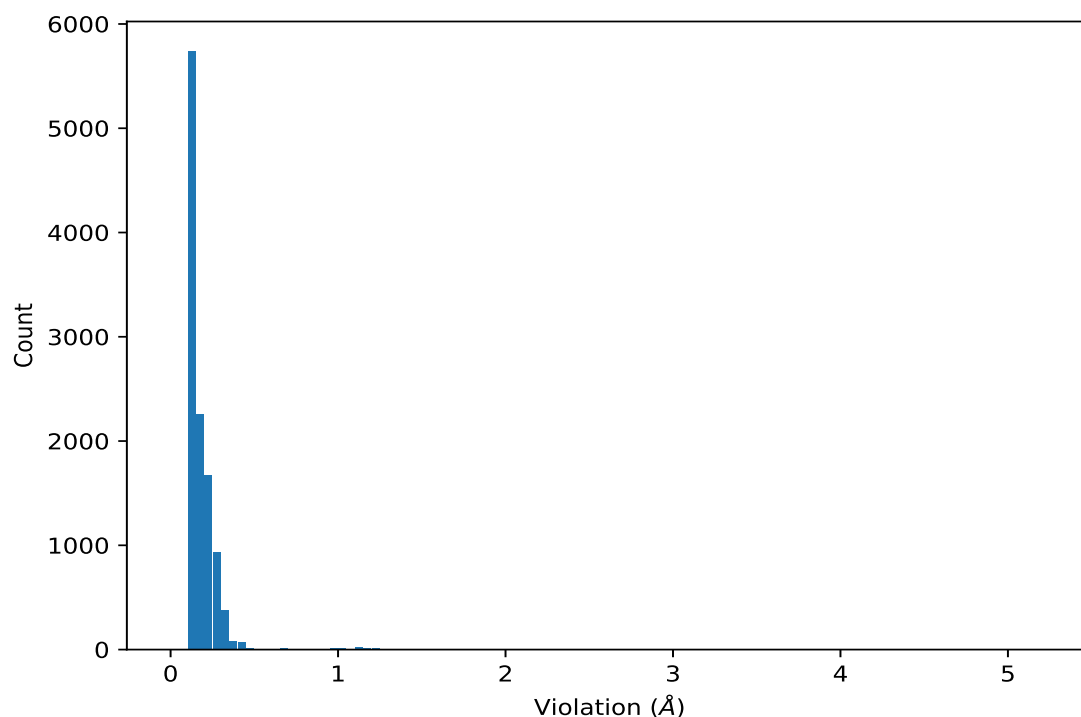
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,564)	1:127:A:VAL:HB	1:128:A:ALA:H	2	0.11	0.0	0.11
(1,1873)	1:22:B:ALA:H	1:35:B:VAL:HB	2	0.11	0.0	0.11
(1,2316)	1:19:A:VAL:HG11	1:106:A:LEU:H	2	0.11	0.0	0.11
(1,2316)	1:19:A:VAL:HG12	1:106:A:LEU:H	2	0.11	0.0	0.11
(1,2316)	1:19:A:VAL:HG13	1:106:A:LEU:H	2	0.11	0.0	0.11
(1,2316)	1:19:A:VAL:HG21	1:106:A:LEU:H	2	0.11	0.0	0.11
(1,2316)	1:19:A:VAL:HG22	1:106:A:LEU:H	2	0.11	0.0	0.11
(1,2316)	1:19:A:VAL:HG23	1:106:A:LEU:H	2	0.11	0.0	0.11
(1,2566)	1:76:A:LYS:HA	1:76:A:LYS:HD2	2	0.11	0.0	0.11
(1,2566)	1:76:A:LYS:HA	1:76:A:LYS:HD3	2	0.11	0.0	0.11
(1,491)	1:74:A:GLU:H	1:74:A:GLU:HG3	2	0.1	0.0	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG21	2	0.1	0.0	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG22	2	0.1	0.0	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG23	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)
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	20	5.21
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	4	5.06
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	20	4.99
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	4	4.98
(1,226)	1:111:B:MET:HA	1:112:B:LYS:HE2	20	4.18
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	20	4.15
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	20	4.15
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	20	3.88
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	20	3.88
(1,1353)	1:111:A:MET:HA	1:112:A:LYS:HE2	20	3.86
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	4	3.52
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	4	3.52
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	4	3.45
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	4	3.45
(1,226)	1:111:B:MET:HA	1:112:B:LYS:HE2	4	3.32
(1,1353)	1:111:A:MET:HA	1:112:A:LYS:HE2	4	3.25
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	3	3.05
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	3	3.05
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	12	3.05
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	12	3.05
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	7	2.83
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	7	2.83
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	10	2.82
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	10	2.82
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	14	2.3
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	14	2.3
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	15	2.3
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	15	2.3
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	9	2.28
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	9	2.28
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	9	2.28
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	9	2.28
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	10	2.14
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	10	2.14
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	10	2.14
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	10	2.14
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	12	2.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	12	2.11
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	12	2.11
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	12	2.11
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	8	2.05
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	8	2.03
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	7	1.99
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	7	1.99
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	7	1.99
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	7	1.99
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	3	1.94
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	3	1.94
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	3	1.94
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	3	1.94
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	3	1.85
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	3	1.85
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	16	1.81
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	16	1.81
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	13	1.75
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	13	1.75
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	12	1.74
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	12	1.74
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	10	1.64
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	10	1.64
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	13	1.61
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	13	1.61
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	13	1.61
(1,2199)	1:120:B:ILE:HG13	1:125:B:ASN:HD21	15	1.54
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	15	1.51
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	15	1.51
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	15	1.51
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	7	1.5
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	7	1.5
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	16	1.5
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	16	1.5
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	16	1.5
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	14	1.46
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	14	1.46
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	14	1.46
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	1	1.46
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	1	1.43
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	1	1.43
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	9	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	9	1.4
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	9	1.4
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG21	2	1.36
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG22	2	1.36
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG23	2	1.36
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG21	2	1.35
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG22	2	1.35
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG23	2	1.35
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG21	9	1.33
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG22	9	1.33
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG23	9	1.33
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	13	1.29
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	13	1.29
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	9	1.27
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	9	1.27
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	18	1.26
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	18	1.26
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	9	1.26
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	15	1.24
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG21	9	1.24
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG22	9	1.24
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG23	9	1.24
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	13	1.23
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	13	1.23
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	13	1.23
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	15	1.23
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	16	1.22
(1,2199)	1:120:B:ILE:HG13	1:125:B:ASN:HD21	16	1.22
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG21	6	1.18
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG22	6	1.18
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG23	6	1.18
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	16	1.18
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	16	1.18
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	16	1.18
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	14	1.17
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	1	1.16
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	5	1.16
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	8	1.16
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	8	1.15
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG21	6	1.14
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG22	6	1.14
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG23	6	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG21	8	1.14
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG22	8	1.14
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG23	8	1.14
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	7	1.14
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	5	1.13
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	5	1.13
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG21	8	1.13
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG22	8	1.13
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG23	8	1.13
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	7	1.13
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	2	1.13
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	11	1.13
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	20	1.12
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	20	1.12
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	15	1.12
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	15	1.12
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	15	1.12
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	1	1.12
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	5	1.11
(1,1047)	1:120:A:ILE:HG13	1:125:A:ASN:HD21	15	1.11
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	10	1.1
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	14	1.1
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	14	1.1
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	14	1.1
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	10	1.09
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	11	1.08
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	17	1.06
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	17	1.06
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	2	1.06
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	5	1.06
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	3	1.06
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	17	1.06
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	1	1.05
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	18	1.04
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	18	1.04
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	3	1.04
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	6	1.04
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	18	1.02
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	5	1.02
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	16	1.01
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	12	1.0
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	17	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	3	1.0
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	3	1.0
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	3	1.0
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	12	1.0
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	4	0.98
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	4	0.98
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	19	0.97
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	19	0.97
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	7	0.97
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	7	0.97
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	7	0.97
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	7	0.97
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	6	0.97
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	16	0.97
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	18	0.97
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	14	0.94
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	16	0.93
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	15	0.92
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	9	0.92
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	14	0.89
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	15	0.89
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	19	0.89
(1,1354)	1:111:A:MET:HA	1:112:A:LYS:HE3	19	0.88
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	20	0.87
(1,227)	1:111:B:MET:HA	1:112:B:LYS:HE3	14	0.85
(1,1047)	1:120:A:ILE:HG13	1:125:A:ASN:HD21	16	0.8
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	20	0.8
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	20	0.79
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	13	0.76
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	10	0.75
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	10	0.75
(1,2279)	1:73:B:ILE:HG13	1:78:B:TYR:HD1	4	0.71
(1,2279)	1:73:B:ILE:HG13	1:78:B:TYR:HD2	4	0.71
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	7	0.71
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	7	0.71
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	7	0.71
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	13	0.71
(1,1126)	1:73:A:ILE:HG13	1:78:A:TYR:HD1	4	0.69
(1,1126)	1:73:A:ILE:HG13	1:78:A:TYR:HD2	4	0.69
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	8	0.69
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	8	0.69
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	3	0.68
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	3	0.68
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	8	0.68
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	8	0.68
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	8	0.68
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	2	0.67
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	2	0.67
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	11	0.66
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	6	0.65
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	6	0.65
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	7	0.65
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	7	0.65
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	3	0.64
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	11	0.63
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	3	0.63
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	12	0.61
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	12	0.61
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	11	0.59
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	11	0.59
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	16	0.59
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB2	8	0.56
(1,3246)	1:120:B:ILE:HG13	1:121:B:SER:HB3	8	0.56
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	18	0.55
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	15	0.53
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	13	0.52
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	15	0.52
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	20	0.52
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	18	0.51
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	7	0.51
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	13	0.51
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	9	0.5
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	16	0.5
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	6	0.49
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	12	0.49
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	7	0.48
(1,2199)	1:120:B:ILE:HG13	1:125:B:ASN:HD21	13	0.47
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	7	0.46
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	7	0.46
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	7	0.46
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	7	0.46
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	7	0.46
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	6	0.46
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	8	0.46
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	8	0.45
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	8	0.45
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	8	0.45
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	20	0.45
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	12	0.45
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	9	0.45
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	10	0.44
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	2	0.44
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	8	0.44
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	2	0.44
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	2	0.43
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	17	0.43
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	2	0.43
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD11	1	0.43
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD12	1	0.43
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD13	1	0.43
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD11	17	0.43
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD12	17	0.43
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD13	17	0.43
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD11	16	0.43
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD12	16	0.43
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD13	16	0.43
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD11	17	0.43
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD12	17	0.43
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD13	17	0.43
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	3	0.42
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	3	0.42
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	3	0.42
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	3	0.42
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	19	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD11	16	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD12	16	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD13	16	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD11	18	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD12	18	0.42
(1,1237)	1:21:B:LEU:HA	1:21:B:LEU:HD13	18	0.42
(1,1047)	1:120:A:ILE:HG13	1:125:A:ASN:HD21	20	0.42
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD11	1	0.42
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD12	1	0.42
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD13	1	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2860)	1:23:B:ASP:HB2	1:25:B:SER:H	7	0.41
(1,2860)	1:23:B:ASP:HB3	1:25:B:SER:H	7	0.41
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	14	0.41
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	14	0.41
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	14	0.41
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	14	0.41
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB1	13	0.41
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB2	13	0.41
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB3	13	0.41
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	13	0.41
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	13	0.41
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	13	0.41
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	7	0.41
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	7	0.41
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	7	0.41
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	7	0.41
(1,2642)	1:98:A:ARG:H	1:98:A:ARG:HG2	13	0.41
(1,2642)	1:98:A:ARG:H	1:98:A:ARG:HG3	13	0.41
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	8	0.41
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	1	0.41
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	5	0.41
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	4	0.41
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	8	0.41
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	8	0.41
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	8	0.41
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	17	0.41
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	1	0.41
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD11	18	0.41
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD12	18	0.41
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD13	18	0.41
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	5	0.4
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	5	0.4
(1,3138)	1:98:B:ARG:H	1:98:B:ARG:HG2	13	0.4
(1,3138)	1:98:B:ARG:H	1:98:B:ARG:HG3	13	0.4
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	5	0.4
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	5	0.4
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	15	0.4
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	15	0.4
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	15	0.4
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	19	0.4
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	10	0.39
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	10	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	10	0.39
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	10	0.39
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	1	0.39
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	1	0.39
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	8	0.39
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	8	0.39
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	16	0.39
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	16	0.39
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	16	0.39
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	16	0.39
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	13	0.39
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	9	0.39
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	10	0.39
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	10	0.39
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	13	0.38
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	13	0.38
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	8	0.38
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	8	0.38
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	18	0.38
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	5	0.38
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	5	0.38
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	5	0.38
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	8	0.38
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD11	15	0.38
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD12	15	0.38
(1,112)	1:21:A:LEU:HA	1:21:A:LEU:HD13	15	0.38
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	12	0.37
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	12	0.37
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	12	0.37
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	12	0.37
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	13	0.37
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	13	0.37
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	13	0.37
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	13	0.37
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	4	0.37
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	4	0.37
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	9	0.37
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	9	0.37
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	10	0.37
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	8	0.37
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD11	8	0.36
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD12	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD13	8	0.36
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD21	8	0.36
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD22	8	0.36
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD23	8	0.36
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD11	8	0.36
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD12	8	0.36
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD13	8	0.36
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD21	8	0.36
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD22	8	0.36
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD23	8	0.36
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	18	0.36
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	18	0.36
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	15	0.36
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	15	0.36
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	15	0.36
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	15	0.36
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	9	0.36
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	9	0.36
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	9	0.36
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	9	0.36
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	13	0.36
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	13	0.36
(1,2187)	1:57:B:ALA:H	1:92:B:ARG:H	8	0.36
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	5	0.36
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	5	0.36
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	5	0.36
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	7	0.36
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE1	5	0.36
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE2	5	0.36
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE3	5	0.36
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	18	0.36
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	18	0.36
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	18	0.36
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	14	0.36
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE1	5	0.36
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE2	5	0.36
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE3	5	0.36
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	1	0.35
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	1	0.35
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	3	0.35
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	3	0.35
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	12	0.35
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	4	0.35
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	4	0.35
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	4	0.35
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	4	0.35
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	4	0.35
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	4	0.35
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	4	0.35
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	4	0.35
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	4	0.35
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	4	0.35
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	4	0.35
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	4	0.35
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	4	0.35
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	4	0.35
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	4	0.35
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	4	0.35
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	4	0.35
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	4	0.35
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	17	0.35
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	17	0.35
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	18	0.35
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	18	0.35
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD11	8	0.35
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD12	8	0.35
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD13	8	0.35
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD21	8	0.35
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD22	8	0.35
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD23	8	0.35
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD11	8	0.35
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD12	8	0.35
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD13	8	0.35
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD21	8	0.35
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD22	8	0.35
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD23	8	0.35
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	3	0.35
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	3	0.35
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	12	0.35
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	12	0.35
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	11	0.35
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	11	0.35
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	8	0.35
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	8	0.35
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	8	0.35
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	14	0.35
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	17	0.35
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	17	0.35
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	17	0.35
(1,1037)	1:57:A:ALA:H	1:92:A:ARG:H	8	0.35
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	7	0.35
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	9	0.35
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	9	0.35
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	9	0.35
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	17	0.35
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	17	0.35
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	17	0.35
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	19	0.35
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	19	0.35
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	19	0.35
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	18	0.35
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	18	0.35
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	18	0.35
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	4	0.34
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	4	0.34
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	4	0.34
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	4	0.34
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	4	0.34
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	4	0.34
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	4	0.34
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	4	0.34
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	4	0.34
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	4	0.34
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	4	0.34
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	4	0.34
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	4	0.34
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	4	0.34
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	4	0.34
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	4	0.34
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	4	0.34
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	4	0.34
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	11	0.34
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	11	0.34
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	9	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	9	0.34
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	3	0.34
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	3	0.34
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	6	0.34
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	6	0.34
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	16	0.34
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	16	0.34
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	16	0.34
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	16	0.34
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	16	0.34
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	16	0.34
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	2	0.34
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	2	0.34
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	2	0.34
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	2	0.34
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	2	0.34
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	2	0.34
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	2	0.34
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	2	0.34
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	2	0.34
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	2	0.34
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	2	0.34
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	2	0.34
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	2	0.34
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	2	0.34
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	2	0.34
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	2	0.34
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	2	0.34
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	2	0.34
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	5	0.34
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	5	0.34
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	11	0.34
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	11	0.34
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	8	0.34
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	8	0.34
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	3	0.34
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	3	0.34
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	6	0.34
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	6	0.34
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	13	0.34
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	13	0.34
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	14	0.34
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	14	0.34
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	14	0.34
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	5	0.34
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	9	0.34
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	9	0.34
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	9	0.34
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	13	0.34
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	13	0.34
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	13	0.34
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	19	0.34
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	19	0.34
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	19	0.34
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE1	17	0.34
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE2	17	0.34
(1,1399)	1:41:B:ILE:HG13	1:111:B:MET:HE3	17	0.34
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	4	0.34
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	4	0.34
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	4	0.34
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	11	0.34
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	11	0.34
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	11	0.34
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	8	0.34
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	8	0.34
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	8	0.34
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	2	0.33
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	2	0.33
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	2	0.33
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	2	0.33
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	2	0.33
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	2	0.33
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	2	0.33
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	2	0.33
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	2	0.33
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	2	0.33
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	2	0.33
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	2	0.33
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	2	0.33
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	2	0.33
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	2	0.33
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	2	0.33
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	2	0.33
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	8	0.33
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	8	0.33
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	2	0.33
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	2	0.33
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	4	0.33
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	4	0.33
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	9	0.33
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	9	0.33
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	4	0.33
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	4	0.33
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	4	0.33
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	4	0.33
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	4	0.33
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	4	0.33
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	1	0.33
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	1	0.33
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	1	0.33
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	1	0.33
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	4	0.33
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	4	0.33
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	9	0.33
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	9	0.33
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	1	0.33
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	1	0.33
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	1	0.33
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	4	0.33
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	4	0.33
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	4	0.33
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	15	0.33
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	15	0.33
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	10	0.33
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	20	0.33
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	20	0.33
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	20	0.33
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD11	9	0.33
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD12	9	0.33
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD13	9	0.33
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	20	0.33
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	20	0.33
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	20	0.33
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	1	0.33
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	1	0.33
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	20	0.33
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	20	0.33
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	20	0.33
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	9	0.33
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	9	0.33
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	9	0.33
(1,592)	1:90:B:GLN:HB3	1:90:B:GLN:HE22	3	0.33
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	20	0.33
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	20	0.33
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	20	0.33
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	2	0.32
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	2	0.32
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	9	0.32
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	9	0.32
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	10	0.32
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	10	0.32
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	15	0.32
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	15	0.32
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	2	0.32
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	2	0.32
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	13	0.32
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	13	0.32
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	2	0.32
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	2	0.32
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	19	0.32
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	19	0.32
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB1	16	0.32
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB2	16	0.32
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB3	16	0.32
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	16	0.32
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	16	0.32
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	16	0.32
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	10	0.32
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	10	0.32
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	10	0.32
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	10	0.32
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	1	0.32
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	1	0.32
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	10	0.32
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	2	0.32
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	2	0.32
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	2	0.32
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	2	0.32
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	13	0.32
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	13	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	4	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	4	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	4	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	4	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	4	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	4	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	16	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	16	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	16	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	16	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	16	0.32
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	16	0.32
(1,2274)	1:20:B:TYR:HE1	1:40:B:ILE:HG13	8	0.32
(1,2274)	1:20:B:TYR:HE2	1:40:B:ILE:HG13	8	0.32
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	20	0.32
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	20	0.32
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	20	0.32
(1,2088)	1:103:B:LEU:HD11	1:104:B:THR:H	5	0.32
(1,2088)	1:103:B:LEU:HD12	1:104:B:THR:H	5	0.32
(1,2088)	1:103:B:LEU:HD13	1:104:B:THR:H	5	0.32
(1,2088)	1:103:B:LEU:HD11	1:104:B:THR:H	8	0.32
(1,2088)	1:103:B:LEU:HD12	1:104:B:THR:H	8	0.32
(1,2088)	1:103:B:LEU:HD13	1:104:B:THR:H	8	0.32
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	16	0.32
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	8	0.32
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	7	0.32
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	7	0.32
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	7	0.32
(1,1121)	1:20:A:TYR:HE1	1:40:A:ILE:HG13	8	0.32
(1,1121)	1:20:A:TYR:HE2	1:40:A:ILE:HG13	8	0.32
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	5	0.32
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	5	0.32
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	5	0.32
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	8	0.32
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	20	0.32
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	5	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	5	0.32
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	5	0.32
(1,942)	1:103:A:LEU:HD11	1:104:A:THR:H	5	0.32
(1,942)	1:103:A:LEU:HD12	1:104:A:THR:H	5	0.32
(1,942)	1:103:A:LEU:HD13	1:104:A:THR:H	5	0.32
(1,942)	1:103:A:LEU:HD11	1:104:A:THR:H	8	0.32
(1,942)	1:103:A:LEU:HD12	1:104:A:THR:H	8	0.32
(1,942)	1:103:A:LEU:HD13	1:104:A:THR:H	8	0.32
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	10	0.32
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	10	0.32
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	10	0.32
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	16	0.32
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	15	0.32
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	13	0.32
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	13	0.32
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	13	0.32
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	18	0.32
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	18	0.32
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	18	0.32
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	20	0.32
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	20	0.32
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	20	0.32
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	4	0.32
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	5	0.32
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	17	0.31
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	17	0.31
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	2	0.31
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	2	0.31
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	17	0.31
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	17	0.31
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	6	0.31
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	6	0.31
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	18	0.31
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	18	0.31
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	13	0.31
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	13	0.31
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	13	0.31
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	13	0.31
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	13	0.31
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	13	0.31
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	1	0.31
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	7	0.31
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	7	0.31
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	15	0.31
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	15	0.31
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	6	0.31
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	6	0.31
(1,2274)	1:20:B:TYR:HE1	1:40:B:ILE:HG13	2	0.31
(1,2274)	1:20:B:TYR:HE2	1:40:B:ILE:HG13	2	0.31
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	9	0.31
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	5	0.31
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	5	0.31
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	5	0.31
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	12	0.31
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	12	0.31
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	12	0.31
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	9	0.31
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	9	0.31
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	9	0.31
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	5	0.31
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	5	0.31
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	5	0.31
(1,1977)	1:57:B:ALA:H	1:91:B:ILE:HA	8	0.31
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	6	0.31
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	6	0.31
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	6	0.31
(1,1499)	1:48:B:LYS:H	1:48:B:LYS:HD3	1	0.31
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	5	0.31
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	5	0.31
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	5	0.31
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	12	0.31
(1,831)	1:57:A:ALA:H	1:91:A:ILE:HA	8	0.31
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	9	0.31
(1,364)	1:48:A:LYS:H	1:48:A:LYS:HD3	1	0.31
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE1	17	0.31
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE2	17	0.31
(1,272)	1:41:A:ILE:HG13	1:111:A:MET:HE3	17	0.31
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	1	0.31
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	1	0.31
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	1	0.31
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	7	0.31
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	7	0.31
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	7	0.3
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	7	0.3
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	11	0.3
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	11	0.3
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	18	0.3
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	18	0.3
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	19	0.3
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	19	0.3
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	14	0.3
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	14	0.3
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	10	0.3
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	10	0.3
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	3	0.3
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	3	0.3
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	3	0.3
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	3	0.3
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	3	0.3
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	3	0.3
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	6	0.3
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	6	0.3
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	8	0.3
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	8	0.3
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	12	0.3
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	12	0.3
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	11	0.3
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	11	0.3
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	18	0.3
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	18	0.3
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	18	0.3
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	18	0.3
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	5	0.3
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	18	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	3	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	3	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	3	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	13	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	13	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	13	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	18	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	18	0.3
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	18	0.3
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	5	0.3
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	5	0.3
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	1	0.3
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	12	0.3
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	9	0.3
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	17	0.3
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	20	0.3
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	5	0.3
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	5	0.3
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	5	0.3
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	7	0.3
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	7	0.3
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	7	0.3
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	10	0.3
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	10	0.3
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	10	0.3
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	11	0.3
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	11	0.3
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	11	0.3
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	18	0.3
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	18	0.3
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	18	0.3
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	4	0.3
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	17	0.3
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD11	8	0.3
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD12	8	0.3
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD13	8	0.3
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	1	0.3
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	1	0.3
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	1	0.3
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	9	0.3
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	9	0.3
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	9	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	12	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	12	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	12	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	13	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	13	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	13	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	14	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	14	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	18	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	18	0.3
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	18	0.3
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	4	0.3
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	4	0.3
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	4	0.3
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	1	0.3
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	5	0.3
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	8	0.3
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	20	0.3
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	1	0.3
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	1	0.3
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	1	0.3
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	6	0.3
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	6	0.3
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	6	0.3
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	7	0.3
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	7	0.3
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	7	0.3
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	2	0.3
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	18	0.3
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	9	0.3
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	9	0.3
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	9	0.3
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	3	0.29
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	3	0.29
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	20	0.29
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	20	0.29
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	14	0.29
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	14	0.29
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	10	0.29
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	10	0.29
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	17	0.29
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	17	0.29
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	17	0.29
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	17	0.29
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	17	0.29
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	17	0.29
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	10	0.29
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	16	0.29
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	16	0.29
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2157)	1:113:B:GLU:HA	1:116:B:ASN:HD21	3	0.29
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	6	0.29
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	14	0.29
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	14	0.29
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	14	0.29
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	19	0.29
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	19	0.29
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	19	0.29
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	3	0.29
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	3	0.29
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	3	0.29
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	3	0.29
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	3	0.29
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	3	0.29
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	1	0.29
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	1	0.29
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	1	0.29
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	5	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD21	6	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD22	6	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD23	6	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD21	7	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD22	7	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD23	7	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD21	10	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD22	10	0.29
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD23	10	0.29
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	11	0.29
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	11	0.29
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	11	0.29
(1,1121)	1:20:A:TYR:HE1	1:40:A:ILE:HG13	2	0.29
(1,1121)	1:20:A:TYR:HE2	1:40:A:ILE:HG13	2	0.29
(1,1066)	1:32:B:GLN:HB3	1:32:B:GLN:HE21	19	0.29
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	6	0.29
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	10	0.29
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	10	0.29
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	10	0.29
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	19	0.29
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	19	0.29
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	19	0.29
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	1	0.29
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	1	0.29
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	3	0.29
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	3	0.29
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	3	0.29
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	10	0.29
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	17	0.29
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	5	0.29
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	5	0.29
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	5	0.29
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	11	0.29
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	11	0.29
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	11	0.29
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD11	8	0.29
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD12	8	0.29
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD13	8	0.29
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD21	7	0.29
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD22	7	0.29
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD23	7	0.29
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD21	10	0.29
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD22	10	0.29
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD23	10	0.29
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	11	0.29
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	11	0.29
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	11	0.29
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	12	0.28
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	12	0.28
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	16	0.28
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	16	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	14	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	14	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	14	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	14	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	14	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	14	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	18	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	18	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	18	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	18	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	18	0.28
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	18	0.28
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	1	0.28
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	8	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	8	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	8	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	8	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	8	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	8	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	17	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	17	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	17	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	17	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	17	0.28
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	17	0.28
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	5	0.28
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	5	0.28
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	5	0.28
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	5	0.28
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	20	0.28
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	20	0.28
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	20	0.28
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	20	0.28
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	18	0.28
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	18	0.28
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	18	0.28
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	18	0.28
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	2	0.28
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	2	0.28
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	16	0.28
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	16	0.28
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	17	0.28
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	17	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	14	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	14	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	14	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	14	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	14	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	14	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	18	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	18	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	18	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	18	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	18	0.28
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	18	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	3	0.28
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	3	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	3	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	3	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	3	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	3	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	3	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	3	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	8	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	8	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	8	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	8	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	8	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	8	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	13	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	13	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	13	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	13	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	13	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	13	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	15	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	15	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	15	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	15	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	15	0.28
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	15	0.28
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	11	0.28
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	17	0.28
(1,2157)	1:113:B:GLU:HA	1:116:B:ASN:HD21	12	0.28
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	19	0.28
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	1	0.28
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	1	0.28
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	1	0.28
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	2	0.28
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	2	0.28
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	2	0.28
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	4	0.28
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	4	0.28
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	4	0.28
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	13	0.28
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	13	0.28
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	18	0.28
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	18	0.28
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	18	0.28
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	17	0.28
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	17	0.28
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	17	0.28
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	17	0.28
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	17	0.28
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	17	0.28
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	10	0.28
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	10	0.28
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	10	0.28
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	19	0.28
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	1	0.28
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	15	0.28
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	16	0.28
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	3	0.28
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	3	0.28
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	3	0.28
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	9	0.28
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	9	0.28
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	9	0.28
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	11	0.28
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	11	0.28
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	11	0.28
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD21	12	0.28
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD22	12	0.28
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD23	12	0.28
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	19	0.28
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	19	0.28
(1,1041)	1:119:A:MET:HG2	1:124:A:LEU:H	12	0.28
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	19	0.28
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	7	0.28
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	7	0.28
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	7	0.28
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	3	0.28
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	3	0.28
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	3	0.28
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	7	0.28
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	7	0.28
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	7	0.28
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	2	0.28
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	2	0.28
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	2	0.28
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	12	0.28
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	12	0.28
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	12	0.28
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	3	0.28
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	3	0.28
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	3	0.28
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	1	0.28
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	12	0.28
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	14	0.28
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	15	0.28
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	16	0.28
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	10	0.28
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	10	0.28
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	10	0.28
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	17	0.28
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	9	0.28
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	9	0.28
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	9	0.28
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	11	0.28
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	11	0.28
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	11	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD21	6	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD22	6	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD23	6	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD21	12	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD22	12	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD23	12	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD21	15	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD22	15	0.28
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD23	15	0.28
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	6	0.27
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	6	0.27
(1,3093)	1:82:B:LYS:HA	1:82:B:LYS:HE2	8	0.27
(1,3093)	1:82:B:LYS:HA	1:82:B:LYS:HE3	8	0.27
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	20	0.27
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	20	0.27
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD11	1	0.27
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD12	1	0.27
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD13	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD21	1	0.27
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD22	1	0.27
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD23	1	0.27
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	9	0.27
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	9	0.27
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	9	0.27
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	9	0.27
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	18	0.27
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	18	0.27
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	18	0.27
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	18	0.27
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB1	15	0.27
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB2	15	0.27
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB3	15	0.27
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	15	0.27
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	15	0.27
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	15	0.27
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD21	15	0.27
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD22	15	0.27
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	12	0.27
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	12	0.27
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	19	0.27
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	19	0.27
(1,2682)	1:109:A:ASP:HA	1:112:A:LYS:HB2	5	0.27
(1,2682)	1:109:A:ASP:HA	1:112:A:LYS:HB3	5	0.27
(1,2593)	1:82:A:LYS:HA	1:82:A:LYS:HE2	8	0.27
(1,2593)	1:82:A:LYS:HA	1:82:A:LYS:HE3	8	0.27
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	20	0.27
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	20	0.27
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD1	6	0.27
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD2	6	0.27
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	9	0.27
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	9	0.27
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	1	0.27
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	9	0.27
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	9	0.27
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	9	0.27
(1,2193)	1:119:B:MET:HG2	1:124:B:LEU:H	12	0.27
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	3	0.27
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	3	0.27
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	3	0.27
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	7	0.27
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	7	0.27
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	7	0.27
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	7	0.27
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	7	0.27
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	10	0.27
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	10	0.27
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	10	0.27
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	7	0.27
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	7	0.27
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	7	0.27
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	12	0.27
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	12	0.27
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	12	0.27
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	15	0.27
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	15	0.27
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	15	0.27
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	20	0.27
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	20	0.27
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	20	0.27
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	19	0.27
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	19	0.27
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	19	0.27
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	12	0.27
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	15	0.27
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	19	0.27
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	3	0.27
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	14	0.27
(1,1710)	1:127:B:VAL:HA	1:128:B:ALA:H	6	0.27
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	15	0.27
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	15	0.27
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	15	0.27
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	8	0.27
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	12	0.27
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	6	0.27
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	6	0.27
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	6	0.27
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	13	0.27
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	13	0.27
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	13	0.27
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	9	0.27
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:112:A:LYS:HB3	1:116:A:ASN:HD22	5	0.27
(1,1011)	1:113:A:GLU:HA	1:116:A:ASN:HD21	7	0.27
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	15	0.27
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	15	0.27
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	15	0.27
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	17	0.27
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	17	0.27
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	17	0.27
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	7	0.27
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	7	0.27
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	7	0.27
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	13	0.27
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	13	0.27
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	13	0.27
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	15	0.27
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	15	0.27
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	15	0.27
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	18	0.27
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	18	0.27
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	18	0.27
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	19	0.27
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	19	0.27
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	19	0.27
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	20	0.27
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	20	0.27
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	20	0.27
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	17	0.27
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	17	0.27
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	17	0.27
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	17	0.27
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	17	0.27
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	17	0.27
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	19	0.27
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	19	0.27
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	19	0.27
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	12	0.27
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	19	0.27
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	19	0.27
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	2	0.27
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	3	0.27
(1,567)	1:127:A:VAL:HA	1:128:A:ALA:H	6	0.27
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	14	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	14	0.27
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	14	0.27
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	5	0.27
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	7	0.27
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	12	0.27
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD21	14	0.27
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD22	14	0.27
(1,171)	1:80:A:LEU:HA	1:80:A:LEU:HD23	14	0.27
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	6	0.27
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	6	0.27
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	6	0.27
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	11	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	11	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	11	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	11	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	11	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	11	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	11	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	11	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	11	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	11	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	11	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	11	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	11	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	11	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	11	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	11	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	11	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	11	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	17	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	17	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	17	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	17	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	17	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	17	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	17	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	17	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	17	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	17	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	17	0.26
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	17	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	17	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	17	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	17	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	17	0.26
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	17	0.26
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	19	0.26
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	19	0.26
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	8	0.26
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	8	0.26
(1,3165)	1:106:B:LEU:H	1:106:B:LEU:HD11	10	0.26
(1,3165)	1:106:B:LEU:H	1:106:B:LEU:HD12	10	0.26
(1,3165)	1:106:B:LEU:H	1:106:B:LEU:HD13	10	0.26
(1,3165)	1:106:B:LEU:H	1:106:B:LEU:HD21	10	0.26
(1,3165)	1:106:B:LEU:H	1:106:B:LEU:HD22	10	0.26
(1,3165)	1:106:B:LEU:H	1:106:B:LEU:HD23	10	0.26
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	7	0.26
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	7	0.26
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	15	0.26
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	15	0.26
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	15	0.26
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	15	0.26
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	15	0.26
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	15	0.26
(1,2876)	1:24:B:LEU:HD11	1:90:B:GLN:HE21	6	0.26
(1,2876)	1:24:B:LEU:HD12	1:90:B:GLN:HE21	6	0.26
(1,2876)	1:24:B:LEU:HD13	1:90:B:GLN:HE21	6	0.26
(1,2876)	1:24:B:LEU:HD21	1:90:B:GLN:HE21	6	0.26
(1,2876)	1:24:B:LEU:HD22	1:90:B:GLN:HE21	6	0.26
(1,2876)	1:24:B:LEU:HD23	1:90:B:GLN:HE21	6	0.26
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD11	5	0.26
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD12	5	0.26
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD13	5	0.26
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD21	5	0.26
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD22	5	0.26
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD23	5	0.26
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	19	0.26
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	19	0.26
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	19	0.26
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	19	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	11	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	11	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	11	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	11	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	11	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	11	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	11	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	11	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	11	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	11	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	11	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	11	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	11	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	11	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	11	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	11	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	11	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	17	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	17	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	17	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	17	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	17	0.26
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	17	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	17	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	17	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	17	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	17	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	17	0.26
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	17	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	17	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	17	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	17	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	17	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	17	0.26
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	17	0.26
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD21	14	0.26
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD22	14	0.26
(1,2369)	1:24:A:LEU:HD11	1:90:A:GLN:HE21	6	0.26
(1,2369)	1:24:A:LEU:HD12	1:90:A:GLN:HE21	6	0.26
(1,2369)	1:24:A:LEU:HD13	1:90:A:GLN:HE21	6	0.26
(1,2369)	1:24:A:LEU:HD21	1:90:A:GLN:HE21	6	0.26
(1,2369)	1:24:A:LEU:HD22	1:90:A:GLN:HE21	6	0.26
(1,2369)	1:24:A:LEU:HD23	1:90:A:GLN:HE21	6	0.26
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	19	0.26
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	8	0.26
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	20	0.26
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	12	0.26
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	20	0.26
(1,2157)	1:113:B:GLU:HA	1:116:B:ASN:HD21	10	0.26
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	8	0.26
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	8	0.26
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	8	0.26
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	15	0.26
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	15	0.26
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	15	0.26
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	17	0.26
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	17	0.26
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	17	0.26
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	19	0.26
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	19	0.26
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	19	0.26
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	19	0.26
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	6	0.26
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	6	0.26
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	6	0.26
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	8	0.26
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	8	0.26
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	8	0.26
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	17	0.26
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	4	0.26
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	5	0.26
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	7	0.26
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	13	0.26
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	18	0.26
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	12	0.26
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	12	0.26
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	12	0.26
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	14	0.26
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	14	0.26
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	14	0.26
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	4	0.26
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	13	0.26
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	5	0.26
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	5	0.26
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	15	0.26
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD21	14	0.26
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD22	14	0.26
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD23	14	0.26
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD21	15	0.26
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD22	15	0.26
(1,1297)	1:80:B:LEU:HA	1:80:B:LEU:HD23	15	0.26
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	4	0.26
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	4	0.26
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	4	0.26
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	14	0.26
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	14	0.26
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	14	0.26
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	6	0.26
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	6	0.26
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	3	0.26
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	3	0.26
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	3	0.26
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	3	0.26
(1,916)	1:95:A:ASP:HB3	1:97:A:LYS:H	16	0.26
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	19	0.26
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	17	0.26
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	17	0.26
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	17	0.26
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	6	0.26
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	6	0.26
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	6	0.26
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	7	0.26
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	7	0.26
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	7	0.26
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	8	0.26
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	8	0.26
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	8	0.26
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	17	0.26
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	18	0.26
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	5	0.26
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	18	0.26
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	3	0.26
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	3	0.26
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	3	0.26
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	15	0.26
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	15	0.26
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	15	0.26
(1,266)	1:119:A:MET:HE1	1:125:A:ASN:HB3	4	0.26
(1,266)	1:119:A:MET:HE2	1:125:A:ASN:HB3	4	0.26
(1,266)	1:119:A:MET:HE3	1:125:A:ASN:HB3	4	0.26
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	5	0.26
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	5	0.26
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	5	0.26
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	14	0.26
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	14	0.26
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	14	0.26
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	20	0.26
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	20	0.26
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	20	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	13	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	13	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	13	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	18	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	18	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	18	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	19	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	19	0.26
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	19	0.26
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	6	0.25
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	6	0.25
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	6	0.25
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	6	0.25
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	6	0.25
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	6	0.25
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	6	0.25
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	6	0.25
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	6	0.25
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	6	0.25
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	6	0.25
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	6	0.25
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	6	0.25
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	6	0.25
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	6	0.25
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	6	0.25
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	6	0.25
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	6	0.25
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	9	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	9	0.25
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	9	0.25
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	9	0.25
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	4	0.25
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	4	0.25
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	5	0.25
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	5	0.25
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	11	0.25
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	11	0.25
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	11	0.25
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	11	0.25
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	11	0.25
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	11	0.25
(1,2869)	1:24:B:LEU:HD11	1:32:B:GLN:H	12	0.25
(1,2869)	1:24:B:LEU:HD12	1:32:B:GLN:H	12	0.25
(1,2869)	1:24:B:LEU:HD13	1:32:B:GLN:H	12	0.25
(1,2869)	1:24:B:LEU:HD21	1:32:B:GLN:H	12	0.25
(1,2869)	1:24:B:LEU:HD22	1:32:B:GLN:H	12	0.25
(1,2869)	1:24:B:LEU:HD23	1:32:B:GLN:H	12	0.25
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	4	0.25
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	4	0.25
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	4	0.25
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	4	0.25
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	6	0.25
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	6	0.25
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	6	0.25
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	6	0.25
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	6	0.25
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	6	0.25
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	6	0.25
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	6	0.25
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	6	0.25
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	6	0.25
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	6	0.25
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	6	0.25
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	6	0.25
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	6	0.25
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	6	0.25
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	6	0.25
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	6	0.25
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	6	0.25
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	3	0.25
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	3	0.25
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	3	0.25
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	3	0.25
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	3	0.25
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD21	13	0.25
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD22	13	0.25
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD21	16	0.25
(1,2720)	1:116:A:ASN:H	1:116:A:ASN:HD22	16	0.25
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	9	0.25
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	9	0.25
(1,2669)	1:106:A:LEU:H	1:106:A:LEU:HD11	10	0.25
(1,2669)	1:106:A:LEU:H	1:106:A:LEU:HD12	10	0.25
(1,2669)	1:106:A:LEU:H	1:106:A:LEU:HD13	10	0.25
(1,2669)	1:106:A:LEU:H	1:106:A:LEU:HD21	10	0.25
(1,2669)	1:106:A:LEU:H	1:106:A:LEU:HD22	10	0.25
(1,2669)	1:106:A:LEU:H	1:106:A:LEU:HD23	10	0.25
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	5	0.25
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	5	0.25
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD11	1	0.25
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD12	1	0.25
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD13	1	0.25
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD21	1	0.25
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD22	1	0.25
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD23	1	0.25
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	6	0.25
(1,2161)	1:112:B:LYS:HB3	1:116:B:ASN:HD22	5	0.25
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG11	16	0.25
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG12	16	0.25
(1,2116)	1:113:B:GLU:H	1:114:B:VAL:HG13	16	0.25
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	3	0.25
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	2	0.25
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	2	0.25
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	2	0.25
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	1	0.25
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	1	0.25
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	1	0.25
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	17	0.25
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	17	0.25
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	17	0.25
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	14	0.25
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1863)	1:19:B:VAL:H	1:104:B:THR:HG21	17	0.25
(1,1863)	1:19:B:VAL:H	1:104:B:THR:HG22	17	0.25
(1,1863)	1:19:B:VAL:H	1:104:B:THR:HG23	17	0.25
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	2	0.25
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	7	0.25
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	2	0.25
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	6	0.25
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	12	0.25
(1,1710)	1:127:B:VAL:HA	1:128:B:ALA:H	5	0.25
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	4	0.25
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	6	0.25
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	2	0.25
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	2	0.25
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	2	0.25
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	4	0.25
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	4	0.25
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	4	0.25
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	2	0.25
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	4	0.25
(1,1393)	1:119:B:MET:HE1	1:125:B:ASN:HB3	4	0.25
(1,1393)	1:119:B:MET:HE2	1:125:B:ASN:HB3	4	0.25
(1,1393)	1:119:B:MET:HE3	1:125:B:ASN:HB3	4	0.25
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	1	0.25
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	1	0.25
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	1	0.25
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	4	0.25
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	4	0.25
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	4	0.25
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	7	0.25
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	7	0.25
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	7	0.25
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	7	0.25
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	11	0.25
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	11	0.25
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	11	0.25
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	20	0.25
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	20	0.25
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	20	0.25
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	3	0.25
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	3	0.25
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	3	0.25
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	18	0.25
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	18	0.25
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	11	0.25
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG11	16	0.25
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG12	16	0.25
(1,970)	1:113:A:GLU:H	1:114:A:VAL:HG13	16	0.25
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	2	0.25
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	2	0.25
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	2	0.25
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	8	0.25
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	15	0.25
(1,717)	1:19:A:VAL:H	1:104:A:THR:HG21	17	0.25
(1,717)	1:19:A:VAL:H	1:104:A:THR:HG22	17	0.25
(1,717)	1:19:A:VAL:H	1:104:A:THR:HG23	17	0.25
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	2	0.25
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	7	0.25
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	4	0.25
(1,567)	1:127:A:VAL:HA	1:128:A:ALA:H	5	0.25
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	2	0.25
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	2	0.25
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	2	0.25
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	12	0.25
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	12	0.25
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	12	0.25
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	16	0.25
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	16	0.25
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	16	0.25
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	3	0.25
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	4	0.25
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	1	0.25
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	1	0.25
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	1	0.25
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	4	0.25
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	4	0.25
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	4	0.25
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	11	0.25
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	11	0.25
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	11	0.25
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	7	0.25
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	7	0.25
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	7	0.25
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	11	0.25
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	11	0.25
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD11	4	0.25
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD12	4	0.25
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD13	4	0.25
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	3	0.25
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	3	0.25
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	3	0.25
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	10	0.25
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	10	0.25
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	10	0.25
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	17	0.25
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	17	0.25
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	17	0.25
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	3	0.24
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	3	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	20	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	20	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	20	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	20	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	20	0.24
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	20	0.24
(1,2876)	1:24:B:LEU:HD11	1:90:B:GLN:HE21	13	0.24
(1,2876)	1:24:B:LEU:HD12	1:90:B:GLN:HE21	13	0.24
(1,2876)	1:24:B:LEU:HD13	1:90:B:GLN:HE21	13	0.24
(1,2876)	1:24:B:LEU:HD21	1:90:B:GLN:HE21	13	0.24
(1,2876)	1:24:B:LEU:HD22	1:90:B:GLN:HE21	13	0.24
(1,2876)	1:24:B:LEU:HD23	1:90:B:GLN:HE21	13	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	13	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	13	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	13	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	13	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	13	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	13	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	15	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	15	0.24
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	15	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	15	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	15	0.24
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	15	0.24
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	8	0.24
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	8	0.24
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	8	0.24
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	3	0.24
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	3	0.24
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	6	0.24
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	6	0.24
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	20	0.24
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	20	0.24
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	20	0.24
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	20	0.24
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	20	0.24
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	20	0.24
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	20	0.24
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	20	0.24
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	20	0.24
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	20	0.24
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	20	0.24
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	20	0.24
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	5	0.24
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	5	0.24
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	8	0.24
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	8	0.24
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	20	0.24
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	20	0.24
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	20	0.24
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	20	0.24
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	20	0.24
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	20	0.24
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD11	5	0.24
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD12	5	0.24
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD13	5	0.24
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD21	5	0.24
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD22	5	0.24
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD23	5	0.24
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE1	3	0.24
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE2	3	0.24
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE1	3	0.24
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE2	3	0.24
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE1	3	0.24
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE2	3	0.24
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	2	0.24
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2196)	1:119:B:MET:HE1	1:125:B:ASN:HD21	4	0.24
(1,2196)	1:119:B:MET:HE2	1:125:B:ASN:HD21	4	0.24
(1,2196)	1:119:B:MET:HE3	1:125:B:ASN:HD21	4	0.24
(1,2159)	1:112:A:LYS:HB2	1:116:A:ASN:HD21	3	0.24
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	15	0.24
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	15	0.24
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	15	0.24
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	4	0.24
(1,2062)	1:95:B:ASP:HB3	1:97:B:LYS:H	16	0.24
(1,2053)	1:93:B:THR:H	1:94:B:LEU:HG	8	0.24
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	11	0.24
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	11	0.24
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	11	0.24
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	20	0.24
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	20	0.24
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	20	0.24
(1,1978)	1:57:B:ALA:H	1:90:B:GLN:HB3	8	0.24
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	15	0.24
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	15	0.24
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	15	0.24
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	7	0.24
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	7	0.24
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	7	0.24
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	8	0.24
(1,1634)	1:15:B:ARG:H	1:15:B:ARG:HG3	1	0.24
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE1	5	0.24
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE2	5	0.24
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE3	5	0.24
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	16	0.24
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	16	0.24
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	16	0.24
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	8	0.24
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	8	0.24
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	8	0.24
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	11	0.24
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	11	0.24
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	11	0.24
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	19	0.24
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	19	0.24
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	19	0.24
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	7	0.24
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	3	0.24
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	3	0.24
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	15	0.24
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	15	0.24
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	15	0.24
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	16	0.24
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	16	0.24
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	16	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	10	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	10	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	10	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	12	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	12	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	12	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	14	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	14	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	14	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	19	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	19	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	19	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	20	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	20	0.24
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	20	0.24
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	17	0.24
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	17	0.24
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	17	0.24
(1,1109)	1:67:A:ILE:HD11	1:69:A:THR:H	6	0.24
(1,1109)	1:67:A:ILE:HD12	1:69:A:THR:H	6	0.24
(1,1109)	1:67:A:ILE:HD13	1:69:A:THR:H	6	0.24
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	20	0.24
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	8	0.24
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	8	0.24
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	8	0.24
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	5	0.24
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	1	0.24
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	1	0.24
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	1	0.24
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	20	0.24
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	20	0.24
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	20	0.24
(1,832)	1:57:A:ALA:H	1:90:A:GLN:HB3	8	0.24
(1,766)	1:35:A:VAL:HG21	1:36:A:ARG:H	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,766)	1:35:A:VAL:HG22	1:36:A:ARG:H	10	0.24
(1,766)	1:35:A:VAL:HG23	1:36:A:ARG:H	10	0.24
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	15	0.24
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	15	0.24
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	15	0.24
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	1	0.24
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	4	0.24
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	9	0.24
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	14	0.24
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	3	0.24
(1,582)	1:116:A:ASN:HA	1:116:A:ASN:HD21	13	0.24
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	6	0.24
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	7	0.24
(1,478)	1:111:A:MET:H	1:111:A:MET:HE1	5	0.24
(1,478)	1:111:A:MET:H	1:111:A:MET:HE2	5	0.24
(1,478)	1:111:A:MET:H	1:111:A:MET:HE3	5	0.24
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	6	0.24
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	4	0.24
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	4	0.24
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	4	0.24
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	5	0.24
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	16	0.24
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	8	0.24
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	8	0.24
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	8	0.24
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	6	0.24
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	6	0.24
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	6	0.24
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	19	0.24
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	19	0.24
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	19	0.24
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	15	0.24
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	8	0.24
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	8	0.24
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	8	0.24
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	16	0.24
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	16	0.24
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	16	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	2	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	2	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	2	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	12	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	12	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	14	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	14	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	14	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	20	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	20	0.24
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	20	0.24
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	4	0.23
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	4	0.23
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	4	0.23
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	4	0.23
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE2	14	0.23
(1,3186)	1:111:B:MET:HA	1:112:B:LYS:HE3	14	0.23
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	2	0.23
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	2	0.23
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	2	0.23
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	2	0.23
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	2	0.23
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	2	0.23
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	20	0.23
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	20	0.23
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	20	0.23
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	20	0.23
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	20	0.23
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	20	0.23
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	20	0.23
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	20	0.23
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	20	0.23
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	20	0.23
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	20	0.23
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	20	0.23
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	8	0.23
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	8	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	5	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	5	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	5	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	5	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	5	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	5	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	14	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	14	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	14	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	14	0.23
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	14	0.23
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	8	0.23
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	8	0.23
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	8	0.23
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	8	0.23
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	10	0.23
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	10	0.23
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	13	0.23
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	13	0.23
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE2	14	0.23
(1,2690)	1:111:A:MET:HA	1:112:A:LYS:HE3	14	0.23
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	2	0.23
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	2	0.23
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	2	0.23
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	2	0.23
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	2	0.23
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	2	0.23
(1,2362)	1:24:A:LEU:HD11	1:32:A:GLN:H	12	0.23
(1,2362)	1:24:A:LEU:HD12	1:32:A:GLN:H	12	0.23
(1,2362)	1:24:A:LEU:HD13	1:32:A:GLN:H	12	0.23
(1,2362)	1:24:A:LEU:HD21	1:32:A:GLN:H	12	0.23
(1,2362)	1:24:A:LEU:HD22	1:32:A:GLN:H	12	0.23
(1,2362)	1:24:A:LEU:HD23	1:32:A:GLN:H	12	0.23
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	15	0.23
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	15	0.23
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	15	0.23
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	15	0.23
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	15	0.23
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	15	0.23
(1,2262)	1:67:B:ILE:HD11	1:69:B:THR:H	6	0.23
(1,2262)	1:67:B:ILE:HD12	1:69:B:THR:H	6	0.23
(1,2262)	1:67:B:ILE:HD13	1:69:B:THR:H	6	0.23
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD11	9	0.23
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD12	9	0.23
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD13	9	0.23
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	8	0.23
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	11	0.23
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	6	0.23
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	6	0.23
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	5	0.23
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	20	0.23
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	20	0.23
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	20	0.23
(1,2039)	1:87:B:LEU:H	1:90:B:GLN:H	8	0.23
(1,2019)	1:73:B:ILE:HB	1:84:B:SER:H	4	0.23
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	13	0.23
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	13	0.23
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	13	0.23
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	12	0.23
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	12	0.23
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	12	0.23
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	1	0.23
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	4	0.23
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	9	0.23
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	9	0.23
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	10	0.23
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	19	0.23
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	2	0.23
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	18	0.23
(1,1535)	1:19:B:VAL:HG21	1:103:B:LEU:H	8	0.23
(1,1535)	1:19:B:VAL:HG22	1:103:B:LEU:H	8	0.23
(1,1535)	1:19:B:VAL:HG23	1:103:B:LEU:H	8	0.23
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	5	0.23
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	8	0.23
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	6	0.23
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	7	0.23
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	16	0.23
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	17	0.23
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	19	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	4	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	4	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	4	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	7	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	7	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	7	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	9	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	9	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	9	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	13	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	13	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	15	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	15	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	15	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	20	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	20	0.23
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	20	0.23
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	6	0.23
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	6	0.23
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	6	0.23
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	2	0.23
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	3	0.23
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	3	0.23
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	3	0.23
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD1	4	0.23
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD2	4	0.23
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	1	0.23
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	1	0.23
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	1	0.23
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	6	0.23
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	6	0.23
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	6	0.23
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	8	0.23
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	8	0.23
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	8	0.23
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	10	0.23
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	10	0.23
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	10	0.23
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	12	0.23
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	12	0.23
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	12	0.23
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	12	0.23
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	12	0.23
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	12	0.23
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	13	0.23
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	13	0.23
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	13	0.23
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	2	0.23
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	2	0.23
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	2	0.23
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	4	0.23
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	4	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	4	0.23
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	3	0.23
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	3	0.23
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	8	0.23
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	8	0.23
(1,1108)	1:67:A:ILE:HG21	1:69:A:THR:H	6	0.23
(1,1108)	1:67:A:ILE:HG22	1:69:A:THR:H	6	0.23
(1,1108)	1:67:A:ILE:HG23	1:69:A:THR:H	6	0.23
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE1	3	0.23
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE2	3	0.23
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE1	3	0.23
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE2	3	0.23
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE1	3	0.23
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE2	3	0.23
(1,1011)	1:113:A:GLU:HA	1:116:A:ASN:HD21	9	0.23
(1,907)	1:93:A:THR:H	1:94:A:LEU:HG	8	0.23
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	20	0.23
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	20	0.23
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	20	0.23
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	11	0.23
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	11	0.23
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	11	0.23
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	20	0.23
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	20	0.23
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	20	0.23
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	7	0.23
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	4	0.23
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	13	0.23
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	19	0.23
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	2	0.23
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	4	0.23
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	8	0.23
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	4	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	7	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	7	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	7	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	13	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	13	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	13	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	15	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	15	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	20	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	20	0.23
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	20	0.23
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	15	0.23
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	15	0.23
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	15	0.23
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	7	0.23
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	1	0.23
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	1	0.23
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	1	0.23
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	16	0.23
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	16	0.23
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	16	0.23
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	19	0.23
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	19	0.23
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	19	0.23
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	10	0.23
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	10	0.23
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	10	0.23
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	13	0.23
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	13	0.23
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	13	0.23
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	15	0.23
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	15	0.23
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	15	0.23
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	19	0.23
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	19	0.23
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	19	0.23
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	4	0.23
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	4	0.23
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	4	0.23
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	15	0.23
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	15	0.23
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	15	0.23
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	19	0.23
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	19	0.23
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	19	0.23
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	16	0.22
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	16	0.22
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	16	0.22
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	16	0.22
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	16	0.22
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	12	0.22
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	12	0.22
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	2	0.22
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	2	0.22
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	2	0.22
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	2	0.22
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	2	0.22
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	2	0.22
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD11	11	0.22
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD12	11	0.22
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD13	11	0.22
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD21	11	0.22
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD22	11	0.22
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD23	11	0.22
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	14	0.22
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	14	0.22
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	14	0.22
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	14	0.22
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	14	0.22
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	14	0.22
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB1	14	0.22
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB2	14	0.22
(1,2727)	1:116:A:ASN:HD21	1:117:A:ALA:HB3	14	0.22
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	14	0.22
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	14	0.22
(1,2727)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	14	0.22
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	1	0.22
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	1	0.22
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	1	0.22
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	1	0.22
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	16	0.22
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	16	0.22
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	16	0.22
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	16	0.22
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	16	0.22
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	16	0.22
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	12	0.22
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	12	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	7	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	7	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	7	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	7	0.22
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	7	0.22
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD11	11	0.22
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD12	11	0.22
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD13	11	0.22
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD21	11	0.22
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD22	11	0.22
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD23	11	0.22
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	4	0.22
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	4	0.22
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	4	0.22
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	4	0.22
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	4	0.22
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	4	0.22
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	3	0.22
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	3	0.22
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	16	0.22
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	16	0.22
(1,2261)	1:67:B:ILE:HG21	1:69:B:THR:H	6	0.22
(1,2261)	1:67:B:ILE:HG22	1:69:B:THR:H	6	0.22
(1,2261)	1:67:B:ILE:HG23	1:69:B:THR:H	6	0.22
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	11	0.22
(1,2157)	1:113:B:GLU:HA	1:116:B:ASN:HD21	4	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	9	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	9	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	9	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	14	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	14	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	14	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	16	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	16	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	16	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	19	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	19	0.22
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	19	0.22
(1,2102)	1:110:B:LYS:H	1:113:B:GLU:H	5	0.22
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	16	0.22
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	16	0.22
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	16	0.22
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	11	0.22
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	11	0.22
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	2	0.22
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	2	0.22
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	2	0.22
(1,1912)	1:35:B:VAL:HG21	1:36:B:ARG:H	10	0.22
(1,1912)	1:35:B:VAL:HG22	1:36:B:ARG:H	10	0.22
(1,1912)	1:35:B:VAL:HG23	1:36:B:ARG:H	10	0.22
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	20	0.22
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	20	0.22
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	20	0.22
(1,1897)	1:24:B:LEU:HD21	1:32:B:GLN:H	18	0.22
(1,1897)	1:24:B:LEU:HD22	1:32:B:GLN:H	18	0.22
(1,1897)	1:24:B:LEU:HD23	1:32:B:GLN:H	18	0.22
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	12	0.22
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	12	0.22
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	12	0.22
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	4	0.22
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	3	0.22
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	7	0.22
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	13	0.22
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	15	0.22
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	16	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	1	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	1	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	1	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	14	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	14	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	14	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	16	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	16	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	16	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	18	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	18	0.22
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	18	0.22
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	13	0.22
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	13	0.22
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	13	0.22
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	14	0.22
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	14	0.22
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	14	0.22
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	15	0.22
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	15	0.22
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	1	0.22
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	1	0.22
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	1	0.22
(1,1234)	1:22:B:ALA:HB1	1:24:B:LEU:HG	13	0.22
(1,1234)	1:22:B:ALA:HB2	1:24:B:LEU:HG	13	0.22
(1,1234)	1:22:B:ALA:HB3	1:24:B:LEU:HG	13	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	2	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	2	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	2	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	9	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	9	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	9	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	13	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	13	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	13	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	15	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	15	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	15	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	16	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	16	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	16	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	18	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	18	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	18	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	19	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	19	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	19	0.22
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	20	0.22
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	20	0.22
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	20	0.22
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	19	0.22
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	19	0.22
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	19	0.22
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	2	0.22
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	2	0.22
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	2	0.22
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	15	0.22
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	15	0.22
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	15	0.22
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	19	0.22
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	19	0.22
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	2	0.22
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	2	0.22
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	2	0.22
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	6	0.22
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	6	0.22
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	6	0.22
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	9	0.22
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	9	0.22
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	9	0.22
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	18	0.22
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	18	0.22
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	18	0.22
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	19	0.22
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	19	0.22
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	19	0.22
(1,1172)	1:117:B:ALA:HB1	1:118:B:LEU:HB2	2	0.22
(1,1172)	1:117:B:ALA:HB2	1:118:B:LEU:HB2	2	0.22
(1,1172)	1:117:B:ALA:HB3	1:118:B:LEU:HB2	2	0.22
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	15	0.22
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	15	0.22
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	15	0.22
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	16	0.22
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	16	0.22
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	16	0.22
(1,1141)	1:111:B:MET:HE1	1:114:B:VAL:HB	6	0.22
(1,1141)	1:111:B:MET:HE2	1:114:B:VAL:HB	6	0.22
(1,1141)	1:111:B:MET:HE3	1:114:B:VAL:HB	6	0.22
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	16	0.22
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	16	0.22
(1,1044)	1:119:A:MET:HE1	1:125:A:ASN:HD21	4	0.22
(1,1044)	1:119:A:MET:HE2	1:125:A:ASN:HD21	4	0.22
(1,1044)	1:119:A:MET:HE3	1:125:A:ASN:HD21	4	0.22
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	15	0.22
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	15	0.22
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	15	0.22
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	4	0.22
(1,1011)	1:113:A:GLU:HA	1:116:A:ASN:HD21	10	0.22
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	8	0.22
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	16	0.22
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	16	0.22
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	13	0.22
(1,893)	1:87:A:LEU:H	1:90:A:GLN:H	8	0.22
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	2	0.22
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	2	0.22
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	2	0.22
(1,766)	1:35:A:VAL:HG21	1:36:A:ARG:H	2	0.22
(1,766)	1:35:A:VAL:HG22	1:36:A:ARG:H	2	0.22
(1,766)	1:35:A:VAL:HG23	1:36:A:ARG:H	2	0.22
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	4	0.22
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	4	0.22
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	4	0.22
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	13	0.22
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	13	0.22
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	13	0.22
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	12	0.22
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	12	0.22
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	12	0.22
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	12	0.22
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	11	0.22
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	9	0.22
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	10	0.22
(1,579)	1:101:A:GLU:H	1:102:A:LYS:H	11	0.22
(1,495)	1:15:A:ARG:H	1:15:A:ARG:HG3	1	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	1	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	4	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	7	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	12	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	13	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	15	0.22
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	16	0.22
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	17	0.22
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	17	0.22
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	17	0.22
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	20	0.22
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	9	0.22
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	10	0.22
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	17	0.22
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	19	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	4	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	4	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	4	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	9	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	9	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	14	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	14	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	14	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	16	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	16	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	16	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	18	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	18	0.22
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	18	0.22
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	13	0.22
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	13	0.22
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	13	0.22
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	2	0.22
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	8	0.22
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	1	0.22
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	1	0.22
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	1	0.22
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	3	0.22
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	3	0.22
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	3	0.22
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	9	0.22
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	9	0.22
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	9	0.22
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	17	0.22
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	17	0.22
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	17	0.22
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	15	0.22
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	15	0.22
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	15	0.22
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	2	0.22
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	2	0.22
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	2	0.22
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	9	0.22
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	9	0.22
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	9	0.22
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	11	0.22
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	11	0.22
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	11	0.22
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	13	0.22
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	13	0.22
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	15	0.22
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	15	0.22
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	15	0.22
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	20	0.22
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	20	0.22
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	20	0.22
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	6	0.22
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	6	0.22
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	6	0.22
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	12	0.22
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	12	0.22
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	12	0.22
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	15	0.22
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	15	0.22
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	15	0.22
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	6	0.22
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	6	0.22
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	6	0.22
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	9	0.22
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	9	0.22
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	9	0.22
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	12	0.22
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	12	0.22
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	12	0.22
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	18	0.22
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	18	0.22
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	18	0.22
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	16	0.22
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	16	0.22
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	16	0.22
(1,14)	1:111:A:MET:HE1	1:114:A:VAL:HB	6	0.22
(1,14)	1:111:A:MET:HE2	1:114:A:VAL:HB	6	0.22
(1,14)	1:111:A:MET:HE3	1:114:A:VAL:HB	6	0.22
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	10	0.21
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	10	0.21
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	10	0.21
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	10	0.21
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	10	0.21
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	10	0.21
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	10	0.21
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	10	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	10	0.21
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	10	0.21
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	10	0.21
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	10	0.21
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	10	0.21
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	10	0.21
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	10	0.21
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	10	0.21
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	10	0.21
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	10	0.21
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB2	7	0.21
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB3	7	0.21
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB2	7	0.21
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB3	7	0.21
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	6	0.21
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	6	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	6	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	6	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	6	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	6	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	6	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	6	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	11	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	11	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	11	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	11	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	11	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	11	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	15	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	15	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	15	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	15	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	15	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	15	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	20	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	20	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	20	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	20	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	20	0.21
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	20	0.21
(1,3042)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	4	0.21
(1,3042)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3042)	1:73:B:ILE:HG13	1:78:B:TYR:HD1	4	0.21
(1,3042)	1:73:B:ILE:HG13	1:78:B:TYR:HD2	4	0.21
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	9	0.21
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	9	0.21
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	11	0.21
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	11	0.21
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	17	0.21
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	17	0.21
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	17	0.21
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	17	0.21
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	17	0.21
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	17	0.21
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	3	0.21
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	3	0.21
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	3	0.21
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	3	0.21
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	10	0.21
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	10	0.21
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	10	0.21
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	10	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	10	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	10	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	10	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	10	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	10	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	10	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	10	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	10	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	10	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	10	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	10	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	10	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	10	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	10	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	10	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	10	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	10	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	10	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	18	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	18	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	18	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	18	0.21
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	18	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	18	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	18	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	18	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	18	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	18	0.21
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	18	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	18	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	18	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	18	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	18	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	18	0.21
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	18	0.21
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	16	0.21
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	16	0.21
(1,2729)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	16	0.21
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	16	0.21
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	16	0.21
(1,2729)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	16	0.21
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	16	0.21
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	16	0.21
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB2	3	0.21
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB3	3	0.21
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB2	3	0.21
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB3	3	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	5	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	5	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	5	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	5	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	5	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	5	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	11	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	11	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	11	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	11	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	11	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	11	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	15	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	15	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	15	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	15	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	15	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	20	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	20	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	20	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	20	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	20	0.21
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	20	0.21
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	11	0.21
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	11	0.21
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	15	0.21
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	15	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	1	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	1	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	1	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	1	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	1	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	1	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	11	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	11	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	11	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	11	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	11	0.21
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	11	0.21
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	2	0.21
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	2	0.21
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	2	0.21
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	2	0.21
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	2	0.21
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	2	0.21
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	17	0.21
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	17	0.21
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	17	0.21
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	17	0.21
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	17	0.21
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	17	0.21
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	8	0.21
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	8	0.21
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	4	0.21
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	8	0.21
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	8	0.21
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	20	0.21
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	3	0.21
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	3	0.21
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	3	0.21
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	14	0.21
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	14	0.21
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	14	0.21
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	13	0.21
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	20	0.21
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	3	0.21
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	3	0.21
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	3	0.21
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	17	0.21
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	17	0.21
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	17	0.21
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	18	0.21
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	18	0.21
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	18	0.21
(1,1912)	1:35:B:VAL:HG21	1:36:B:ARG:H	2	0.21
(1,1912)	1:35:B:VAL:HG22	1:36:B:ARG:H	2	0.21
(1,1912)	1:35:B:VAL:HG23	1:36:B:ARG:H	2	0.21
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	4	0.21
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	4	0.21
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	4	0.21
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	5	0.21
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	5	0.21
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	5	0.21
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	7	0.21
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	7	0.21
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	7	0.21
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	19	0.21
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	19	0.21
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	19	0.21
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	12	0.21
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	11	0.21
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	20	0.21
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	18	0.21
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	1	0.21
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	17	0.21
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	11	0.21
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	17	0.21
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	4	0.21
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	12	0.21
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	14	0.21
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	18	0.21
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	19	0.21
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	10	0.21
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	10	0.21
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	10	0.21
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	17	0.21
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	17	0.21
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	17	0.21
(1,1499)	1:48:B:LYS:H	1:48:B:LYS:HD3	8	0.21
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	3	0.21
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	9	0.21
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	18	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	6	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	6	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	6	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	10	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	10	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	10	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	12	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	12	0.21
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	12	0.21
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	2	0.21
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	2	0.21
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	2	0.21
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	3	0.21
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	3	0.21
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	3	0.21
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	4	0.21
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	4	0.21
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	4	0.21
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	6	0.21
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	6	0.21
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	6	0.21
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	8	0.21
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	8	0.21
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	8	0.21
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	11	0.21
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	11	0.21
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	17	0.21
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	17	0.21
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	17	0.21
(1,1218)	1:119:B:MET:HG2	1:124:B:LEU:HD11	8	0.21
(1,1218)	1:119:B:MET:HG2	1:124:B:LEU:HD12	8	0.21
(1,1218)	1:119:B:MET:HG2	1:124:B:LEU:HD13	8	0.21
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	5	0.21
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	5	0.21
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	5	0.21
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	3	0.21
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	3	0.21
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	3	0.21
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	4	0.21
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	4	0.21
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	4	0.21
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	14	0.21
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	14	0.21
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	14	0.21
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	16	0.21
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	16	0.21
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	16	0.21
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	18	0.21
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	18	0.21
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	18	0.21
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	7	0.21
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	7	0.21
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	7	0.21
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	1	0.21
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	1	0.21
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	1	0.21
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	19	0.21
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	19	0.21
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	19	0.21
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	2	0.21
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	2	0.21
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	15	0.21
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	15	0.21
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	18	0.21
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	11	0.21
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	11	0.21
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	11	0.21
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	12	0.21
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	5	0.21
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	19	0.21
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	6	0.21
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	6	0.21
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	6	0.21
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	14	0.21
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	14	0.21
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	14	0.21
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	20	0.21
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	3	0.21
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	3	0.21
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	3	0.21
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	11	0.21
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	11	0.21
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	11	0.21
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	14	0.21
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	14	0.21
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	14	0.21
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	17	0.21
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	17	0.21
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	17	0.21
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	5	0.21
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	5	0.21
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	5	0.21
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	7	0.21
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	7	0.21
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	7	0.21
(1,751)	1:24:A:LEU:HD21	1:32:A:GLN:H	18	0.21
(1,751)	1:24:A:LEU:HD22	1:32:A:GLN:H	18	0.21
(1,751)	1:24:A:LEU:HD23	1:32:A:GLN:H	18	0.21
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	1	0.21
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	8	0.21
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	15	0.21
(1,525)	1:132:A:ASN:H	1:132:A:ASN:HD22	5	0.21
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	11	0.21
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	18	0.21
(1,400)	1:19:A:VAL:HG21	1:103:A:LEU:H	8	0.21
(1,400)	1:19:A:VAL:HG22	1:103:A:LEU:H	8	0.21
(1,400)	1:19:A:VAL:HG23	1:103:A:LEU:H	8	0.21
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	3	0.21
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	18	0.21
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	19	0.21
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	20	0.21
(1,364)	1:48:A:LYS:H	1:48:A:LYS:HD3	19	0.21
(1,356)	1:115:B:ASP:HB2	1:116:B:ASN:H	6	0.21
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	13	0.21
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	13	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	6	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	6	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	6	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	10	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	10	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	10	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	12	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	12	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	12	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	19	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	19	0.21
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	19	0.21
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	2	0.21
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	2	0.21
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	2	0.21
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	14	0.21
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	14	0.21
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	14	0.21
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	14	0.21
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	14	0.21
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	14	0.21
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	3	0.21
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	17	0.21
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	6	0.21
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	6	0.21
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	6	0.21
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	18	0.21
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	18	0.21
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	18	0.21
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	14	0.21
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	14	0.21
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	14	0.21
(1,109)	1:22:A:ALA:HB1	1:24:A:LEU:HG	13	0.21
(1,109)	1:22:A:ALA:HB2	1:24:A:LEU:HG	13	0.21
(1,109)	1:22:A:ALA:HB3	1:24:A:LEU:HG	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	3	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	3	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	3	0.21
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	4	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	4	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	4	0.21
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	6	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	6	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	6	0.21
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	8	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	8	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	8	0.21
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	10	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	10	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	10	0.21
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	17	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	17	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	17	0.21
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	18	0.21
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	18	0.21
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	18	0.21
(1,93)	1:119:A:MET:HG2	1:124:A:LEU:HD11	8	0.21
(1,93)	1:119:A:MET:HG2	1:124:A:LEU:HD12	8	0.21
(1,93)	1:119:A:MET:HG2	1:124:A:LEU:HD13	8	0.21
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	2	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	2	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	2	0.21
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	3	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	3	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	3	0.21
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	4	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	4	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	4	0.21
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	13	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	13	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	13	0.21
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	16	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	16	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	16	0.21
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	18	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	18	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	19	0.21
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	19	0.21
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	19	0.21
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	2	0.21
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	2	0.21
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	2	0.21
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	3	0.21
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	3	0.21
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	3	0.21
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	4	0.21
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	4	0.21
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	4	0.21
(1,36)	1:42:A:GLN:HB3	1:54:A:ILE:HG21	13	0.21
(1,36)	1:42:A:GLN:HB3	1:54:A:ILE:HG22	13	0.21
(1,36)	1:42:A:GLN:HB3	1:54:A:ILE:HG23	13	0.21
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	18	0.2
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	18	0.2
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	18	0.2
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	18	0.2
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	18	0.2
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	18	0.2
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	18	0.2
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	18	0.2
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	18	0.2
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	18	0.2
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	18	0.2
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	18	0.2
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	18	0.2
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	18	0.2
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	18	0.2
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	18	0.2
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	18	0.2
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	18	0.2
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	4	0.2
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	4	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	4	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	4	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	4	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	4	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	4	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	4	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	5	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	5	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	5	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	5	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	5	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	17	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	17	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	17	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	17	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	17	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	17	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	19	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	19	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	19	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	19	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	19	0.2
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	19	0.2
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	7	0.2
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	7	0.2
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	15	0.2
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	15	0.2
(1,2871)	1:24:B:LEU:HD11	1:32:B:GLN:HG2	1	0.2
(1,2871)	1:24:B:LEU:HD11	1:32:B:GLN:HG3	1	0.2
(1,2871)	1:24:B:LEU:HD12	1:32:B:GLN:HG2	1	0.2
(1,2871)	1:24:B:LEU:HD12	1:32:B:GLN:HG3	1	0.2
(1,2871)	1:24:B:LEU:HD13	1:32:B:GLN:HG2	1	0.2
(1,2871)	1:24:B:LEU:HD13	1:32:B:GLN:HG3	1	0.2
(1,2871)	1:24:B:LEU:HD21	1:32:B:GLN:HG2	1	0.2
(1,2871)	1:24:B:LEU:HD21	1:32:B:GLN:HG3	1	0.2
(1,2871)	1:24:B:LEU:HD22	1:32:B:GLN:HG2	1	0.2
(1,2871)	1:24:B:LEU:HD22	1:32:B:GLN:HG3	1	0.2
(1,2871)	1:24:B:LEU:HD23	1:32:B:GLN:HG2	1	0.2
(1,2871)	1:24:B:LEU:HD23	1:32:B:GLN:HG3	1	0.2
(1,2869)	1:24:B:LEU:HD11	1:32:B:GLN:H	7	0.2
(1,2869)	1:24:B:LEU:HD12	1:32:B:GLN:H	7	0.2
(1,2869)	1:24:B:LEU:HD13	1:32:B:GLN:H	7	0.2
(1,2869)	1:24:B:LEU:HD21	1:32:B:GLN:H	7	0.2
(1,2869)	1:24:B:LEU:HD22	1:32:B:GLN:H	7	0.2
(1,2869)	1:24:B:LEU:HD23	1:32:B:GLN:H	7	0.2
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	4	0.2
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	4	0.2
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	4	0.2
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	4	0.2
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	4	0.2
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	9	0.2
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	9	0.2
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	9	0.2
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	9	0.2
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	9	0.2
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	9	0.2
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	16	0.2
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	16	0.2
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	16	0.2
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	16	0.2
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	16	0.2
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	16	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	13	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	13	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	13	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	13	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	13	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	13	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	13	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	13	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	13	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	13	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	13	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	13	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	13	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	13	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	13	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	13	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	13	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	13	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	15	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	15	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	15	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	15	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	15	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	15	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	15	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	15	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	15	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	15	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	15	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	15	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	15	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	15	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	15	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	15	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	15	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	19	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	19	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	19	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	19	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	19	0.2
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	19	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	19	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	19	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	19	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	19	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	19	0.2
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	19	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	19	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	19	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	19	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	19	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	19	0.2
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	19	0.2
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	8	0.2
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	8	0.2
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	2	0.2
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	2	0.2
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	2	0.2
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	2	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	6	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	6	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	6	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	6	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	6	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	6	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	8	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	8	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	8	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	8	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	8	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	10	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	10	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	10	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	10	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	10	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	10	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	19	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	19	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	19	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	19	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	19	0.2
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	19	0.2
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	1	0.2
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	1	0.2
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	7	0.2
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	7	0.2
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	9	0.2
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	9	0.2
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE21	12	0.2
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE22	12	0.2
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE21	12	0.2
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE22	12	0.2
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	14	0.2
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	14	0.2
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	5	0.2
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	5	0.2
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	5	0.2
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	5	0.2
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	5	0.2
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	5	0.2
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	1	0.2
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	1	0.2
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	1	0.2
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	1	0.2
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	1	0.2
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	1	0.2
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	7	0.2
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	7	0.2
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	7	0.2
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	7	0.2
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	7	0.2
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	16	0.2
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	16	0.2
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	16	0.2
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	16	0.2
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	16	0.2
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	16	0.2
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	2	0.2
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	2	0.2
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	11	0.2
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	11	0.2
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	17	0.2
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	19	0.2
(1,2218)	1:32:A:GLN:HB3	1:32:A:GLN:HE21	6	0.2
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	15	0.2
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	15	0.2
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	15	0.2
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	6	0.2
(1,2157)	1:113:B:GLU:HA	1:116:B:ASN:HD21	7	0.2
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	5	0.2
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	14	0.2
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	10	0.2
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	10	0.2
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	10	0.2
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	11	0.2
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	11	0.2
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	11	0.2
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	7	0.2
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	9	0.2
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	1	0.2
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	1	0.2
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	1	0.2
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	5	0.2
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	5	0.2
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	5	0.2
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	14	0.2
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	14	0.2
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	14	0.2
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	3	0.2
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	3	0.2
(1,2003)	1:73:B:ILE:HG21	1:74:B:GLU:H	19	0.2
(1,2003)	1:73:B:ILE:HG22	1:74:B:GLU:H	19	0.2
(1,2003)	1:73:B:ILE:HG23	1:74:B:GLU:H	19	0.2
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	5	0.2
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	5	0.2
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	5	0.2
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	3	0.2
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	3	0.2
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	3	0.2
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	8	0.2
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	8	0.2
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	8	0.2
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	8	0.2
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	16	0.2
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	18	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD11	3	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD12	3	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD13	3	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD11	18	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD12	18	0.2
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD13	18	0.2
(1,1722)	1:101:B:GLU:H	1:102:B:LYS:H	11	0.2
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	15	0.2
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	15	0.2
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	19	0.2
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	9	0.2
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	20	0.2
(1,1499)	1:48:B:LYS:H	1:48:B:LYS:HD3	11	0.2
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	5	0.2
(1,1419)	1:28:B:GLN:HG2	1:28:B:GLN:HE22	6	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	2	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	2	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	2	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	11	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	11	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	11	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	19	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	19	0.2
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	19	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	4	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	4	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	14	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	14	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	14	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	17	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	17	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	17	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	19	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	19	0.2
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	19	0.2
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	17	0.2
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	6	0.2
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	6	0.2
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	6	0.2
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	9	0.2
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	9	0.2
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	9	0.2
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	18	0.2
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	18	0.2
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	18	0.2
(1,1347)	1:72:B:GLU:HA	1:85:B:VAL:HG11	13	0.2
(1,1347)	1:72:B:GLU:HA	1:85:B:VAL:HG12	13	0.2
(1,1347)	1:72:B:GLU:HA	1:85:B:VAL:HG13	13	0.2
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD21	4	0.2
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD22	4	0.2
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD23	4	0.2
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	5	0.2
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	5	0.2
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	5	0.2
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	10	0.2
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	10	0.2
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	10	0.2
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	14	0.2
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	14	0.2
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	14	0.2
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG21	13	0.2
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG22	13	0.2
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG23	13	0.2
(1,1145)	1:27:A:VAL:HG21	1:33:A:GLY:HA3	19	0.2
(1,1145)	1:27:A:VAL:HG22	1:33:A:GLY:HA3	19	0.2
(1,1145)	1:27:A:VAL:HG23	1:33:A:GLY:HA3	19	0.2
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	14	0.2
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	11	0.2
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	11	0.2
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	6	0.2
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	17	0.2
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	2	0.2
(1,1011)	1:113:A:GLU:HA	1:116:A:ASN:HD21	3	0.2
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	12	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	9	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	9	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	9	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	14	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	14	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	14	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	15	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	15	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	15	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	16	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	16	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	16	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	19	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	19	0.2
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	19	0.2
(1,956)	1:110:A:LYS:H	1:113:A:GLU:H	5	0.2
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	10	0.2
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	10	0.2
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	10	0.2
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	11	0.2
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	11	0.2
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	11	0.2
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	7	0.2
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	1	0.2
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	1	0.2
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	1	0.2
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	5	0.2
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	5	0.2
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	5	0.2
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	18	0.2
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	18	0.2
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	18	0.2
(1,873)	1:73:A:ILE:HB	1:84:A:SER:H	4	0.2
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	3	0.2
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	3	0.2
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	5	0.2
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	5	0.2
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	5	0.2
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	18	0.2
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	18	0.2
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	18	0.2
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	5	0.2
(1,857)	1:73:A:ILE:HG21	1:74:A:GLU:H	19	0.2
(1,857)	1:73:A:ILE:HG22	1:74:A:GLU:H	19	0.2
(1,857)	1:73:A:ILE:HG23	1:74:A:GLU:H	19	0.2
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	11	0.2
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	5	0.2
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	5	0.2
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	5	0.2
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	8	0.2
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	8	0.2
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	8	0.2
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	19	0.2
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	19	0.2
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	19	0.2
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	5	0.2
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	11	0.2
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	11	0.2
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	11	0.2
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	12	0.2
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	12	0.2
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	12	0.2
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	20	0.2
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	18	0.2
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	16	0.2
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	17	0.2
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	18	0.2
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	12	0.2
(1,472)	1:90:A:GLN:HB3	1:90:A:GLN:HE21	3	0.2
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	19	0.2
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	9	0.2
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	10	0.2
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	11	0.2
(1,394)	1:118:A:LEU:H	1:118:A:LEU:HG	17	0.2
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	2	0.2
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	11	0.2
(1,292)	1:28:A:GLN:HA	1:28:A:GLN:HE22	18	0.2
(1,290)	1:28:A:GLN:HG2	1:28:A:GLN:HE22	6	0.2
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	1	0.2
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	1	0.2
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	1	0.2
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	11	0.2
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	11	0.2
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	11	0.2
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	17	0.2
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	17	0.2
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	17	0.2
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	19	0.2
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	19	0.2
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	19	0.2
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	10	0.2
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	14	0.2
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	13	0.2
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	13	0.2
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	13	0.2
(1,220)	1:72:A:GLU:HA	1:85:A:VAL:HG11	13	0.2
(1,220)	1:72:A:GLU:HA	1:85:A:VAL:HG12	13	0.2
(1,220)	1:72:A:GLU:HA	1:85:A:VAL:HG13	13	0.2
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	20	0.2
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	20	0.2
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	20	0.2
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	5	0.2
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	14	0.2
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	5	0.2
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	5	0.2
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	5	0.2
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	14	0.2
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	14	0.2
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	14	0.2
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	5	0.2
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	5	0.2
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	5	0.2
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	14	0.2
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	14	0.2
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	14	0.2
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	7	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	7	0.2
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	7	0.2
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	1	0.2
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	1	0.2
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	1	0.2
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	8	0.2
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	8	0.2
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	8	0.2
(1,19)	1:27:B:VAL:HG21	1:33:B:GLY:HA3	19	0.2
(1,19)	1:27:B:VAL:HG22	1:33:B:GLY:HA3	19	0.2
(1,19)	1:27:B:VAL:HG23	1:33:B:GLY:HA3	19	0.2
(1,3178)	1:109:B:ASP:HA	1:112:B:LYS:HB2	5	0.19
(1,3178)	1:109:B:ASP:HA	1:112:B:LYS:HB3	5	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	8	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	8	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	8	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	8	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	8	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	8	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	9	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	9	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	9	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	9	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	9	0.19
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	9	0.19
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	17	0.19
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	17	0.19
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	18	0.19
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	18	0.19
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB2	4	0.19
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB3	4	0.19
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB2	4	0.19
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB3	4	0.19
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB2	4	0.19
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB3	4	0.19
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB2	4	0.19
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB3	4	0.19
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB2	4	0.19
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB3	4	0.19
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB2	4	0.19
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB3	4	0.19
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	15	0.19
(1,2866)	1:24:B:LEU:HB2	1:25:B:SER:H	4	0.19
(1,2866)	1:24:B:LEU:HB3	1:25:B:SER:H	4	0.19
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	1	0.19
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	1	0.19
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	1	0.19
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	1	0.19
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	1	0.19
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	1	0.19
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	14	0.19
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	14	0.19
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	14	0.19
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	14	0.19
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	14	0.19
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	14	0.19
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB2	10	0.19
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB3	10	0.19
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	4	0.19
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	4	0.19
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	17	0.19
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	17	0.19
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	17	0.19
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	17	0.19
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	17	0.19
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	17	0.19
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	11	0.19
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	11	0.19
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	11	0.19
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	11	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	4	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	4	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	4	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	4	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	4	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	4	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	17	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	17	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	17	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	17	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	17	0.19
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	17	0.19
(1,2633)	1:95:A:ASP:HB2	1:30:B:SER:H	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2633)	1:95:A:ASP:HB3	1:30:B:SER:H	20	0.19
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	18	0.19
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	18	0.19
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	10	0.19
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE3	10	0.19
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	10	0.19
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE3	10	0.19
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	15	0.19
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	15	0.19
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD11	6	0.19
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD12	6	0.19
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD13	6	0.19
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD21	6	0.19
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD22	6	0.19
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD23	6	0.19
(1,2401)	1:32:A:GLN:HB2	1:57:A:ALA:HB1	4	0.19
(1,2401)	1:32:A:GLN:HB2	1:57:A:ALA:HB2	4	0.19
(1,2401)	1:32:A:GLN:HB2	1:57:A:ALA:HB3	4	0.19
(1,2401)	1:32:A:GLN:HB3	1:57:A:ALA:HB1	4	0.19
(1,2401)	1:32:A:GLN:HB3	1:57:A:ALA:HB2	4	0.19
(1,2401)	1:32:A:GLN:HB3	1:57:A:ALA:HB3	4	0.19
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD2	12	0.19
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD3	12	0.19
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD2	12	0.19
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD3	12	0.19
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	12	0.19
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	12	0.19
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	12	0.19
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	12	0.19
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	12	0.19
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	12	0.19
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	8	0.19
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	8	0.19
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	8	0.19
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	8	0.19
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	8	0.19
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	8	0.19
(1,2359)	1:24:A:LEU:HB2	1:25:A:SER:H	4	0.19
(1,2359)	1:24:A:LEU:HB3	1:25:A:SER:H	4	0.19
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	9	0.19
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	9	0.19
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	9	0.19
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	9	0.19
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	9	0.19
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	12	0.19
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	12	0.19
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	12	0.19
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	12	0.19
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	12	0.19
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	12	0.19
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	14	0.19
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	14	0.19
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	14	0.19
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	14	0.19
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	14	0.19
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	14	0.19
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD1	14	0.19
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD2	14	0.19
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	6	0.19
(1,2194)	1:119:A:MET:HG3	1:124:A:LEU:H	19	0.19
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	12	0.19
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	12	0.19
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	12	0.19
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	11	0.19
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	11	0.19
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	11	0.19
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	2	0.19
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	10	0.19
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	19	0.19
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	13	0.19
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	13	0.19
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	13	0.19
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	19	0.19
(1,2096)	1:19:A:VAL:HG11	1:105:A:TYR:H	17	0.19
(1,2096)	1:19:A:VAL:HG12	1:105:A:TYR:H	17	0.19
(1,2096)	1:19:A:VAL:HG13	1:105:A:TYR:H	17	0.19
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	8	0.19
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	20	0.19
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	20	0.19
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	20	0.19
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	4	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	4	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	6	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	6	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	6	0.19
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	7	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	7	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	7	0.19
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	9	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	9	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	9	0.19
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	10	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	10	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	10	0.19
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	18	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	18	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	18	0.19
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	19	0.19
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	19	0.19
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	19	0.19
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	5	0.19
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	5	0.19
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	5	0.19
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	5	0.19
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	11	0.19
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	11	0.19
(1,1912)	1:35:B:VAL:HG21	1:36:B:ARG:H	18	0.19
(1,1912)	1:35:B:VAL:HG22	1:36:B:ARG:H	18	0.19
(1,1912)	1:35:B:VAL:HG23	1:36:B:ARG:H	18	0.19
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	14	0.19
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	14	0.19
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	14	0.19
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	11	0.19
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	11	0.19
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	11	0.19
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	3	0.19
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	10	0.19
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	17	0.19
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	5	0.19
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	7	0.19
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	15	0.19
(1,1727)	1:91:A:ILE:H	1:91:A:ILE:HD11	17	0.19
(1,1727)	1:91:A:ILE:H	1:91:A:ILE:HD12	17	0.19
(1,1727)	1:91:A:ILE:H	1:91:A:ILE:HD13	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1725)	1:116:B:ASN:HA	1:116:B:ASN:HD21	13	0.19
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD21	3	0.19
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD22	3	0.19
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD23	3	0.19
(1,1666)	1:132:B:ASN:H	1:132:B:ASN:HD22	5	0.19
(1,1610)	1:90:B:GLN:H	1:90:B:GLN:HE21	15	0.19
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	1	0.19
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	9	0.19
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	15	0.19
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	10	0.19
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	11	0.19
(1,1529)	1:118:B:LEU:H	1:118:B:LEU:HG	17	0.19
(1,1499)	1:48:B:LYS:H	1:48:B:LYS:HD3	19	0.19
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	17	0.19
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	19	0.19
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	2	0.19
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	3	0.19
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	15	0.19
(1,1484)	1:120:B:ILE:H	1:120:B:ILE:HG13	19	0.19
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	7	0.19
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	3	0.19
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	3	0.19
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	3	0.19
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	17	0.19
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	17	0.19
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	17	0.19
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	3	0.19
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	10	0.19
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	13	0.19
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	13	0.19
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	13	0.19
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	17	0.19
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	17	0.19
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	17	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	4	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	4	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	4	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	17	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	17	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	17	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	20	0.19
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	20	0.19
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	4	0.19
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	3	0.19
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	5	0.19
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	8	0.19
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	12	0.19
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	13	0.19
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	14	0.19
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	16	0.19
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	1	0.19
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	1	0.19
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	1	0.19
(1,1234)	1:22:B:ALA:HB1	1:24:B:LEU:HG	18	0.19
(1,1234)	1:22:B:ALA:HB2	1:24:B:LEU:HG	18	0.19
(1,1234)	1:22:B:ALA:HB3	1:24:B:LEU:HG	18	0.19
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	7	0.19
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	7	0.19
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	7	0.19
(1,1221)	1:38:A:VAL:HG11	1:57:A:ALA:HA	12	0.19
(1,1221)	1:38:A:VAL:HG12	1:57:A:ALA:HA	12	0.19
(1,1221)	1:38:A:VAL:HG13	1:57:A:ALA:HA	12	0.19
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	14	0.19
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	14	0.19
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	14	0.19
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	13	0.19
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	13	0.19
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	13	0.19
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	4	0.19
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	4	0.19
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	4	0.19
(1,1172)	1:117:B:ALA:HB1	1:118:B:LEU:HB2	6	0.19
(1,1172)	1:117:B:ALA:HB2	1:118:B:LEU:HB2	6	0.19
(1,1172)	1:117:B:ALA:HB3	1:118:B:LEU:HB2	6	0.19
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	8	0.19
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	8	0.19
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	8	0.19
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	14	0.19
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	14	0.19
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	14	0.19
(1,1145)	1:27:A:VAL:HG21	1:33:A:GLY:HA3	12	0.19
(1,1145)	1:27:A:VAL:HG22	1:33:A:GLY:HA3	12	0.19
(1,1145)	1:27:A:VAL:HG23	1:33:A:GLY:HA3	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	8	0.19
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	1	0.19
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	16	0.19
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	3	0.19
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	3	0.19
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	3	0.19
(1,950)	1:19:B:VAL:HG11	1:105:B:TYR:H	17	0.19
(1,950)	1:19:B:VAL:HG12	1:105:B:TYR:H	17	0.19
(1,950)	1:19:B:VAL:HG13	1:105:B:TYR:H	17	0.19
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	8	0.19
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	10	0.19
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	9	0.19
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	20	0.19
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	20	0.19
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	20	0.19
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	4	0.19
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	4	0.19
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	4	0.19
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	6	0.19
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	6	0.19
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	6	0.19
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	7	0.19
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	7	0.19
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	7	0.19
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	9	0.19
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	9	0.19
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	9	0.19
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	10	0.19
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	10	0.19
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	10	0.19
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	7	0.19
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	7	0.19
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	7	0.19
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	11	0.19
(1,766)	1:35:A:VAL:HG21	1:36:A:ARG:H	18	0.19
(1,766)	1:35:A:VAL:HG22	1:36:A:ARG:H	18	0.19
(1,766)	1:35:A:VAL:HG23	1:36:A:ARG:H	18	0.19
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	14	0.19
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	14	0.19
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	14	0.19
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	3	0.19
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	17	0.19
(1,604)	1:24:B:LEU:HB3	1:25:B:SER:H	7	0.19
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	7	0.19
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	9	0.19
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	11	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD11	3	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD12	3	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD13	3	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD11	18	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD12	18	0.19
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD13	18	0.19
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	11	0.19
(1,471)	1:90:A:GLN:H	1:90:A:GLN:HE21	19	0.19
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	1	0.19
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	8	0.19
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	15	0.19
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	17	0.19
(1,434)	1:113:A:GLU:H	1:113:A:GLU:HG2	5	0.19
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	11	0.19
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	11	0.19
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	11	0.19
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	5	0.19
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	5	0.19
(1,364)	1:48:A:LYS:H	1:48:A:LYS:HD3	8	0.19
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	6	0.19
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	15	0.19
(1,290)	1:28:A:GLN:HG2	1:28:A:GLN:HE22	11	0.19
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	2	0.19
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	2	0.19
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	2	0.19
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	17	0.19
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	17	0.19
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	17	0.19
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	4	0.19
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	4	0.19
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	4	0.19
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	17	0.19
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	17	0.19
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	17	0.19
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	12	0.19
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD21	4	0.19
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD22	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD23	4	0.19
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD1	4	0.19
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD2	4	0.19
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	3	0.19
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	12	0.19
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	13	0.19
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	16	0.19
(1,109)	1:22:A:ALA:HB1	1:24:A:LEU:HG	18	0.19
(1,109)	1:22:A:ALA:HB2	1:24:A:LEU:HG	18	0.19
(1,109)	1:22:A:ALA:HB3	1:24:A:LEU:HG	18	0.19
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	7	0.19
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	7	0.19
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	7	0.19
(1,96)	1:38:B:VAL:HG11	1:57:B:ALA:HA	12	0.19
(1,96)	1:38:B:VAL:HG12	1:57:B:ALA:HA	12	0.19
(1,96)	1:38:B:VAL:HG13	1:57:B:ALA:HA	12	0.19
(1,46)	1:117:A:ALA:HB1	1:118:A:LEU:HB2	2	0.19
(1,46)	1:117:A:ALA:HB2	1:118:A:LEU:HB2	2	0.19
(1,46)	1:117:A:ALA:HB3	1:118:A:LEU:HB2	2	0.19
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	14	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	14	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	14	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	14	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	14	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	14	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	14	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	14	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	14	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	14	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	14	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	14	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	14	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	14	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	14	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	14	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	14	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	14	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	19	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	19	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	19	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	19	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	19	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	19	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	19	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	19	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	19	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	19	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	19	0.18
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	19	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	19	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	19	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	19	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	19	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	19	0.18
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	19	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD11	1	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD12	1	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD13	1	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD21	1	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD22	1	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD23	1	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD11	1	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD12	1	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD13	1	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD21	1	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD22	1	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD23	1	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD11	20	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD12	20	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD13	20	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD21	20	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD22	20	0.18
(1,3239)	1:119:B:MET:HG2	1:124:B:LEU:HD23	20	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD11	20	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD12	20	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD13	20	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD21	20	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD22	20	0.18
(1,3239)	1:119:B:MET:HG3	1:124:B:LEU:HD23	20	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	5	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	5	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	5	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	5	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	5	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	18	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	18	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	18	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	18	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	18	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	18	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	20	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	20	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	20	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	20	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	20	0.18
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	20	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	1	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	1	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	1	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	1	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	1	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	1	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	3	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	3	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	3	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	3	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	3	0.18
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	3	0.18
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	19	0.18
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	19	0.18
(1,3050)	1:74:B:GLU:HG2	1:76:B:LYS:H	4	0.18
(1,3050)	1:74:B:GLU:HG3	1:76:B:LYS:H	4	0.18
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	4	0.18
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	4	0.18
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	6	0.18
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	6	0.18
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	13	0.18
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	13	0.18
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD11	6	0.18
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD12	6	0.18
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD13	6	0.18
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD21	6	0.18
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD22	6	0.18
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD23	6	0.18
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	14	0.18
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	1	0.18
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	1	0.18
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	1	0.18
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	1	0.18
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	1	0.18
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	1	0.18
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	12	0.18
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	12	0.18
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	12	0.18
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	12	0.18
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	12	0.18
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	12	0.18
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	18	0.18
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	18	0.18
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	18	0.18
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	18	0.18
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	18	0.18
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	18	0.18
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	20	0.18
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	20	0.18
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	20	0.18
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	20	0.18
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	20	0.18
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	20	0.18
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB2	11	0.18
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB3	11	0.18
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	11	0.18
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	11	0.18
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	11	0.18
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	11	0.18
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD11	20	0.18
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD12	20	0.18
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD13	20	0.18
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD21	20	0.18
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD22	20	0.18
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD23	20	0.18
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD11	20	0.18
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD12	20	0.18
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD13	20	0.18
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD21	20	0.18
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD22	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD23	20	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	4	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	4	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	4	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	4	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	4	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	4	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	18	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	18	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	18	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	18	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	18	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	18	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	20	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	20	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	20	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	20	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	20	0.18
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	20	0.18
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	14	0.18
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	14	0.18
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD21	10	0.18
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD22	10	0.18
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD21	10	0.18
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD22	10	0.18
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	4	0.18
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	4	0.18
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	4	0.18
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	4	0.18
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	17	0.18
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	17	0.18
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	17	0.18
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	17	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	1	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	1	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	1	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	1	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	1	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	1	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	3	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	3	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	3	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	3	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	3	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	13	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	13	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	13	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	13	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	13	0.18
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	13	0.18
(1,2587)	1:80:A:LEU:HD11	1:84:A:SER:HB2	4	0.18
(1,2587)	1:80:A:LEU:HD11	1:84:A:SER:HB3	4	0.18
(1,2587)	1:80:A:LEU:HD12	1:84:A:SER:HB2	4	0.18
(1,2587)	1:80:A:LEU:HD12	1:84:A:SER:HB3	4	0.18
(1,2587)	1:80:A:LEU:HD13	1:84:A:SER:HB2	4	0.18
(1,2587)	1:80:A:LEU:HD13	1:84:A:SER:HB3	4	0.18
(1,2587)	1:80:A:LEU:HD21	1:84:A:SER:HB2	4	0.18
(1,2587)	1:80:A:LEU:HD21	1:84:A:SER:HB3	4	0.18
(1,2587)	1:80:A:LEU:HD22	1:84:A:SER:HB2	4	0.18
(1,2587)	1:80:A:LEU:HD22	1:84:A:SER:HB3	4	0.18
(1,2587)	1:80:A:LEU:HD23	1:84:A:SER:HB2	4	0.18
(1,2587)	1:80:A:LEU:HD23	1:84:A:SER:HB3	4	0.18
(1,2548)	1:74:A:GLU:HB2	1:77:A:LYS:H	5	0.18
(1,2548)	1:74:A:GLU:HB3	1:77:A:LYS:H	5	0.18
(1,2542)	1:73:A:ILE:HG12	1:78:A:TYR:HD1	4	0.18
(1,2542)	1:73:A:ILE:HG12	1:78:A:TYR:HD2	4	0.18
(1,2542)	1:73:A:ILE:HG13	1:78:A:TYR:HD1	4	0.18
(1,2542)	1:73:A:ILE:HG13	1:78:A:TYR:HD2	4	0.18
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	4	0.18
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	4	0.18
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	6	0.18
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	6	0.18
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	18	0.18
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	18	0.18
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	14	0.18
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	14	0.18
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	14	0.18
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	14	0.18
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	14	0.18
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	14	0.18
(1,2362)	1:24:A:LEU:HD11	1:32:A:GLN:H	7	0.18
(1,2362)	1:24:A:LEU:HD12	1:32:A:GLN:H	7	0.18
(1,2362)	1:24:A:LEU:HD13	1:32:A:GLN:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2362)	1:24:A:LEU:HD21	1:32:A:GLN:H	7	0.18
(1,2362)	1:24:A:LEU:HD22	1:32:A:GLN:H	7	0.18
(1,2362)	1:24:A:LEU:HD23	1:32:A:GLN:H	7	0.18
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	10	0.18
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	10	0.18
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	10	0.18
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	10	0.18
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	10	0.18
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	10	0.18
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	18	0.18
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	18	0.18
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	18	0.18
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	18	0.18
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	18	0.18
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	18	0.18
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB2	11	0.18
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB3	11	0.18
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	15	0.18
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	15	0.18
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	18	0.18
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	8	0.18
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	8	0.18
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	8	0.18
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	8	0.18
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	8	0.18
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	8	0.18
(1,2152)	1:123:B:GLY:H	1:125:B:ASN:H	19	0.18
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	1	0.18
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	1	0.18
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	1	0.18
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	20	0.18
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	20	0.18
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	20	0.18
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	6	0.18
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	8	0.18
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	9	0.18
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	12	0.18
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	4	0.18
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	4	0.18
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	4	0.18
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	9	0.18
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	9	0.18
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	20	0.18
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	20	0.18
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	20	0.18
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	10	0.18
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	8	0.18
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	2	0.18
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	2	0.18
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	2	0.18
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	13	0.18
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	13	0.18
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	13	0.18
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	15	0.18
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	15	0.18
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	15	0.18
(1,2047)	1:91:B:ILE:HG21	1:92:B:ARG:H	16	0.18
(1,2047)	1:91:B:ILE:HG22	1:92:B:ARG:H	16	0.18
(1,2047)	1:91:B:ILE:HG23	1:92:B:ARG:H	16	0.18
(1,2044)	1:93:A:THR:HB	1:91:B:ILE:H	20	0.18
(1,2001)	1:74:B:GLU:H	1:78:B:TYR:HD1	20	0.18
(1,2001)	1:74:B:GLU:H	1:78:B:TYR:HD2	20	0.18
(1,1938)	1:42:B:GLN:HE21	1:45:B:THR:H	19	0.18
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	7	0.18
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	7	0.18
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	7	0.18
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	11	0.18
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	1	0.18
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	1	0.18
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	1	0.18
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	5	0.18
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	6	0.18
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	19	0.18
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	9	0.18
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	9	0.18
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	9	0.18
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	6	0.18
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	7	0.18
(1,1775)	1:73:A:ILE:H	1:73:A:ILE:HG13	7	0.18
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	6	0.18
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	9	0.18
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	11	0.18
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	11	0.18
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	12	0.18
(1,1710)	1:127:B:VAL:HA	1:128:B:ALA:H	13	0.18
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	12	0.18
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	11	0.18
(1,1610)	1:90:B:GLN:H	1:90:B:GLN:HE21	19	0.18
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	10	0.18
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	8	0.18
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	11	0.18
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	11	0.18
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	11	0.18
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	5	0.18
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	5	0.18
(1,1498)	1:48:B:LYS:H	1:48:B:LYS:HD2	15	0.18
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	18	0.18
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	7	0.18
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	10	0.18
(1,1456)	1:14:A:ILE:H	1:14:A:ILE:HG13	16	0.18
(1,1419)	1:28:B:GLN:HG2	1:28:B:GLN:HE22	11	0.18
(1,1417)	1:75:B:LYS:H	1:75:B:LYS:HD3	20	0.18
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	19	0.18
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	19	0.18
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	19	0.18
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	19	0.18
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	19	0.18
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	19	0.18
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	19	0.18
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	19	0.18
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	19	0.18
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	3	0.18
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	3	0.18
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	3	0.18
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	10	0.18
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	10	0.18
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	10	0.18
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	1	0.18
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	14	0.18
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG21	5	0.18
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG22	5	0.18
(1,1356)	1:111:A:MET:HA	1:114:A:VAL:HG23	5	0.18
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	2	0.18
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	2	0.18
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	5	0.18
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	5	0.18
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	5	0.18
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	12	0.18
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	12	0.18
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	12	0.18
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	14	0.18
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	14	0.18
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	14	0.18
(1,1342)	1:91:A:ILE:HG21	1:93:B:THR:HB	16	0.18
(1,1342)	1:91:A:ILE:HG22	1:93:B:THR:HB	16	0.18
(1,1342)	1:91:A:ILE:HG23	1:93:B:THR:HB	16	0.18
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	12	0.18
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	13	0.18
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD11	12	0.18
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD12	12	0.18
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD13	12	0.18
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	4	0.18
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	17	0.18
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	19	0.18
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	20	0.18
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	20	0.18
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	20	0.18
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD21	18	0.18
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD22	18	0.18
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD23	18	0.18
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	20	0.18
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	20	0.18
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	20	0.18
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	10	0.18
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	10	0.18
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	10	0.18
(1,1145)	1:27:A:VAL:HG21	1:33:A:GLY:HA3	8	0.18
(1,1145)	1:27:A:VAL:HG22	1:33:A:GLY:HA3	8	0.18
(1,1145)	1:27:A:VAL:HG23	1:33:A:GLY:HA3	8	0.18
(1,1141)	1:111:B:MET:HE1	1:114:B:VAL:HB	9	0.18
(1,1141)	1:111:B:MET:HE2	1:114:B:VAL:HB	9	0.18
(1,1141)	1:111:B:MET:HE3	1:114:B:VAL:HB	9	0.18
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	1	0.18
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	1	0.18
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	13	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	13	0.18
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	19	0.18
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	17	0.18
(1,1071)	1:24:A:LEU:HD11	1:32:A:GLN:H	4	0.18
(1,1071)	1:24:A:LEU:HD12	1:32:A:GLN:H	4	0.18
(1,1071)	1:24:A:LEU:HD13	1:32:A:GLN:H	4	0.18
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	18	0.18
(1,1042)	1:119:B:MET:HG3	1:124:B:LEU:H	19	0.18
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG21	12	0.18
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG22	12	0.18
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG23	12	0.18
(1,1027)	1:42:A:GLN:HE21	1:53:A:VAL:HG21	8	0.18
(1,1027)	1:42:A:GLN:HE21	1:53:A:VAL:HG22	8	0.18
(1,1027)	1:42:A:GLN:HE21	1:53:A:VAL:HG23	8	0.18
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	4	0.18
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	4	0.18
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	4	0.18
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	20	0.18
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	20	0.18
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	20	0.18
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	6	0.18
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	4	0.18
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	4	0.18
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	4	0.18
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	13	0.18
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	13	0.18
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	13	0.18
(1,942)	1:103:A:LEU:HD11	1:104:A:THR:H	11	0.18
(1,942)	1:103:A:LEU:HD12	1:104:A:THR:H	11	0.18
(1,942)	1:103:A:LEU:HD13	1:104:A:THR:H	11	0.18
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	2	0.18
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	2	0.18
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	2	0.18
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	13	0.18
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	13	0.18
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	13	0.18
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	15	0.18
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	15	0.18
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	15	0.18
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	16	0.18
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	16	0.18
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	16	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,901)	1:91:A:ILE:HG21	1:92:A:ARG:H	19	0.18
(1,901)	1:91:A:ILE:HG22	1:92:A:ARG:H	19	0.18
(1,901)	1:91:A:ILE:HG23	1:92:A:ARG:H	19	0.18
(1,898)	1:91:A:ILE:H	1:93:B:THR:HB	20	0.18
(1,792)	1:42:A:GLN:HE21	1:45:A:THR:H	19	0.18
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	11	0.18
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	9	0.18
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	9	0.18
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	9	0.18
(1,751)	1:24:A:LEU:HD21	1:32:A:GLN:H	13	0.18
(1,751)	1:24:A:LEU:HD22	1:32:A:GLN:H	13	0.18
(1,751)	1:24:A:LEU:HD23	1:32:A:GLN:H	13	0.18
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	6	0.18
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	7	0.18
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	7	0.18
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	7	0.18
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	9	0.18
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	9	0.18
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	9	0.18
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	20	0.18
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	20	0.18
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	20	0.18
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	6	0.18
(1,625)	1:96:B:LYS:HB2	1:97:B:LYS:H	20	0.18
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	2	0.18
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	5	0.18
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	6	0.18
(1,585)	1:91:B:ILE:H	1:91:B:ILE:HD11	17	0.18
(1,585)	1:91:B:ILE:H	1:91:B:ILE:HD12	17	0.18
(1,585)	1:91:B:ILE:H	1:91:B:ILE:HD13	17	0.18
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	12	0.18
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	11	0.18
(1,471)	1:90:A:GLN:H	1:90:A:GLN:HE21	15	0.18
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	10	0.18
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	9	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	4	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	4	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	4	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	10	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	10	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	10	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	18	0.18
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	18	0.18
(1,363)	1:48:A:LYS:H	1:48:A:LYS:HD2	15	0.18
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	10	0.18
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	3	0.18
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	3	0.18
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	3	0.18
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD11	14	0.18
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD12	14	0.18
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD13	14	0.18
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	10	0.18
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	10	0.18
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	10	0.18
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	1	0.18
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	12	0.18
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	12	0.18
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	12	0.18
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	15	0.18
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	15	0.18
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	15	0.18
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	4	0.18
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	4	0.18
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	4	0.18
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	7	0.18
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	7	0.18
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	7	0.18
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG21	16	0.18
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG22	16	0.18
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG23	16	0.18
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	16	0.18
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD11	12	0.18
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD12	12	0.18
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD13	12	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	1	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	4	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	8	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	9	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	11	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	17	0.18
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	19	0.18
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	1	0.18
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	1	0.18
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	20	0.18
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	20	0.18
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	20	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	4	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	4	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	4	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	17	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	17	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	17	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	20	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	20	0.18
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	20	0.18
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	18	0.18
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	18	0.18
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	18	0.18
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	14	0.18
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	14	0.18
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	14	0.18
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	10	0.18
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	10	0.18
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	10	0.18
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	14	0.18
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	14	0.18
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	14	0.18
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	13	0.17
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	13	0.17
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	13	0.17
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	13	0.17
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	13	0.17
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	13	0.17
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	13	0.17
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	13	0.17
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	13	0.17
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	13	0.17
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	13	0.17
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	13	0.17
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	13	0.17
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	13	0.17
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	13	0.17
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	13	0.17
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	13	0.17
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	2	0.17
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	2	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	1	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	1	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	1	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	1	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	1	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	1	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	10	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	10	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	10	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	10	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	10	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	10	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	11	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	11	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	11	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	11	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	11	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	11	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	17	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	17	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	17	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	17	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	17	0.17
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	17	0.17
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	13	0.17
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	13	0.17
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	15	0.17
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	15	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	7	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	7	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	7	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	7	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	7	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	7	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	10	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	10	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	10	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	10	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	10	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	13	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	13	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	13	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	13	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	13	0.17
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	13	0.17
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	11	0.17
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	11	0.17
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	11	0.17
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	11	0.17
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	11	0.17
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	11	0.17
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	11	0.17
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	11	0.17
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	11	0.17
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	11	0.17
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	11	0.17
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	11	0.17
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE2	10	0.17
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE3	10	0.17
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE2	10	0.17
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE3	10	0.17
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	1	0.17
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	1	0.17
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	14	0.17
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	14	0.17
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	16	0.17
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	16	0.17
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	17	0.17
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	17	0.17
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	18	0.17
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	18	0.17
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	18	0.17
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	18	0.17
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	18	0.17
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	18	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	9	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	9	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	9	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	9	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	9	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	12	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	12	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	12	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	12	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	12	0.17
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	12	0.17
(1,2876)	1:24:B:LEU:HD11	1:90:B:GLN:HE21	12	0.17
(1,2876)	1:24:B:LEU:HD12	1:90:B:GLN:HE21	12	0.17
(1,2876)	1:24:B:LEU:HD13	1:90:B:GLN:HE21	12	0.17
(1,2876)	1:24:B:LEU:HD21	1:90:B:GLN:HE21	12	0.17
(1,2876)	1:24:B:LEU:HD22	1:90:B:GLN:HE21	12	0.17
(1,2876)	1:24:B:LEU:HD23	1:90:B:GLN:HE21	12	0.17
(1,2874)	1:24:B:LEU:HD11	1:32:B:GLN:HE22	11	0.17
(1,2874)	1:24:B:LEU:HD12	1:32:B:GLN:HE22	11	0.17
(1,2874)	1:24:B:LEU:HD13	1:32:B:GLN:HE22	11	0.17
(1,2874)	1:24:B:LEU:HD21	1:32:B:GLN:HE22	11	0.17
(1,2874)	1:24:B:LEU:HD22	1:32:B:GLN:HE22	11	0.17
(1,2874)	1:24:B:LEU:HD23	1:32:B:GLN:HE22	11	0.17
(1,2869)	1:24:B:LEU:HD11	1:32:B:GLN:H	8	0.17
(1,2869)	1:24:B:LEU:HD12	1:32:B:GLN:H	8	0.17
(1,2869)	1:24:B:LEU:HD13	1:32:B:GLN:H	8	0.17
(1,2869)	1:24:B:LEU:HD21	1:32:B:GLN:H	8	0.17
(1,2869)	1:24:B:LEU:HD22	1:32:B:GLN:H	8	0.17
(1,2869)	1:24:B:LEU:HD23	1:32:B:GLN:H	8	0.17
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	2	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	2	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	2	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	2	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	2	0.17
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	2	0.17
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	5	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	5	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	5	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	5	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	5	0.17
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	5	0.17
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	6	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	6	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	6	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	6	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	6	0.17
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	7	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	7	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	7	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	7	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	7	0.17
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	7	0.17
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	8	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	8	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	8	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	8	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	8	0.17
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	8	0.17
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	11	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	11	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	11	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	11	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	11	0.17
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	11	0.17
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	15	0.17
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	15	0.17
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	15	0.17
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	15	0.17
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	15	0.17
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	15	0.17
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	7	0.17
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	7	0.17
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	7	0.17
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	7	0.17
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	17	0.17
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	17	0.17
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	17	0.17
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	17	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	8	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	8	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	8	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	8	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	8	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	8	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	8	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	8	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	8	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	8	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	8	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	8	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	8	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	8	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	8	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	8	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	8	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	14	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	14	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	14	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	14	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	14	0.17
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	14	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	14	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	14	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	14	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	14	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	14	0.17
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	14	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	14	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	14	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	14	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	14	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	14	0.17
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	14	0.17
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	2	0.17
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	2	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	1	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	1	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	1	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	1	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	1	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	1	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	5	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	5	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	5	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	5	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	5	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	5	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	8	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	8	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	8	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	8	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	8	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	11	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	11	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	11	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	11	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	11	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	11	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	12	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	12	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	12	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	12	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	12	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	12	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	19	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	19	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	19	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	19	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	19	0.17
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	19	0.17
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	5	0.17
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	5	0.17
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	19	0.17
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	19	0.17
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	19	0.17
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	19	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	7	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	7	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	7	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	7	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	7	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	7	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	9	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	9	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	9	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	9	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	9	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	9	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD11	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD12	12	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD13	12	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD21	12	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD22	12	0.17
(1,2635)	1:96:A:LYS:HA	1:99:A:LEU:HD23	12	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	3	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	3	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	3	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	3	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	3	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	3	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	3	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	3	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	3	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	3	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	3	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	3	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	5	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	5	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	5	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	5	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	5	0.17
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	5	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	5	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	5	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	5	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	5	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	5	0.17
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	5	0.17
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	17	0.17
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	17	0.17
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	19	0.17
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	19	0.17
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	16	0.17
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE3	16	0.17
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	16	0.17
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE3	16	0.17
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	10	0.17
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	10	0.17
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	14	0.17
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	14	0.17
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	16	0.17
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	17	0.17
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	17	0.17
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB2	20	0.17
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB3	20	0.17
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	9	0.17
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	9	0.17
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	9	0.17
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	9	0.17
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	9	0.17
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	9	0.17
(1,2362)	1:24:A:LEU:HD11	1:32:A:GLN:H	8	0.17
(1,2362)	1:24:A:LEU:HD12	1:32:A:GLN:H	8	0.17
(1,2362)	1:24:A:LEU:HD13	1:32:A:GLN:H	8	0.17
(1,2362)	1:24:A:LEU:HD21	1:32:A:GLN:H	8	0.17
(1,2362)	1:24:A:LEU:HD22	1:32:A:GLN:H	8	0.17
(1,2362)	1:24:A:LEU:HD23	1:32:A:GLN:H	8	0.17
(1,2359)	1:24:A:LEU:HB2	1:25:A:SER:H	18	0.17
(1,2359)	1:24:A:LEU:HB3	1:25:A:SER:H	18	0.17
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	6	0.17
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	6	0.17
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	6	0.17
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	6	0.17
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	6	0.17
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	6	0.17
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	20	0.17
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	20	0.17
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	20	0.17
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	20	0.17
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	20	0.17
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	20	0.17
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB2	10	0.17
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB3	10	0.17
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD1	1	0.17
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD2	1	0.17
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	13	0.17
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	13	0.17
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	11	0.17
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	17	0.17
(1,2224)	1:24:B:LEU:HD11	1:32:B:GLN:H	4	0.17
(1,2224)	1:24:B:LEU:HD12	1:32:B:GLN:H	4	0.17
(1,2224)	1:24:B:LEU:HD13	1:32:B:GLN:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	3	0.17
(1,2218)	1:32:A:GLN:HB3	1:32:A:GLN:HE21	19	0.17
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	18	0.17
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	20	0.17
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	17	0.17
(1,2157)	1:113:B:GLU:HA	1:116:B:ASN:HD21	9	0.17
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	12	0.17
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	1	0.17
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	16	0.17
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	12	0.17
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	12	0.17
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	12	0.17
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	14	0.17
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	14	0.17
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	14	0.17
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	16	0.17
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	16	0.17
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	16	0.17
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	17	0.17
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	17	0.17
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	17	0.17
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	18	0.17
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	18	0.17
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	18	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	1	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	1	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	1	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	11	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	11	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	11	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	20	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	20	0.17
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	20	0.17
(1,2107)	1:112:B:LYS:H	1:115:B:ASP:H	2	0.17
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	12	0.17
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	5	0.17
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	12	0.17
(1,2088)	1:103:B:LEU:HD11	1:104:B:THR:H	7	0.17
(1,2088)	1:103:B:LEU:HD12	1:104:B:THR:H	7	0.17
(1,2088)	1:103:B:LEU:HD13	1:104:B:THR:H	7	0.17
(1,2088)	1:103:B:LEU:HD11	1:104:B:THR:H	11	0.17
(1,2088)	1:103:B:LEU:HD12	1:104:B:THR:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:103:B:LEU:HD13	1:104:B:THR:H	11	0.17
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	1	0.17
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	1	0.17
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	1	0.17
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	8	0.17
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	16	0.17
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	16	0.17
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	16	0.17
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	15	0.17
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	9	0.17
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	9	0.17
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	9	0.17
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	12	0.17
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	12	0.17
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	12	0.17
(1,1897)	1:24:B:LEU:HD21	1:32:B:GLN:H	13	0.17
(1,1897)	1:24:B:LEU:HD22	1:32:B:GLN:H	13	0.17
(1,1897)	1:24:B:LEU:HD23	1:32:B:GLN:H	13	0.17
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	13	0.17
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	14	0.17
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	18	0.17
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	18	0.17
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	18	0.17
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	20	0.17
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	20	0.17
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	20	0.17
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	2	0.17
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	13	0.17
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	5	0.17
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	9	0.17
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	16	0.17
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	2	0.17
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	3	0.17
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	4	0.17
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	10	0.17
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	12	0.17
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	19	0.17
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	13	0.17
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	6	0.17
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	10	0.17
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	3	0.17
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	18	0.17
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	18	0.17
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	20	0.17
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	20	0.17
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	20	0.17
(1,1490)	1:115:A:ASP:HB2	1:116:A:ASN:H	6	0.17
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	6	0.17
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	16	0.17
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	16	0.17
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	16	0.17
(1,1406)	1:99:B:LEU:HA	1:100:B:LYS:HG3	19	0.17
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	5	0.17
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	5	0.17
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	5	0.17
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	5	0.17
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	5	0.17
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	5	0.17
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	5	0.17
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	5	0.17
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	5	0.17
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	7	0.17
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	7	0.17
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	7	0.17
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	15	0.17
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	15	0.17
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	15	0.17
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	9	0.17
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	4	0.17
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	4	0.17
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	4	0.17
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	15	0.17
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	15	0.17
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	15	0.17
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	1	0.17
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	1	0.17
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	1	0.17
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	7	0.17
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	7	0.17
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	7	0.17
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	3	0.17
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	16	0.17
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	9	0.17
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	11	0.17
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	15	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	1	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	1	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	1	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	17	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	17	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	17	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	20	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	20	0.17
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	20	0.17
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD21	1	0.17
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD22	1	0.17
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD23	1	0.17
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD21	17	0.17
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD22	17	0.17
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD23	17	0.17
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	1	0.17
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	1	0.17
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	1	0.17
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	10	0.17
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	10	0.17
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	10	0.17
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	13	0.17
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	13	0.17
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	13	0.17
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD1	14	0.17
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD2	14	0.17
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE1	16	0.17
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE2	16	0.17
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE1	16	0.17
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE2	16	0.17
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE1	16	0.17
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE2	16	0.17
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	11	0.17
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	8	0.17
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	8	0.17
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	8	0.17
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	20	0.17
(1,1047)	1:120:A:ILE:HG13	1:125:A:ASN:HD21	13	0.17
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	15	0.17
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	15	0.17
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	7	0.17
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	7	0.17
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	7	0.17
(1,1006)	1:123:A:GLY:H	1:125:A:ASN:H	19	0.17
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	12	0.17
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	12	0.17
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	12	0.17
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	5	0.17
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	12	0.17
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	14	0.17
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	20	0.17
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	20	0.17
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	20	0.17
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	5	0.17
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	18	0.17
(1,942)	1:103:A:LEU:HD11	1:104:A:THR:H	7	0.17
(1,942)	1:103:A:LEU:HD12	1:104:A:THR:H	7	0.17
(1,942)	1:103:A:LEU:HD13	1:104:A:THR:H	7	0.17
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	8	0.17
(1,916)	1:95:A:ASP:HB3	1:97:A:LYS:H	14	0.17
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	16	0.17
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	16	0.17
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	16	0.17
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	15	0.17
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	3	0.17
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	3	0.17
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	3	0.17
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	12	0.17
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	12	0.17
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	12	0.17
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	14	0.17
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	14	0.17
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	14	0.17
(1,736)	1:24:A:LEU:HD21	1:25:A:SER:H	18	0.17
(1,736)	1:24:A:LEU:HD22	1:25:A:SER:H	18	0.17
(1,736)	1:24:A:LEU:HD23	1:25:A:SER:H	18	0.17
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	5	0.17
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	7	0.17
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	9	0.17
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	16	0.17
(1,633)	1:73:B:ILE:H	1:73:B:ILE:HG13	7	0.17
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	3	0.17
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	4	0.17
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	10	0.17
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	12	0.17
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	13	0.17
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	19	0.17
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	20	0.17
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	13	0.17
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD21	3	0.17
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD22	3	0.17
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD23	3	0.17
(1,532)	1:76:A:LYS:H	1:76:A:LYS:HD2	10	0.17
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	10	0.17
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	11	0.17
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	3	0.17
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	3	0.17
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	14	0.17
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	16	0.17
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	4	0.17
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	8	0.17
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	20	0.17
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	20	0.17
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	20	0.17
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	20	0.17
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	20	0.17
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	20	0.17
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	5	0.17
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	3	0.17
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	4	0.17
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	16	0.17
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	16	0.17
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	16	0.17
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD11	5	0.17
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD12	5	0.17
(1,273)	1:86:A:ILE:HA	1:86:A:ILE:HD13	5	0.17
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD11	3	0.17
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD12	3	0.17
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD13	3	0.17
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	3	0.17
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	3	0.17
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	7	0.17
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	7	0.17
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	7	0.17
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	5	0.17
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG21	5	0.17
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG22	5	0.17
(1,229)	1:111:B:MET:HA	1:114:B:VAL:HG23	5	0.17
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	2	0.17
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	2	0.17
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	2	0.17
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	4	0.17
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	4	0.17
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	4	0.17
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG11	5	0.17
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG12	5	0.17
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG13	5	0.17
(1,158)	1:116:A:ASN:HB2	1:120:A:ILE:HD11	3	0.17
(1,158)	1:116:A:ASN:HB2	1:120:A:ILE:HD12	3	0.17
(1,158)	1:116:A:ASN:HB2	1:120:A:ILE:HD13	3	0.17
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	10	0.17
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	15	0.17
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	8	0.17
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	8	0.17
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	8	0.17
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	1	0.17
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	1	0.17
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	1	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	1	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	1	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	1	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	16	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	16	0.17
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	16	0.17
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	6	0.17
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	6	0.17
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	6	0.17
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	16	0.17
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	16	0.17
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	16	0.17
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	9	0.17
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	9	0.17
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	5	0.17
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	5	0.17
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	5	0.17
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	20	0.17
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	20	0.17
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	20	0.17
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	1	0.17
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	1	0.17
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	1	0.17
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	20	0.17
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	20	0.17
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	20	0.17
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	13	0.17
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	13	0.17
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	13	0.17
(1,19)	1:27:B:VAL:HG21	1:33:B:GLY:HA3	8	0.17
(1,19)	1:27:B:VAL:HG22	1:33:B:GLY:HA3	8	0.17
(1,19)	1:27:B:VAL:HG23	1:33:B:GLY:HA3	8	0.17
(1,3248)	1:120:B:ILE:HD11	1:125:B:ASN:HD21	4	0.16
(1,3248)	1:120:B:ILE:HD11	1:125:B:ASN:HD22	4	0.16
(1,3248)	1:120:B:ILE:HD12	1:125:B:ASN:HD21	4	0.16
(1,3248)	1:120:B:ILE:HD12	1:125:B:ASN:HD22	4	0.16
(1,3248)	1:120:B:ILE:HD13	1:125:B:ASN:HD21	4	0.16
(1,3248)	1:120:B:ILE:HD13	1:125:B:ASN:HD22	4	0.16
(1,3240)	1:119:B:MET:HE1	1:124:B:LEU:HB2	9	0.16
(1,3240)	1:119:B:MET:HE1	1:124:B:LEU:HB3	9	0.16
(1,3240)	1:119:B:MET:HE2	1:124:B:LEU:HB2	9	0.16
(1,3240)	1:119:B:MET:HE2	1:124:B:LEU:HB3	9	0.16
(1,3240)	1:119:B:MET:HE3	1:124:B:LEU:HB2	9	0.16
(1,3240)	1:119:B:MET:HE3	1:124:B:LEU:HB3	9	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	3	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	3	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	3	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	3	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	3	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	3	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	7	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	7	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	7	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	7	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	7	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	8	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	8	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	8	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	8	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	8	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	8	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	12	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	12	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	12	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	12	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	12	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	12	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	19	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	19	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	19	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	19	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	19	0.16
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	19	0.16
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD11	12	0.16
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD12	12	0.16
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD13	12	0.16
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD21	12	0.16
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD22	12	0.16
(1,3131)	1:96:B:LYS:HA	1:99:B:LEU:HD23	12	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	5	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	5	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	5	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	5	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	5	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	5	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	5	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	5	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	5	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	5	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	5	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	5	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	10	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	10	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	10	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	10	0.16
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	10	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	10	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	10	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	10	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	10	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	10	0.16
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	10	0.16
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE2	16	0.16
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE3	16	0.16
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE2	16	0.16
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE3	16	0.16
(1,3048)	1:74:B:GLU:HB2	1:77:B:LYS:H	5	0.16
(1,3048)	1:74:B:GLU:HB3	1:77:B:LYS:H	5	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD11	14	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD12	14	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD13	14	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD21	14	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD22	14	0.16
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD23	14	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD11	14	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD12	14	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD13	14	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD21	14	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD22	14	0.16
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD23	14	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD11	14	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD12	14	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD13	14	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD21	14	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD22	14	0.16
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD23	14	0.16
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG12	18	0.16
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	18	0.16
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG12	18	0.16
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	18	0.16
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG12	18	0.16
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	18	0.16
(1,2960)	1:45:B:THR:HG21	1:48:B:LYS:HG2	8	0.16
(1,2960)	1:45:B:THR:HG21	1:48:B:LYS:HG3	8	0.16
(1,2960)	1:45:B:THR:HG22	1:48:B:LYS:HG2	8	0.16
(1,2960)	1:45:B:THR:HG22	1:48:B:LYS:HG3	8	0.16
(1,2960)	1:45:B:THR:HG23	1:48:B:LYS:HG2	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2960)	1:45:B:THR:HG23	1:48:B:LYS:HG3	8	0.16
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	3	0.16
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	3	0.16
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	3	0.16
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	3	0.16
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	3	0.16
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	3	0.16
(1,2944)	1:42:B:GLN:HB2	1:54:B:ILE:H	10	0.16
(1,2944)	1:42:B:GLN:HB3	1:54:B:ILE:H	10	0.16
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	10	0.16
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	10	0.16
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	10	0.16
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	10	0.16
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	10	0.16
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	10	0.16
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	9	0.16
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	9	0.16
(1,2874)	1:24:B:LEU:HD11	1:32:B:GLN:HE22	8	0.16
(1,2874)	1:24:B:LEU:HD12	1:32:B:GLN:HE22	8	0.16
(1,2874)	1:24:B:LEU:HD13	1:32:B:GLN:HE22	8	0.16
(1,2874)	1:24:B:LEU:HD21	1:32:B:GLN:HE22	8	0.16
(1,2874)	1:24:B:LEU:HD22	1:32:B:GLN:HE22	8	0.16
(1,2874)	1:24:B:LEU:HD23	1:32:B:GLN:HE22	8	0.16
(1,2866)	1:24:B:LEU:HB2	1:25:B:SER:H	18	0.16
(1,2866)	1:24:B:LEU:HB3	1:25:B:SER:H	18	0.16
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	10	0.16
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	10	0.16
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	10	0.16
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	10	0.16
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	10	0.16
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	10	0.16
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	13	0.16
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	13	0.16
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	13	0.16
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	13	0.16
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	13	0.16
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	13	0.16
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	2	0.16
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	2	0.16
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	2	0.16
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	2	0.16
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	6	0.16
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	6	0.16
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	6	0.16
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	16	0.16
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	16	0.16
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	16	0.16
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	16	0.16
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	16	0.16
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	16	0.16
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	16	0.16
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	16	0.16
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	16	0.16
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	16	0.16
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	16	0.16
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	16	0.16
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	16	0.16
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	16	0.16
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	16	0.16
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	16	0.16
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	16	0.16
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	16	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	7	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	7	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	7	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	7	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	7	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	7	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	10	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	10	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	10	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	10	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	10	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	10	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	13	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	13	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	13	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	13	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	13	0.16
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	13	0.16
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	19	0.16
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	19	0.16
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	15	0.16
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	17	0.16
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	17	0.16
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	17	0.16
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	17	0.16
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD11	12	0.16
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD12	12	0.16
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD13	12	0.16
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD21	12	0.16
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD22	12	0.16
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD23	12	0.16
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD11	12	0.16
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD12	12	0.16
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD13	12	0.16
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD21	12	0.16
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD22	12	0.16
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD23	12	0.16
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	16	0.16
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	16	0.16
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	13	0.16
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE3	13	0.16
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	13	0.16
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE3	13	0.16
(1,2548)	1:74:A:GLU:HB2	1:77:A:LYS:H	15	0.16
(1,2548)	1:74:A:GLU:HB3	1:77:A:LYS:H	15	0.16
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD11	14	0.16
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD12	14	0.16
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD13	14	0.16
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD21	14	0.16
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD22	14	0.16
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD23	14	0.16
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD11	14	0.16
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD12	14	0.16
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD13	14	0.16
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD21	14	0.16
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD22	14	0.16
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD23	14	0.16
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD11	14	0.16
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD12	14	0.16
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD13	14	0.16
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD21	14	0.16
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD22	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD23	14	0.16
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG12	18	0.16
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	18	0.16
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG12	18	0.16
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	18	0.16
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG12	18	0.16
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	18	0.16
(1,2475)	1:48:A:LYS:HE2	1:49:A:TYR:HE1	5	0.16
(1,2475)	1:48:A:LYS:HE2	1:49:A:TYR:HE2	5	0.16
(1,2475)	1:48:A:LYS:HE3	1:49:A:TYR:HE1	5	0.16
(1,2475)	1:48:A:LYS:HE3	1:49:A:TYR:HE2	5	0.16
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	3	0.16
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	3	0.16
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	3	0.16
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG21	3	0.16
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG22	3	0.16
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG23	3	0.16
(1,2442)	1:42:A:GLN:HB2	1:54:A:ILE:H	13	0.16
(1,2442)	1:42:A:GLN:HB3	1:54:A:ILE:H	13	0.16
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	1	0.16
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	1	0.16
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	1	0.16
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	1	0.16
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	1	0.16
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	1	0.16
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	10	0.16
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	10	0.16
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	10	0.16
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	10	0.16
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	10	0.16
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	10	0.16
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	18	0.16
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	18	0.16
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	18	0.16
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	18	0.16
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	18	0.16
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	18	0.16
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	19	0.16
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	19	0.16
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	19	0.16
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	19	0.16
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	19	0.16
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	11	0.16
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	11	0.16
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	11	0.16
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	11	0.16
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	11	0.16
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	11	0.16
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	17	0.16
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	17	0.16
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	17	0.16
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	17	0.16
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	17	0.16
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	17	0.16
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	2	0.16
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	2	0.16
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	2	0.16
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	2	0.16
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	2	0.16
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	2	0.16
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	5	0.16
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	5	0.16
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	5	0.16
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	5	0.16
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	5	0.16
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	5	0.16
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	8	0.16
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	8	0.16
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	8	0.16
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	8	0.16
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	8	0.16
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	8	0.16
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	11	0.16
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	11	0.16
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	11	0.16
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	11	0.16
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	11	0.16
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	11	0.16
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	13	0.16
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	13	0.16
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	13	0.16
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	13	0.16
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	13	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	13	0.16
(1,2256)	1:73:B:ILE:HD11	1:78:B:TYR:HD1	1	0.16
(1,2256)	1:73:B:ILE:HD11	1:78:B:TYR:HD2	1	0.16
(1,2256)	1:73:B:ILE:HD12	1:78:B:TYR:HD1	1	0.16
(1,2256)	1:73:B:ILE:HD12	1:78:B:TYR:HD2	1	0.16
(1,2256)	1:73:B:ILE:HD13	1:78:B:TYR:HD1	1	0.16
(1,2256)	1:73:B:ILE:HD13	1:78:B:TYR:HD2	1	0.16
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE1	8	0.16
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE2	8	0.16
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE1	8	0.16
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE2	8	0.16
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE1	8	0.16
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE2	8	0.16
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE1	16	0.16
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE2	16	0.16
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE1	16	0.16
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE2	16	0.16
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE1	16	0.16
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE2	16	0.16
(1,2236)	1:76:B:LYS:H	1:80:B:LEU:H	9	0.16
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	12	0.16
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	14	0.16
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	16	0.16
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	2	0.16
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	2	0.16
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	2	0.16
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	1	0.16
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	7	0.16
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	7	0.16
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	7	0.16
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	7	0.16
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	12	0.16
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	12	0.16
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	12	0.16
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	16	0.16
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	10	0.16
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	10	0.16
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	10	0.16
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	11	0.16
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	11	0.16
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	11	0.16
(1,2111)	1:111:B:MET:HG3	1:112:B:LYS:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2107)	1:112:B:LYS:H	1:115:B:ASP:H	6	0.16
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	18	0.16
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	1	0.16
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	2	0.16
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	9	0.16
(1,2062)	1:95:B:ASP:HB3	1:97:B:LYS:H	14	0.16
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	12	0.16
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	12	0.16
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	12	0.16
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	19	0.16
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	19	0.16
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	19	0.16
(1,2011)	1:80:B:LEU:HD11	1:82:B:LYS:H	4	0.16
(1,2011)	1:80:B:LEU:HD12	1:82:B:LYS:H	4	0.16
(1,2011)	1:80:B:LEU:HD13	1:82:B:LYS:H	4	0.16
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	3	0.16
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	1	0.16
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	11	0.16
(1,1882)	1:24:B:LEU:HD21	1:25:B:SER:H	14	0.16
(1,1882)	1:24:B:LEU:HD22	1:25:B:SER:H	14	0.16
(1,1882)	1:24:B:LEU:HD23	1:25:B:SER:H	14	0.16
(1,1881)	1:25:B:SER:H	1:35:B:VAL:HA	2	0.16
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	10	0.16
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	3	0.16
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	11	0.16
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	18	0.16
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	14	0.16
(1,1764)	1:96:A:LYS:HB3	1:97:A:LYS:H	2	0.16
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	7	0.16
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	7	0.16
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	7	0.16
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	14	0.16
(1,1735)	1:21:A:LEU:H	1:21:A:LEU:HB3	20	0.16
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	3	0.16
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	17	0.16
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	3	0.16
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	1	0.16
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	7	0.16
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	11	0.16
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	5	0.16
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	3	0.16
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	13	0.16
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	14	0.16
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	16	0.16
(1,1571)	1:113:B:GLU:H	1:113:B:GLU:HG2	5	0.16
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	4	0.16
(1,1539)	1:32:B:GLN:H	1:32:B:GLN:HE21	7	0.16
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	18	0.16
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	1	0.16
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	1	0.16
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	1	0.16
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	19	0.16
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	19	0.16
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	20	0.16
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	20	0.16
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	2	0.16
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	4	0.16
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	20	0.16
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	20	0.16
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	20	0.16
(1,1437)	1:89:A:GLU:HB2	1:90:A:GLN:H	2	0.16
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD11	5	0.16
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD12	5	0.16
(1,1400)	1:86:B:ILE:HA	1:86:B:ILE:HD13	5	0.16
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	8	0.16
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	8	0.16
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	8	0.16
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	8	0.16
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	8	0.16
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	8	0.16
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	8	0.16
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	8	0.16
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	8	0.16
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD21	17	0.16
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD22	17	0.16
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD23	17	0.16
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD21	17	0.16
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD22	17	0.16
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD23	17	0.16
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD21	17	0.16
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD22	17	0.16
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD23	17	0.16
(1,1370)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1370)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	16	0.16
(1,1370)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	16	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	1	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	1	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	1	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	6	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	6	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	6	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	9	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	9	0.16
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	9	0.16
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	5	0.16
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	14	0.16
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	14	0.16
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	14	0.16
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	19	0.16
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	19	0.16
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	19	0.16
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	14	0.16
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	11	0.16
(1,1305)	1:109:B:ASP:HA	1:112:B:LYS:HB2	5	0.16
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD21	12	0.16
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD22	12	0.16
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD23	12	0.16
(1,1277)	1:92:B:ARG:HB3	1:94:B:LEU:HD11	8	0.16
(1,1277)	1:92:B:ARG:HB3	1:94:B:LEU:HD12	8	0.16
(1,1277)	1:92:B:ARG:HB3	1:94:B:LEU:HD13	8	0.16
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	10	0.16
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	20	0.16
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD21	14	0.16
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD22	14	0.16
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD23	14	0.16
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	8	0.16
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	8	0.16
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	8	0.16
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	10	0.16
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	10	0.16
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	10	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD21	5	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD22	5	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD23	5	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD21	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD22	8	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD23	8	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD21	16	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD22	16	0.16
(1,1238)	1:21:B:LEU:HA	1:21:B:LEU:HD23	16	0.16
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	6	0.16
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	6	0.16
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	6	0.16
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	16	0.16
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	16	0.16
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	16	0.16
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	5	0.16
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	5	0.16
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	5	0.16
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB1	9	0.16
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB2	9	0.16
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB3	9	0.16
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB1	9	0.16
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB2	9	0.16
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB3	9	0.16
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB1	9	0.16
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB2	9	0.16
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB3	9	0.16
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	20	0.16
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	20	0.16
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	20	0.16
(1,1141)	1:111:B:MET:HE1	1:114:B:VAL:HB	8	0.16
(1,1141)	1:111:B:MET:HE2	1:114:B:VAL:HB	8	0.16
(1,1141)	1:111:B:MET:HE3	1:114:B:VAL:HB	8	0.16
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	20	0.16
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	20	0.16
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	5	0.16
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	5	0.16
(1,1103)	1:73:A:ILE:HD11	1:78:A:TYR:HD1	1	0.16
(1,1103)	1:73:A:ILE:HD11	1:78:A:TYR:HD2	1	0.16
(1,1103)	1:73:A:ILE:HD12	1:78:A:TYR:HD1	1	0.16
(1,1103)	1:73:A:ILE:HD12	1:78:A:TYR:HD2	1	0.16
(1,1103)	1:73:A:ILE:HD13	1:78:A:TYR:HD1	1	0.16
(1,1103)	1:73:A:ILE:HD13	1:78:A:TYR:HD2	1	0.16
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	2	0.16
(1,1066)	1:32:B:GLN:HB3	1:32:B:GLN:HE21	10	0.16
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1048)	1:119:A:MET:HE1	1:125:A:ASN:HD22	19	0.16
(1,1048)	1:119:A:MET:HE2	1:125:A:ASN:HD22	19	0.16
(1,1048)	1:119:A:MET:HE3	1:125:A:ASN:HD22	19	0.16
(1,1040)	1:112:A:LYS:H	1:114:A:VAL:HG21	5	0.16
(1,1040)	1:112:A:LYS:H	1:114:A:VAL:HG22	5	0.16
(1,1040)	1:112:A:LYS:H	1:114:A:VAL:HG23	5	0.16
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	1	0.16
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	1	0.16
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	1	0.16
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	8	0.16
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	8	0.16
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	8	0.16
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	1	0.16
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	1	0.16
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	1	0.16
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	11	0.16
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	11	0.16
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	11	0.16
(1,961)	1:112:A:LYS:H	1:115:A:ASP:H	6	0.16
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	12	0.16
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	11	0.16
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	15	0.16
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	2	0.16
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	9	0.16
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	17	0.16
(1,898)	1:91:A:ILE:H	1:93:B:THR:HB	18	0.16
(1,893)	1:87:A:LEU:H	1:90:A:GLN:H	18	0.16
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	19	0.16
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	19	0.16
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	19	0.16
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	19	0.16
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	19	0.16
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	19	0.16
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	2	0.16
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	3	0.16
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	11	0.16
(1,754)	1:27:A:VAL:HG11	1:33:A:GLY:H	10	0.16
(1,754)	1:27:A:VAL:HG12	1:33:A:GLY:H	10	0.16
(1,754)	1:27:A:VAL:HG13	1:33:A:GLY:H	10	0.16
(1,751)	1:24:A:LEU:HD21	1:32:A:GLN:H	2	0.16
(1,751)	1:24:A:LEU:HD22	1:32:A:GLN:H	2	0.16
(1,751)	1:24:A:LEU:HD23	1:32:A:GLN:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	14	0.16
(1,742)	1:31:A:GLU:H	1:95:B:ASP:H	16	0.16
(1,735)	1:25:A:SER:H	1:35:A:VAL:HA	2	0.16
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	2	0.16
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	10	0.16
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	11	0.16
(1,622)	1:96:B:LYS:HB3	1:97:B:LYS:H	2	0.16
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	14	0.16
(1,593)	1:21:B:LEU:H	1:21:B:LEU:HB3	15	0.16
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	12	0.16
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	8	0.16
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	6	0.16
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	7	0.16
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	13	0.16
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	1	0.16
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	15	0.16
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	18	0.16
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	1	0.16
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	1	0.16
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	1	0.16
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	20	0.16
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	20	0.16
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	20	0.16
(1,288)	1:75:A:LYS:H	1:75:A:LYS:HD3	20	0.16
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	15	0.16
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	15	0.16
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	15	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	1	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	1	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	1	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	6	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	6	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	6	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	9	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	9	0.16
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	9	0.16
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	9	0.16
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	13	0.16
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	5	0.16
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	5	0.16
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	5	0.16
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	13	0.16
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD21	7	0.16
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD22	7	0.16
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD23	7	0.16
(1,151)	1:92:A:ARG:HB3	1:94:A:LEU:HD11	8	0.16
(1,151)	1:92:A:ARG:HB3	1:94:A:LEU:HD12	8	0.16
(1,151)	1:92:A:ARG:HB3	1:94:A:LEU:HD13	8	0.16
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	6	0.16
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	20	0.16
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD21	14	0.16
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD22	14	0.16
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD23	14	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	5	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	5	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	5	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	8	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	8	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	8	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD21	17	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD22	17	0.16
(1,113)	1:21:A:LEU:HA	1:21:A:LEU:HD23	17	0.16
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	3	0.16
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	3	0.16
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	3	0.16
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	17	0.16
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	17	0.16
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	17	0.16
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	19	0.16
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	19	0.16
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	19	0.16
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	10	0.16
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	10	0.16
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	10	0.16
(1,46)	1:117:A:ALA:HB1	1:118:A:LEU:HB2	6	0.16
(1,46)	1:117:A:ALA:HB2	1:118:A:LEU:HB2	6	0.16
(1,46)	1:117:A:ALA:HB3	1:118:A:LEU:HB2	6	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	1	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	1	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	1	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	3	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	3	0.16
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:111:A:MET:HE1	1:114:A:VAL:HB	9	0.16
(1,14)	1:111:A:MET:HE2	1:114:A:VAL:HB	9	0.16
(1,14)	1:111:A:MET:HE3	1:114:A:VAL:HB	9	0.16
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	16	0.15
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	16	0.15
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	16	0.15
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	16	0.15
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	16	0.15
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	16	0.15
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	16	0.15
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	16	0.15
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	16	0.15
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	16	0.15
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	16	0.15
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	16	0.15
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	16	0.15
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	16	0.15
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	16	0.15
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	16	0.15
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	16	0.15
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	16	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	6	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	6	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	17	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	17	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	18	0.15
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	18	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	4	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	4	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	4	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	4	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	4	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	4	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	13	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	13	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	13	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	13	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	13	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	13	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	16	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	16	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	16	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	16	0.15
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	16	0.15
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	17	0.15
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	17	0.15
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	17	0.15
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	17	0.15
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	20	0.15
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	20	0.15
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	20	0.15
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	20	0.15
(1,3135)	1:97:B:LYS:HB2	1:98:B:ARG:H	5	0.15
(1,3135)	1:97:B:LYS:HB3	1:98:B:ARG:H	5	0.15
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD11	12	0.15
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD12	12	0.15
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD13	12	0.15
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD21	12	0.15
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD22	12	0.15
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD23	12	0.15
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD11	12	0.15
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD12	12	0.15
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD13	12	0.15
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD21	12	0.15
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD22	12	0.15
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD23	12	0.15
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	13	0.15
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	13	0.15
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	15	0.15
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	15	0.15
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	16	0.15
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	16	0.15
(1,3113)	1:88:B:LEU:HA	1:118:B:LEU:HD11	2	0.15
(1,3113)	1:88:B:LEU:HA	1:118:B:LEU:HD12	2	0.15
(1,3113)	1:88:B:LEU:HA	1:118:B:LEU:HD13	2	0.15
(1,3113)	1:88:B:LEU:HA	1:118:B:LEU:HD21	2	0.15
(1,3113)	1:88:B:LEU:HA	1:118:B:LEU:HD22	2	0.15
(1,3113)	1:88:B:LEU:HA	1:118:B:LEU:HD23	2	0.15
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE2	13	0.15
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE3	13	0.15
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE2	13	0.15
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE3	13	0.15
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD3	10	0.15
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD2	12	0.15
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD3	12	0.15
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD11	7	0.15
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD12	7	0.15
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD13	7	0.15
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD21	7	0.15
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD22	7	0.15
(1,3044)	1:73:B:ILE:HD11	1:106:B:LEU:HD23	7	0.15
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD11	7	0.15
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD12	7	0.15
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD13	7	0.15
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD21	7	0.15
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD22	7	0.15
(1,3044)	1:73:B:ILE:HD12	1:106:B:LEU:HD23	7	0.15
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD11	7	0.15
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD12	7	0.15
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD13	7	0.15
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD21	7	0.15
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD22	7	0.15
(1,3044)	1:73:B:ILE:HD13	1:106:B:LEU:HD23	7	0.15
(1,3040)	1:73:B:ILE:HG21	1:106:B:LEU:HD11	20	0.15
(1,3040)	1:73:B:ILE:HG21	1:106:B:LEU:HD12	20	0.15
(1,3040)	1:73:B:ILE:HG21	1:106:B:LEU:HD13	20	0.15
(1,3040)	1:73:B:ILE:HG21	1:106:B:LEU:HD21	20	0.15
(1,3040)	1:73:B:ILE:HG21	1:106:B:LEU:HD22	20	0.15
(1,3040)	1:73:B:ILE:HG21	1:106:B:LEU:HD23	20	0.15
(1,3040)	1:73:B:ILE:HG22	1:106:B:LEU:HD11	20	0.15
(1,3040)	1:73:B:ILE:HG22	1:106:B:LEU:HD12	20	0.15
(1,3040)	1:73:B:ILE:HG22	1:106:B:LEU:HD13	20	0.15
(1,3040)	1:73:B:ILE:HG22	1:106:B:LEU:HD21	20	0.15
(1,3040)	1:73:B:ILE:HG22	1:106:B:LEU:HD22	20	0.15
(1,3040)	1:73:B:ILE:HG22	1:106:B:LEU:HD23	20	0.15
(1,3040)	1:73:B:ILE:HG23	1:106:B:LEU:HD11	20	0.15
(1,3040)	1:73:B:ILE:HG23	1:106:B:LEU:HD12	20	0.15
(1,3040)	1:73:B:ILE:HG23	1:106:B:LEU:HD13	20	0.15
(1,3040)	1:73:B:ILE:HG23	1:106:B:LEU:HD21	20	0.15
(1,3040)	1:73:B:ILE:HG23	1:106:B:LEU:HD22	20	0.15
(1,3040)	1:73:B:ILE:HG23	1:106:B:LEU:HD23	20	0.15
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG11	14	0.15
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG12	14	0.15
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG13	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG21	14	0.15
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG22	14	0.15
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG23	14	0.15
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG11	14	0.15
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG12	14	0.15
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG13	14	0.15
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG21	14	0.15
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG22	14	0.15
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG23	14	0.15
(1,2982)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	1	0.15
(1,2982)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	1	0.15
(1,2982)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	1	0.15
(1,2982)	1:53:B:VAL:HG21	1:94:B:LEU:HB2	1	0.15
(1,2982)	1:53:B:VAL:HG22	1:94:B:LEU:HB2	1	0.15
(1,2982)	1:53:B:VAL:HG23	1:94:B:LEU:HB2	1	0.15
(1,2972)	1:48:B:LYS:HE2	1:49:B:TYR:HE1	5	0.15
(1,2972)	1:48:B:LYS:HE2	1:49:B:TYR:HE2	5	0.15
(1,2972)	1:48:B:LYS:HE3	1:49:B:TYR:HE1	5	0.15
(1,2972)	1:48:B:LYS:HE3	1:49:B:TYR:HE2	5	0.15
(1,2956)	1:43:B:ASN:HD21	1:47:B:ASN:H	17	0.15
(1,2956)	1:43:B:ASN:HD22	1:47:B:ASN:H	17	0.15
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	1	0.15
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	1	0.15
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	1	0.15
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	1	0.15
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	1	0.15
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	1	0.15
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	19	0.15
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	19	0.15
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	19	0.15
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	19	0.15
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	19	0.15
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	19	0.15
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	5	0.15
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	5	0.15
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	5	0.15
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	5	0.15
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	5	0.15
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	5	0.15
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	16	0.15
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	16	0.15
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	16	0.15
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	16	0.15
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	16	0.15
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	3	0.15
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	3	0.15
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	3	0.15
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	3	0.15
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	3	0.15
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	3	0.15
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB2	12	0.15
(1,2758)	1:120:A:ILE:HG12	1:121:A:SER:HB3	12	0.15
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB2	12	0.15
(1,2758)	1:120:A:ILE:HG13	1:121:A:SER:HB3	12	0.15
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB2	1	0.15
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB3	1	0.15
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB2	1	0.15
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB3	1	0.15
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB2	1	0.15
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB3	1	0.15
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	6	0.15
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	6	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	3	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	3	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	3	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	3	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	3	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	3	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	14	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	14	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	14	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	14	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	14	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	14	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	16	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	16	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	16	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	16	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	16	0.15
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	16	0.15
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	7	0.15
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	7	0.15
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD21	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD22	3	0.15
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD21	3	0.15
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD22	3	0.15
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	3	0.15
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	3	0.15
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	3	0.15
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	3	0.15
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	12	0.15
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	12	0.15
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	12	0.15
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	12	0.15
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	19	0.15
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	19	0.15
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	19	0.15
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	19	0.15
(1,2695)	1:112:A:LYS:H	1:112:A:LYS:HB2	5	0.15
(1,2695)	1:112:A:LYS:H	1:112:A:LYS:HB3	5	0.15
(1,2639)	1:97:A:LYS:HB2	1:98:A:ARG:H	5	0.15
(1,2639)	1:97:A:LYS:HB3	1:98:A:ARG:H	5	0.15
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	11	0.15
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	11	0.15
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	11	0.15
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	11	0.15
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	11	0.15
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	11	0.15
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	11	0.15
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	11	0.15
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	11	0.15
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	11	0.15
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	11	0.15
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	11	0.15
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	13	0.15
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	13	0.15
(1,2613)	1:88:A:LEU:HA	1:118:A:LEU:HD11	2	0.15
(1,2613)	1:88:A:LEU:HA	1:118:A:LEU:HD12	2	0.15
(1,2613)	1:88:A:LEU:HA	1:118:A:LEU:HD13	2	0.15
(1,2613)	1:88:A:LEU:HA	1:118:A:LEU:HD21	2	0.15
(1,2613)	1:88:A:LEU:HA	1:118:A:LEU:HD22	2	0.15
(1,2613)	1:88:A:LEU:HA	1:118:A:LEU:HD23	2	0.15
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD2	6	0.15
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD3	6	0.15
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD3	10	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD11	7	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD12	7	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD13	7	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD21	7	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD22	7	0.15
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD23	7	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD11	7	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD12	7	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD13	7	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD21	7	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD22	7	0.15
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD23	7	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD11	7	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD12	7	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD13	7	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD21	7	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD22	7	0.15
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD23	7	0.15
(1,2540)	1:73:A:ILE:HG21	1:106:A:LEU:HD11	20	0.15
(1,2540)	1:73:A:ILE:HG21	1:106:A:LEU:HD12	20	0.15
(1,2540)	1:73:A:ILE:HG21	1:106:A:LEU:HD13	20	0.15
(1,2540)	1:73:A:ILE:HG21	1:106:A:LEU:HD21	20	0.15
(1,2540)	1:73:A:ILE:HG21	1:106:A:LEU:HD22	20	0.15
(1,2540)	1:73:A:ILE:HG21	1:106:A:LEU:HD23	20	0.15
(1,2540)	1:73:A:ILE:HG22	1:106:A:LEU:HD11	20	0.15
(1,2540)	1:73:A:ILE:HG22	1:106:A:LEU:HD12	20	0.15
(1,2540)	1:73:A:ILE:HG22	1:106:A:LEU:HD13	20	0.15
(1,2540)	1:73:A:ILE:HG22	1:106:A:LEU:HD21	20	0.15
(1,2540)	1:73:A:ILE:HG22	1:106:A:LEU:HD22	20	0.15
(1,2540)	1:73:A:ILE:HG22	1:106:A:LEU:HD23	20	0.15
(1,2540)	1:73:A:ILE:HG23	1:106:A:LEU:HD11	20	0.15
(1,2540)	1:73:A:ILE:HG23	1:106:A:LEU:HD12	20	0.15
(1,2540)	1:73:A:ILE:HG23	1:106:A:LEU:HD13	20	0.15
(1,2540)	1:73:A:ILE:HG23	1:106:A:LEU:HD21	20	0.15
(1,2540)	1:73:A:ILE:HG23	1:106:A:LEU:HD22	20	0.15
(1,2540)	1:73:A:ILE:HG23	1:106:A:LEU:HD23	20	0.15
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG11	10	0.15
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG12	10	0.15
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG13	10	0.15
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG21	10	0.15
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG22	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG23	10	0.15
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	5	0.15
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	5	0.15
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	5	0.15
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	5	0.15
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	5	0.15
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	5	0.15
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	16	0.15
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	16	0.15
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	16	0.15
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	16	0.15
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	16	0.15
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	16	0.15
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB2	7	0.15
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB3	7	0.15
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	9	0.15
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	9	0.15
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	20	0.15
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	20	0.15
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	19	0.15
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	19	0.15
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	19	0.15
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	19	0.15
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	19	0.15
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	19	0.15
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	5	0.15
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	5	0.15
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	5	0.15
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	5	0.15
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	5	0.15
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	5	0.15
(1,2362)	1:24:A:LEU:HD11	1:32:A:GLN:H	10	0.15
(1,2362)	1:24:A:LEU:HD12	1:32:A:GLN:H	10	0.15
(1,2362)	1:24:A:LEU:HD13	1:32:A:GLN:H	10	0.15
(1,2362)	1:24:A:LEU:HD21	1:32:A:GLN:H	10	0.15
(1,2362)	1:24:A:LEU:HD22	1:32:A:GLN:H	10	0.15
(1,2362)	1:24:A:LEU:HD23	1:32:A:GLN:H	10	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	3	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	3	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	3	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	3	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	3	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	18	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	18	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	18	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	18	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	18	0.15
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	18	0.15
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	3	0.15
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	3	0.15
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	3	0.15
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	3	0.15
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	3	0.15
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	3	0.15
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	5	0.15
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	5	0.15
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	2	0.15
(1,2224)	1:24:B:LEU:HD11	1:32:B:GLN:H	17	0.15
(1,2224)	1:24:B:LEU:HD12	1:32:B:GLN:H	17	0.15
(1,2224)	1:24:B:LEU:HD13	1:32:B:GLN:H	17	0.15
(1,2220)	1:116:B:ASN:HD21	1:117:B:ALA:HB1	13	0.15
(1,2220)	1:116:B:ASN:HD21	1:117:B:ALA:HB2	13	0.15
(1,2220)	1:116:B:ASN:HD21	1:117:B:ALA:HB3	13	0.15
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	4	0.15
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	8	0.15
(1,2200)	1:119:B:MET:HE1	1:125:B:ASN:HD22	9	0.15
(1,2200)	1:119:B:MET:HE2	1:125:B:ASN:HD22	9	0.15
(1,2200)	1:119:B:MET:HE3	1:125:B:ASN:HD22	9	0.15
(1,2180)	1:23:B:ASP:H	1:100:B:LYS:H	3	0.15
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	9	0.15
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	9	0.15
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	9	0.15
(1,2162)	1:112:A:LYS:HB2	1:116:A:ASN:HD22	18	0.15
(1,2161)	1:112:B:LYS:HB3	1:116:B:ASN:HD22	9	0.15
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD11	7	0.15
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD12	7	0.15
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD13	7	0.15
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	19	0.15
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	19	0.15
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	19	0.15
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	1	0.15
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	5	0.15
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	13	0.15
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	2	0.15
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	2	0.15
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	2	0.15
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	6	0.15
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	6	0.15
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	6	0.15
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	15	0.15
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	15	0.15
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	15	0.15
(1,2104)	1:110:A:LYS:H	1:110:A:LYS:HE3	15	0.15
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	7	0.15
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	17	0.15
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	11	0.15
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	15	0.15
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	5	0.15
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	10	0.15
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	4	0.15
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	4	0.15
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	4	0.15
(1,2044)	1:93:A:THR:HB	1:91:B:ILE:H	18	0.15
(1,2039)	1:87:B:LEU:H	1:90:B:GLN:H	18	0.15
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	4	0.15
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	4	0.15
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	4	0.15
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	9	0.15
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	9	0.15
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	9	0.15
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	18	0.15
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	18	0.15
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	18	0.15
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	13	0.15
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	13	0.15
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	13	0.15
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	19	0.15
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	19	0.15
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	19	0.15
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	15	0.15
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	5	0.15
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	5	0.15
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	5	0.15
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	16	0.15
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	16	0.15
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	3	0.15
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	2	0.15
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	2	0.15
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	2	0.15
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	2	0.15
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	18	0.15
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	18	0.15
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	20	0.15
(1,1897)	1:24:B:LEU:HD21	1:32:B:GLN:H	2	0.15
(1,1897)	1:24:B:LEU:HD22	1:32:B:GLN:H	2	0.15
(1,1897)	1:24:B:LEU:HD23	1:32:B:GLN:H	2	0.15
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	20	0.15
(1,1888)	1:95:A:ASP:H	1:31:B:GLU:H	15	0.15
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	6	0.15
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	8	0.15
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	13	0.15
(1,1767)	1:96:A:LYS:HB2	1:97:A:LYS:H	18	0.15
(1,1767)	1:96:A:LYS:HB2	1:97:A:LYS:H	20	0.15
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	13	0.15
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	13	0.15
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	13	0.15
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD11	11	0.15
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD12	11	0.15
(1,1733)	1:106:A:LEU:H	1:106:A:LEU:HD13	11	0.15
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	17	0.15
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	6	0.15
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	8	0.15
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	15	0.15
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	9	0.15
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	9	0.15
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	9	0.15
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	6	0.15
(1,1611)	1:90:B:GLN:HB3	1:90:B:GLN:HE21	19	0.15
(1,1610)	1:90:B:GLN:H	1:90:B:GLN:HE21	16	0.15
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	17	0.15
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	1	0.15
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	8	0.15
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	3	0.15
(1,1498)	1:48:B:LYS:H	1:48:B:LYS:HD2	18	0.15
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	3	0.15
(1,1466)	1:80:B:LEU:H	1:80:B:LEU:HB2	4	0.15
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	20	0.15
(1,1421)	1:28:B:GLN:HA	1:28:B:GLN:HE22	15	0.15
(1,1397)	1:119:B:MET:HE1	1:126:B:ALA:HB1	17	0.15
(1,1397)	1:119:B:MET:HE1	1:126:B:ALA:HB2	17	0.15
(1,1397)	1:119:B:MET:HE1	1:126:B:ALA:HB3	17	0.15
(1,1397)	1:119:B:MET:HE2	1:126:B:ALA:HB1	17	0.15
(1,1397)	1:119:B:MET:HE2	1:126:B:ALA:HB2	17	0.15
(1,1397)	1:119:B:MET:HE2	1:126:B:ALA:HB3	17	0.15
(1,1397)	1:119:B:MET:HE3	1:126:B:ALA:HB1	17	0.15
(1,1397)	1:119:B:MET:HE3	1:126:B:ALA:HB2	17	0.15
(1,1397)	1:119:B:MET:HE3	1:126:B:ALA:HB3	17	0.15
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	2	0.15
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	2	0.15
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	2	0.15
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	2	0.15
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	2	0.15
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	2	0.15
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	2	0.15
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	2	0.15
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	2	0.15
(1,1369)	1:56:B:ALA:HB1	1:91:B:ILE:HG12	17	0.15
(1,1369)	1:56:B:ALA:HB2	1:91:B:ILE:HG12	17	0.15
(1,1369)	1:56:B:ALA:HB3	1:91:B:ILE:HG12	17	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	2	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	2	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	2	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	3	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	3	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	3	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	11	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	11	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	11	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	18	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	18	0.15
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	18	0.15
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	13	0.15
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	16	0.15
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	20	0.15
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	20	0.15
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG11	5	0.15
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG12	5	0.15
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG13	5	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	2	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	2	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	2	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	3	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	3	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	3	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	6	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	6	0.15
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	6	0.15
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	5	0.15
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	7	0.15
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD11	13	0.15
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD12	13	0.15
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD13	13	0.15
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	9	0.15
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD21	7	0.15
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD22	7	0.15
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD23	7	0.15
(1,1295)	1:27:B:VAL:HG11	1:33:B:GLY:HA2	14	0.15
(1,1295)	1:27:B:VAL:HG12	1:33:B:GLY:HA2	14	0.15
(1,1295)	1:27:B:VAL:HG13	1:33:B:GLY:HA2	14	0.15
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	2	0.15
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	6	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	4	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	4	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	4	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	5	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	5	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	5	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	18	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	18	0.15
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	18	0.15
(1,1234)	1:22:B:ALA:HB1	1:24:B:LEU:HG	2	0.15
(1,1234)	1:22:B:ALA:HB2	1:24:B:LEU:HG	2	0.15
(1,1234)	1:22:B:ALA:HB3	1:24:B:LEU:HG	2	0.15
(1,1219)	1:119:B:MET:HG3	1:124:B:LEU:HD11	11	0.15
(1,1219)	1:119:B:MET:HG3	1:124:B:LEU:HD12	11	0.15
(1,1219)	1:119:B:MET:HG3	1:124:B:LEU:HD13	11	0.15
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	13	0.15
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	13	0.15
(1,1203)	1:71:B:VAL:HG21	1:113:B:GLU:HB3	17	0.15
(1,1203)	1:71:B:VAL:HG22	1:113:B:GLU:HB3	17	0.15
(1,1203)	1:71:B:VAL:HG23	1:113:B:GLU:HB3	17	0.15
(1,1195)	1:19:A:VAL:HG11	1:103:A:LEU:HB3	17	0.15
(1,1195)	1:19:A:VAL:HG12	1:103:A:LEU:HB3	17	0.15
(1,1195)	1:19:A:VAL:HG13	1:103:A:LEU:HB3	17	0.15
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	13	0.15
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	13	0.15
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	13	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	1	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	1	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	1	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	3	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	3	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	3	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	20	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	20	0.15
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	20	0.15
(1,1141)	1:111:B:MET:HE1	1:114:B:VAL:HB	2	0.15
(1,1141)	1:111:B:MET:HE2	1:114:B:VAL:HB	2	0.15
(1,1141)	1:111:B:MET:HE3	1:114:B:VAL:HB	2	0.15
(1,1121)	1:20:A:TYR:HE1	1:40:A:ILE:HG13	18	0.15
(1,1121)	1:20:A:TYR:HE2	1:40:A:ILE:HG13	18	0.15
(1,1116)	1:18:A:ASP:HA	1:105:A:TYR:HA	8	0.15
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	20	0.15
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	20	0.15
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	4	0.15
(1,1051)	1:120:A:ILE:HG13	1:125:A:ASN:HD22	6	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	4	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	4	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	4	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	9	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	9	0.15
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	9	0.15
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	18	0.15
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	7	0.15
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	7	0.15
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	7	0.15
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	8	0.15
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	8	0.15
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	19	0.15
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	19	0.15
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	19	0.15
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	1	0.15
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	11	0.15
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	18	0.15
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	7	0.15
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	9	0.15
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	4	0.15
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	9	0.15
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	12	0.15
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	12	0.15
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	12	0.15
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	4	0.15
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	6	0.15
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	9	0.15
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	1	0.15
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	5	0.15
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	11	0.15
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	4	0.15
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	4	0.15
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	4	0.15
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	17	0.15
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	17	0.15
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	17	0.15
(1,903)	1:92:B:ARG:HG2	1:93:B:THR:H	8	0.15
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	1	0.15
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	1	0.15
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	1	0.15
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	4	0.15
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	4	0.15
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	4	0.15
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	12	0.15
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	12	0.15
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	12	0.15
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	18	0.15
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	18	0.15
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	18	0.15
(1,876)	1:73:B:ILE:HG13	1:84:B:SER:H	14	0.15
(1,865)	1:80:A:LEU:HD11	1:82:A:LYS:H	4	0.15
(1,865)	1:80:A:LEU:HD12	1:82:A:LYS:H	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,865)	1:80:A:LEU:HD13	1:82:A:LYS:H	4	0.15
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	9	0.15
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	9	0.15
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	9	0.15
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	15	0.15
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	16	0.15
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	16	0.15
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	16	0.15
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	3	0.15
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	5	0.15
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	8	0.15
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	2	0.15
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	2	0.15
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	2	0.15
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	18	0.15
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	10	0.15
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	20	0.15
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	8	0.15
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	7	0.15
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	20	0.15
(1,742)	1:31:A:GLU:H	1:95:B:ASP:H	5	0.15
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	13	0.15
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	3	0.15
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	6	0.15
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	8	0.15
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	18	0.15
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	11	0.15
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	7	0.15
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	7	0.15
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	7	0.15
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	13	0.15
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	13	0.15
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	13	0.15
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	17	0.15
(1,582)	1:116:A:ASN:HA	1:116:A:ASN:HD21	16	0.15
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	3	0.15
(1,567)	1:127:A:VAL:HA	1:128:A:ALA:H	13	0.15
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	3	0.15
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG11	10	0.15
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG12	10	0.15
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG13	10	0.15
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	11	0.15
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	11	0.15
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	1	0.15
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	3	0.15
(1,527)	1:75:A:LYS:HB3	1:76:A:LYS:H	4	0.15
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	5	0.15
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	6	0.15
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	10	0.15
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	15	0.15
(1,472)	1:90:A:GLN:HB3	1:90:A:GLN:HE21	19	0.15
(1,471)	1:90:A:GLN:H	1:90:A:GLN:HE21	16	0.15
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	17	0.15
(1,455)	1:105:A:TYR:H	1:106:A:LEU:H	18	0.15
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	12	0.15
(1,418)	1:126:A:ALA:HB1	1:127:A:VAL:H	12	0.15
(1,418)	1:126:A:ALA:HB2	1:127:A:VAL:H	12	0.15
(1,418)	1:126:A:ALA:HB3	1:127:A:VAL:H	12	0.15
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	10	0.15
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	16	0.15
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	15	0.15
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	15	0.15
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	17	0.15
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	17	0.15
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	19	0.15
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	19	0.15
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	7	0.15
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	8	0.15
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	16	0.15
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	2	0.15
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	2	0.15
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	2	0.15
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	7	0.15
(1,308)	1:89:B:GLU:HB2	1:90:B:GLN:H	2	0.15
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	20	0.15
(1,293)	1:28:A:GLN:HG3	1:28:A:GLN:HE22	5	0.15
(1,279)	1:99:A:LEU:HA	1:100:A:LYS:HG3	19	0.15
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD21	17	0.15
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD22	17	0.15
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD23	17	0.15
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD21	17	0.15
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD22	17	0.15
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD23	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD21	17	0.15
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD22	17	0.15
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD23	17	0.15
(1,243)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	16	0.15
(1,243)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	16	0.15
(1,243)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	16	0.15
(1,242)	1:56:A:ALA:HB1	1:91:A:ILE:HG12	17	0.15
(1,242)	1:56:A:ALA:HB2	1:91:A:ILE:HG12	17	0.15
(1,242)	1:56:A:ALA:HB3	1:91:A:ILE:HG12	17	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	3	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	3	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	3	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	18	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	18	0.15
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	18	0.15
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	19	0.15
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	19	0.15
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	19	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	3	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	3	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	3	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	15	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	15	0.15
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	15	0.15
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	5	0.15
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	7	0.15
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	14	0.15
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD21	12	0.15
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD22	12	0.15
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD23	12	0.15
(1,169)	1:27:A:VAL:HG11	1:33:A:GLY:HA2	14	0.15
(1,169)	1:27:A:VAL:HG12	1:33:A:GLY:HA2	14	0.15
(1,169)	1:27:A:VAL:HG13	1:33:A:GLY:HA2	14	0.15
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	2	0.15
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	6	0.15
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	6	0.15
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	6	0.15
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	10	0.15
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	10	0.15
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	10	0.15
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	18	0.15
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	18	0.15
(1,109)	1:22:A:ALA:HB1	1:24:A:LEU:HG	2	0.15
(1,109)	1:22:A:ALA:HB2	1:24:A:LEU:HG	2	0.15
(1,109)	1:22:A:ALA:HB3	1:24:A:LEU:HG	2	0.15
(1,70)	1:19:B:VAL:HG11	1:103:B:LEU:HB3	17	0.15
(1,70)	1:19:B:VAL:HG12	1:103:B:LEU:HB3	17	0.15
(1,70)	1:19:B:VAL:HG13	1:103:B:LEU:HB3	17	0.15
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	9	0.15
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	9	0.15
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	9	0.15
(1,19)	1:27:B:VAL:HG21	1:33:B:GLY:HA3	12	0.15
(1,19)	1:27:B:VAL:HG22	1:33:B:GLY:HA3	12	0.15
(1,19)	1:27:B:VAL:HG23	1:33:B:GLY:HA3	12	0.15
(1,14)	1:111:A:MET:HE1	1:114:A:VAL:HB	2	0.15
(1,14)	1:111:A:MET:HE2	1:114:A:VAL:HB	2	0.15
(1,14)	1:111:A:MET:HE3	1:114:A:VAL:HB	2	0.15
(1,14)	1:111:A:MET:HE1	1:114:A:VAL:HB	8	0.15
(1,14)	1:111:A:MET:HE2	1:114:A:VAL:HB	8	0.15
(1,14)	1:111:A:MET:HE3	1:114:A:VAL:HB	8	0.15
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	15	0.14
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	15	0.14
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	15	0.14
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	15	0.14
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	15	0.14
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	15	0.14
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	15	0.14
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	15	0.14
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	15	0.14
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	15	0.14
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	15	0.14
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	15	0.14
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	15	0.14
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	15	0.14
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	15	0.14
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	15	0.14
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	15	0.14
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	15	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	9	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	9	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	9	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	9	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	9	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	14	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	14	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	14	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	14	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	14	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	14	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD11	15	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD12	15	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD13	15	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD21	15	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD22	15	0.14
(1,3227)	1:118:B:LEU:H	1:118:B:LEU:HD23	15	0.14
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB2	9	0.14
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB3	9	0.14
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB2	9	0.14
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB3	9	0.14
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	6	0.14
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	6	0.14
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	6	0.14
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	6	0.14
(1,3150)	1:100:B:LYS:HD2	1:101:B:GLU:HG2	19	0.14
(1,3150)	1:100:B:LYS:HD2	1:101:B:GLU:HG3	19	0.14
(1,3150)	1:100:B:LYS:HD3	1:101:B:GLU:HG2	19	0.14
(1,3150)	1:100:B:LYS:HD3	1:101:B:GLU:HG3	19	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	2	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	2	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	2	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	2	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	2	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	2	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	2	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	2	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	2	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	2	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	2	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	2	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	3	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	3	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	3	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	3	0.14
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	3	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	3	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	3	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	3	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	3	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	3	0.14
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	3	0.14
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	6	0.14
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	6	0.14
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	8	0.14
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	8	0.14
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	14	0.14
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	14	0.14
(1,3116)	1:89:B:GLU:HA	1:122:B:LEU:HD11	20	0.14
(1,3116)	1:89:B:GLU:HA	1:122:B:LEU:HD12	20	0.14
(1,3116)	1:89:B:GLU:HA	1:122:B:LEU:HD13	20	0.14
(1,3116)	1:89:B:GLU:HA	1:122:B:LEU:HD21	20	0.14
(1,3116)	1:89:B:GLU:HA	1:122:B:LEU:HD22	20	0.14
(1,3116)	1:89:B:GLU:HA	1:122:B:LEU:HD23	20	0.14
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE2	9	0.14
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE3	9	0.14
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE2	9	0.14
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE3	9	0.14
(1,3060)	1:75:B:LYS:HD2	1:82:B:LYS:HB2	4	0.14
(1,3060)	1:75:B:LYS:HD2	1:82:B:LYS:HB3	4	0.14
(1,3060)	1:75:B:LYS:HD3	1:82:B:LYS:HB2	4	0.14
(1,3060)	1:75:B:LYS:HD3	1:82:B:LYS:HB3	4	0.14
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD2	6	0.14
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD3	6	0.14
(1,3048)	1:74:B:GLU:HB2	1:77:B:LYS:H	15	0.14
(1,3048)	1:74:B:GLU:HB3	1:77:B:LYS:H	15	0.14
(1,3004)	1:67:B:ILE:HG21	1:68:B:PRO:HG2	16	0.14
(1,3004)	1:67:B:ILE:HG21	1:68:B:PRO:HG3	16	0.14
(1,3004)	1:67:B:ILE:HG22	1:68:B:PRO:HG2	16	0.14
(1,3004)	1:67:B:ILE:HG22	1:68:B:PRO:HG3	16	0.14
(1,3004)	1:67:B:ILE:HG23	1:68:B:PRO:HG2	16	0.14
(1,3004)	1:67:B:ILE:HG23	1:68:B:PRO:HG3	16	0.14
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	5	0.14
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	5	0.14
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	5	0.14
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	5	0.14
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	5	0.14
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	8	0.14
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	8	0.14
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	19	0.14
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	19	0.14
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	14	0.14
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	14	0.14
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	14	0.14
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	14	0.14
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	14	0.14
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	14	0.14
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	20	0.14
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	20	0.14
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	20	0.14
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	20	0.14
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	20	0.14
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	20	0.14
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	1	0.14
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	1	0.14
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	1	0.14
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	1	0.14
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	1	0.14
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	1	0.14
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	19	0.14
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	19	0.14
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	19	0.14
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	19	0.14
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	19	0.14
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	19	0.14
(1,2874)	1:24:B:LEU:HD11	1:32:B:GLN:HE22	17	0.14
(1,2874)	1:24:B:LEU:HD12	1:32:B:GLN:HE22	17	0.14
(1,2874)	1:24:B:LEU:HD13	1:32:B:GLN:HE22	17	0.14
(1,2874)	1:24:B:LEU:HD21	1:32:B:GLN:HE22	17	0.14
(1,2874)	1:24:B:LEU:HD22	1:32:B:GLN:HE22	17	0.14
(1,2874)	1:24:B:LEU:HD23	1:32:B:GLN:HE22	17	0.14
(1,2872)	1:24:B:LEU:HD21	1:32:B:GLN:HG2	8	0.14
(1,2872)	1:24:B:LEU:HD22	1:32:B:GLN:HG2	8	0.14
(1,2872)	1:24:B:LEU:HD23	1:32:B:GLN:HG2	8	0.14
(1,2866)	1:24:B:LEU:HB2	1:25:B:SER:H	15	0.14
(1,2866)	1:24:B:LEU:HB3	1:25:B:SER:H	15	0.14
(1,2866)	1:24:B:LEU:HB2	1:25:B:SER:H	17	0.14
(1,2866)	1:24:B:LEU:HB3	1:25:B:SER:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	3	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	3	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	3	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	3	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	3	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	3	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	16	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	16	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	16	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	16	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	16	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	16	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	18	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	18	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	18	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	18	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	18	0.14
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	18	0.14
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	19	0.14
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	19	0.14
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	19	0.14
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	19	0.14
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	19	0.14
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	19	0.14
(1,2761)	1:120:A:ILE:HD11	1:125:A:ASN:HD21	4	0.14
(1,2761)	1:120:A:ILE:HD11	1:125:A:ASN:HD22	4	0.14
(1,2761)	1:120:A:ILE:HD12	1:125:A:ASN:HD21	4	0.14
(1,2761)	1:120:A:ILE:HD12	1:125:A:ASN:HD22	4	0.14
(1,2761)	1:120:A:ILE:HD13	1:125:A:ASN:HD21	4	0.14
(1,2761)	1:120:A:ILE:HD13	1:125:A:ASN:HD22	4	0.14
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB2	9	0.14
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB3	9	0.14
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB2	9	0.14
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB3	9	0.14
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB2	9	0.14
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB3	9	0.14
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	17	0.14
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	17	0.14
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	18	0.14
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	18	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	9	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	9	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	9	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	9	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	9	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	15	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	15	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	15	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	15	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	15	0.14
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	15	0.14
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB2	10	0.14
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB3	10	0.14
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB2	10	0.14
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB3	10	0.14
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	1	0.14
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	1	0.14
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	1	0.14
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	1	0.14
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	20	0.14
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	20	0.14
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	20	0.14
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	20	0.14
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	13	0.14
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	13	0.14
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	13	0.14
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	13	0.14
(1,2654)	1:100:A:LYS:HD2	1:101:A:GLU:HG2	19	0.14
(1,2654)	1:100:A:LYS:HD2	1:101:A:GLU:HG3	19	0.14
(1,2654)	1:100:A:LYS:HD3	1:101:A:GLU:HG2	19	0.14
(1,2654)	1:100:A:LYS:HD3	1:101:A:GLU:HG3	19	0.14
(1,2633)	1:95:A:ASP:HB2	1:30:B:SER:H	7	0.14
(1,2633)	1:95:A:ASP:HB3	1:30:B:SER:H	7	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	10	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	10	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	10	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	10	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	10	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	10	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	10	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	10	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	10	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	10	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	10	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	15	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	15	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	15	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	15	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	15	0.14
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	15	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	15	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	15	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	15	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	15	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	15	0.14
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	15	0.14
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	6	0.14
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	6	0.14
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	8	0.14
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	8	0.14
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	14	0.14
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	14	0.14
(1,2616)	1:89:A:GLU:HA	1:122:A:LEU:HD11	20	0.14
(1,2616)	1:89:A:GLU:HA	1:122:A:LEU:HD12	20	0.14
(1,2616)	1:89:A:GLU:HA	1:122:A:LEU:HD13	20	0.14
(1,2616)	1:89:A:GLU:HA	1:122:A:LEU:HD21	20	0.14
(1,2616)	1:89:A:GLU:HA	1:122:A:LEU:HD22	20	0.14
(1,2616)	1:89:A:GLU:HA	1:122:A:LEU:HD23	20	0.14
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	9	0.14
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE3	9	0.14
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	9	0.14
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE3	9	0.14
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD2	7	0.14
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD3	7	0.14
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD2	12	0.14
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD3	12	0.14
(1,2550)	1:74:A:GLU:HG2	1:76:A:LYS:H	4	0.14
(1,2550)	1:74:A:GLU:HG3	1:76:A:LYS:H	4	0.14
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG11	14	0.14
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG12	14	0.14
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG13	14	0.14
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	14	0.14
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	14	0.14
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG11	14	0.14
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG12	14	0.14
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG13	14	0.14
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG21	14	0.14
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG22	14	0.14
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG23	14	0.14
(1,2456)	1:43:A:ASN:HD21	1:47:A:ASN:H	17	0.14
(1,2456)	1:43:A:ASN:HD22	1:47:A:ASN:H	17	0.14
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	8	0.14
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	8	0.14
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	11	0.14
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	11	0.14
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	19	0.14
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	19	0.14
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	14	0.14
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	14	0.14
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	14	0.14
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	14	0.14
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	14	0.14
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	14	0.14
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	20	0.14
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	20	0.14
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	20	0.14
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	20	0.14
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	20	0.14
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	20	0.14
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	1	0.14
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	1	0.14
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	1	0.14
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	1	0.14
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	1	0.14
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	1	0.14
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	6	0.14
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	6	0.14
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	6	0.14
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	6	0.14
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	6	0.14
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	6	0.14
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB2	7	0.14
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB3	7	0.14
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB2	7	0.14
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB2	7	0.14
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB3	7	0.14
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB2	7	0.14
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB3	7	0.14
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB2	7	0.14
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB3	7	0.14
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB2	7	0.14
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB3	7	0.14
(1,2369)	1:24:A:LEU:HD11	1:90:A:GLN:HE21	12	0.14
(1,2369)	1:24:A:LEU:HD12	1:90:A:GLN:HE21	12	0.14
(1,2369)	1:24:A:LEU:HD13	1:90:A:GLN:HE21	12	0.14
(1,2369)	1:24:A:LEU:HD21	1:90:A:GLN:HE21	12	0.14
(1,2369)	1:24:A:LEU:HD22	1:90:A:GLN:HE21	12	0.14
(1,2369)	1:24:A:LEU:HD23	1:90:A:GLN:HE21	12	0.14
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	15	0.14
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	15	0.14
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	15	0.14
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	15	0.14
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	15	0.14
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	15	0.14
(1,2359)	1:24:A:LEU:HB2	1:25:A:SER:H	17	0.14
(1,2359)	1:24:A:LEU:HB3	1:25:A:SER:H	17	0.14
(1,2342)	1:21:A:LEU:HD11	1:103:A:LEU:H	8	0.14
(1,2342)	1:21:A:LEU:HD12	1:103:A:LEU:H	8	0.14
(1,2342)	1:21:A:LEU:HD13	1:103:A:LEU:H	8	0.14
(1,2342)	1:21:A:LEU:HD21	1:103:A:LEU:H	8	0.14
(1,2342)	1:21:A:LEU:HD22	1:103:A:LEU:H	8	0.14
(1,2342)	1:21:A:LEU:HD23	1:103:A:LEU:H	8	0.14
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD1	20	0.14
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD2	20	0.14
(1,2269)	1:18:B:ASP:HA	1:105:B:TYR:HA	8	0.14
(1,2256)	1:73:B:ILE:HD11	1:78:B:TYR:HD1	6	0.14
(1,2256)	1:73:B:ILE:HD11	1:78:B:TYR:HD2	6	0.14
(1,2256)	1:73:B:ILE:HD12	1:78:B:TYR:HD1	6	0.14
(1,2256)	1:73:B:ILE:HD12	1:78:B:TYR:HD2	6	0.14
(1,2256)	1:73:B:ILE:HD13	1:78:B:TYR:HD1	6	0.14
(1,2256)	1:73:B:ILE:HD13	1:78:B:TYR:HD2	6	0.14
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE1	2	0.14
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE2	2	0.14
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE1	2	0.14
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE2	2	0.14
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE1	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE2	2	0.14
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	9	0.14
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	14	0.14
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	14	0.14
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	19	0.14
(1,2198)	1:120:B:ILE:HD11	1:125:B:ASN:HD21	9	0.14
(1,2198)	1:120:B:ILE:HD12	1:125:B:ASN:HD21	9	0.14
(1,2198)	1:120:B:ILE:HD13	1:125:B:ASN:HD21	9	0.14
(1,2192)	1:112:B:LYS:H	1:114:B:VAL:HG21	5	0.14
(1,2192)	1:112:B:LYS:H	1:114:B:VAL:HG22	5	0.14
(1,2192)	1:112:B:LYS:H	1:114:B:VAL:HG23	5	0.14
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	5	0.14
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	5	0.14
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	5	0.14
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	6	0.14
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	6	0.14
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	6	0.14
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG21	1	0.14
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG22	1	0.14
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG23	1	0.14
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	4	0.14
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	4	0.14
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	4	0.14
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	6	0.14
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	6	0.14
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	6	0.14
(1,2163)	1:113:B:GLU:HA	1:116:B:ASN:HD22	3	0.14
(1,2163)	1:113:B:GLU:HA	1:116:B:ASN:HD22	10	0.14
(1,2163)	1:113:B:GLU:HA	1:116:B:ASN:HD22	14	0.14
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD11	3	0.14
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD12	3	0.14
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD13	3	0.14
(1,2155)	1:119:B:MET:HE1	1:126:B:ALA:H	4	0.14
(1,2155)	1:119:B:MET:HE2	1:126:B:ALA:H	4	0.14
(1,2155)	1:119:B:MET:HE3	1:126:B:ALA:H	4	0.14
(1,2152)	1:123:B:GLY:H	1:125:B:ASN:H	9	0.14
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	8	0.14
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	8	0.14
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	8	0.14
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	9	0.14
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	9	0.14
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	13	0.14
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	7	0.14
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	9	0.14
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	2	0.14
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	4	0.14
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	3	0.14
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	3	0.14
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	3	0.14
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	7	0.14
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	7	0.14
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	7	0.14
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	19	0.14
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	19	0.14
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	19	0.14
(1,2111)	1:111:B:MET:HG3	1:112:B:LYS:H	3	0.14
(1,2111)	1:111:B:MET:HG3	1:112:B:LYS:H	4	0.14
(1,2111)	1:111:B:MET:HG3	1:112:B:LYS:H	9	0.14
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	9	0.14
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	19	0.14
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	12	0.14
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	11	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	7	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	7	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	7	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	11	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	11	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	11	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	15	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	15	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	15	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	17	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	17	0.14
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	17	0.14
(1,2049)	1:92:A:ARG:HG2	1:93:A:THR:H	8	0.14
(1,2039)	1:87:B:LEU:H	1:90:B:GLN:H	19	0.14
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	16	0.14
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	16	0.14
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	16	0.14
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	6	0.14
(1,2022)	1:73:A:ILE:HG13	1:84:A:SER:H	14	0.14
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	8	0.14
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	8	0.14
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	9	0.14
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	9	0.14
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	9	0.14
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	12	0.14
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	12	0.14
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	12	0.14
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	2	0.14
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	2	0.14
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	2	0.14
(1,1965)	1:53:B:VAL:HG21	1:54:B:ILE:H	11	0.14
(1,1965)	1:53:B:VAL:HG22	1:54:B:ILE:H	11	0.14
(1,1965)	1:53:B:VAL:HG23	1:54:B:ILE:H	11	0.14
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	12	0.14
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	18	0.14
(1,1933)	1:122:A:LEU:HA	1:43:B:ASN:H	12	0.14
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	6	0.14
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	16	0.14
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	20	0.14
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	2	0.14
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	10	0.14
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	8	0.14
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	12	0.14
(1,1900)	1:27:B:VAL:HG11	1:33:B:GLY:H	7	0.14
(1,1900)	1:27:B:VAL:HG12	1:33:B:GLY:H	7	0.14
(1,1900)	1:27:B:VAL:HG13	1:33:B:GLY:H	7	0.14
(1,1900)	1:27:B:VAL:HG11	1:33:B:GLY:H	10	0.14
(1,1900)	1:27:B:VAL:HG12	1:33:B:GLY:H	10	0.14
(1,1900)	1:27:B:VAL:HG13	1:33:B:GLY:H	10	0.14
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	10	0.14
(1,1888)	1:95:A:ASP:H	1:31:B:GLU:H	5	0.14
(1,1888)	1:95:A:ASP:H	1:31:B:GLU:H	16	0.14
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	7	0.14
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	2	0.14
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	4	0.14
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	19	0.14
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	11	0.14
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	4	0.14
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	4	0.14
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	4	0.14
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	20	0.14
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	20	0.14
(1,1742)	1:42:B:GLN:HE22	1:43:B:ASN:H	7	0.14
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	3	0.14
(1,1715)	1:28:A:GLN:HB3	1:28:A:GLN:HE21	5	0.14
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	7	0.14
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG11	10	0.14
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG12	10	0.14
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG13	10	0.14
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	1	0.14
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	1	0.14
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	1	0.14
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	11	0.14
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	11	0.14
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	11	0.14
(1,1673)	1:76:B:LYS:H	1:76:B:LYS:HD2	10	0.14
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	3	0.14
(1,1668)	1:75:B:LYS:HB3	1:76:B:LYS:H	4	0.14
(1,1634)	1:15:B:ARG:H	1:15:B:ARG:HG3	15	0.14
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	2	0.14
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	10	0.14
(1,1625)	1:122:B:LEU:H	1:122:B:LEU:HG	15	0.14
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	3	0.14
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	5	0.14
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	6	0.14
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	18	0.14
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	20	0.14
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	16	0.14
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	19	0.14
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	19	0.14
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	19	0.14
(1,1506)	1:20:B:TYR:H	1:21:B:LEU:H	17	0.14
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	3	0.14
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	3	0.14
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	7	0.14
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	7	0.14
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	1	0.14
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	5	0.14
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	11	0.14
(1,1491)	1:116:B:ASN:H	1:116:B:ASN:HD22	20	0.14
(1,1489)	1:115:B:ASP:HB3	1:116:B:ASN:H	13	0.14
(1,1488)	1:125:B:ASN:HA	1:125:B:ASN:HD22	4	0.14
(1,1487)	1:125:B:ASN:H	1:125:B:ASN:HD22	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	10	0.14
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	9	0.14
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	9	0.14
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	9	0.14
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	19	0.14
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	2	0.14
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	3	0.14
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	13	0.14
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	20	0.14
(1,1422)	1:28:B:GLN:HG3	1:28:B:GLN:HE22	15	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	6	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	6	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	6	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	6	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	6	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	6	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	6	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	6	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	6	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	11	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	11	0.14
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	11	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	11	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	11	0.14
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	11	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	11	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	11	0.14
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	11	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	5	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	5	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	5	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	7	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	7	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	7	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	12	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	12	0.14
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	12	0.14
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	16	0.14
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	16	0.14
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	16	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	8	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	8	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	9	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	9	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	9	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	15	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	15	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	15	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG21	19	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG22	19	0.14
(1,1343)	1:52:B:THR:HB	1:93:B:THR:HG23	19	0.14
(1,1342)	1:91:A:ILE:HG21	1:93:B:THR:HB	20	0.14
(1,1342)	1:91:A:ILE:HG22	1:93:B:THR:HB	20	0.14
(1,1342)	1:91:A:ILE:HG23	1:93:B:THR:HB	20	0.14
(1,1341)	1:58:B:ILE:HG21	1:84:B:SER:HB3	16	0.14
(1,1341)	1:58:B:ILE:HG22	1:84:B:SER:HB3	16	0.14
(1,1341)	1:58:B:ILE:HG23	1:84:B:SER:HB3	16	0.14
(1,1315)	1:119:B:MET:HA	1:124:B:LEU:HG	15	0.14
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD21	1	0.14
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD22	1	0.14
(1,1298)	1:106:B:LEU:HA	1:106:B:LEU:HD23	1	0.14
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD1	14	0.14
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD2	14	0.14
(1,1257)	1:96:B:LYS:HA	1:99:B:LEU:HG	18	0.14
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	6	0.14
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	6	0.14
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	6	0.14
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	17	0.14
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	17	0.14
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	17	0.14
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	13	0.14
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	13	0.14
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	13	0.14
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	9	0.14
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	9	0.14
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	9	0.14
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	10	0.14
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	10	0.14
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	10	0.14
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	17	0.14
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	17	0.14
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	17	0.14
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	18	0.14
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	18	0.14
(1,1169)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	3	0.14
(1,1169)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	3	0.14
(1,1169)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	3	0.14
(1,1167)	1:73:B:ILE:HG21	1:78:B:TYR:HB3	5	0.14
(1,1167)	1:73:B:ILE:HG22	1:78:B:TYR:HB3	5	0.14
(1,1167)	1:73:B:ILE:HG23	1:78:B:TYR:HB3	5	0.14
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	9	0.14
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	9	0.14
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	9	0.14
(1,1145)	1:27:A:VAL:HG21	1:33:A:GLY:HA3	16	0.14
(1,1145)	1:27:A:VAL:HG22	1:33:A:GLY:HA3	16	0.14
(1,1145)	1:27:A:VAL:HG23	1:33:A:GLY:HA3	16	0.14
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD1	3	0.14
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD2	3	0.14
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD1	18	0.14
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD2	18	0.14
(1,1103)	1:73:A:ILE:HD11	1:78:A:TYR:HD1	6	0.14
(1,1103)	1:73:A:ILE:HD11	1:78:A:TYR:HD2	6	0.14
(1,1103)	1:73:A:ILE:HD12	1:78:A:TYR:HD1	6	0.14
(1,1103)	1:73:A:ILE:HD12	1:78:A:TYR:HD2	6	0.14
(1,1103)	1:73:A:ILE:HD13	1:78:A:TYR:HD1	6	0.14
(1,1103)	1:73:A:ILE:HD13	1:78:A:TYR:HD2	6	0.14
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE1	2	0.14
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE2	2	0.14
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE1	2	0.14
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE2	2	0.14
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE1	2	0.14
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE2	2	0.14
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE1	8	0.14
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE2	8	0.14
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE1	8	0.14
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE2	8	0.14
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE1	8	0.14
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE2	8	0.14
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	9	0.14
(1,1071)	1:24:A:LEU:HD11	1:32:A:GLN:H	17	0.14
(1,1071)	1:24:A:LEU:HD12	1:32:A:GLN:H	17	0.14
(1,1071)	1:24:A:LEU:HD13	1:32:A:GLN:H	17	0.14
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	1	0.14
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	14	0.14
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	19	0.14
(1,1034)	1:23:A:ASP:H	1:100:A:LYS:H	3	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG21	4	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG22	4	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG23	4	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG21	6	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG22	6	0.14
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG23	6	0.14
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	6	0.14
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	6	0.14
(1,1019)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	6	0.14
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	19	0.14
(1,1011)	1:113:A:GLU:HA	1:116:A:ASN:HD21	4	0.14
(1,1011)	1:113:A:GLU:HA	1:116:A:ASN:HD21	12	0.14
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	16	0.14
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	20	0.14
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	2	0.14
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	8	0.14
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	18	0.14
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	18	0.14
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	18	0.14
(1,961)	1:112:A:LYS:H	1:115:A:ASP:H	2	0.14
(1,957)	1:110:B:LYS:H	1:110:B:LYS:HE2	6	0.14
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	7	0.14
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	12	0.14
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	17	0.14
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	19	0.14
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	3	0.14
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	10	0.14
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	20	0.14
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	1	0.14
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	10	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	5	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	5	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	5	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	7	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	7	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	7	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	11	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	11	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	15	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	15	0.14
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	15	0.14
(1,893)	1:87:A:LEU:H	1:90:A:GLN:H	19	0.14
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	13	0.14
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	13	0.14
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	13	0.14
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	15	0.14
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	15	0.14
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	15	0.14
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	16	0.14
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	16	0.14
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	16	0.14
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	8	0.14
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	8	0.14
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	8	0.14
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	4	0.14
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	4	0.14
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	4	0.14
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	7	0.14
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	7	0.14
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	7	0.14
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	12	0.14
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	12	0.14
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	12	0.14
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	2	0.14
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	2	0.14
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	2	0.14
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	5	0.14
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	5	0.14
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	5	0.14
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	12	0.14
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	18	0.14
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	6	0.14
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	9	0.14
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	16	0.14
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	20	0.14
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	2	0.14
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	3	0.14
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	13	0.14
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	6	0.14
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	6	0.14
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	3	0.14
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	16	0.14
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	19	0.14
(1,732)	1:25:A:SER:H	1:27:A:VAL:H	5	0.14
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	4	0.14
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	15	0.14
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	19	0.14
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	20	0.14
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	2	0.14
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	14	0.14
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	16	0.14
(1,625)	1:96:B:LYS:HB2	1:97:B:LYS:H	18	0.14
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	4	0.14
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	4	0.14
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	4	0.14
(1,600)	1:42:A:GLN:HE22	1:43:A:ASN:H	7	0.14
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD11	11	0.14
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD12	11	0.14
(1,591)	1:106:B:LEU:H	1:106:B:LEU:HD13	11	0.14
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	10	0.14
(1,572)	1:28:B:GLN:HB3	1:28:B:GLN:HE21	15	0.14
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	7	0.14
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	12	0.14
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG11	18	0.14
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG12	18	0.14
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG13	18	0.14
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	1	0.14
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	1	0.14
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	1	0.14
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	9	0.14
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	9	0.14
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	9	0.14
(1,486)	1:122:A:LEU:H	1:122:A:LEU:HG	2	0.14
(1,472)	1:90:A:GLN:HB3	1:90:A:GLN:HE21	15	0.14
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	3	0.14
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	5	0.14
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	7	0.14
(1,404)	1:32:A:GLN:H	1:32:A:GLN:HE21	7	0.14
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	10	0.14
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	14	0.14
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	19	0.14
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	19	0.14
(1,371)	1:20:A:TYR:H	1:21:A:LEU:H	17	0.14
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	4	0.14
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	4	0.14
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	7	0.14
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	7	0.14
(1,363)	1:48:A:LYS:H	1:48:A:LYS:HD2	18	0.14
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	16	0.14
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	10	0.14
(1,333)	1:80:A:LEU:H	1:80:A:LEU:HB2	4	0.14
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	20	0.14
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	5	0.14
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	5	0.14
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	5	0.14
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	5	0.14
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	5	0.14
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	5	0.14
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	5	0.14
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	5	0.14
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	5	0.14
(1,232)	1:27:A:VAL:HG11	1:33:A:GLY:HA3	11	0.14
(1,232)	1:27:A:VAL:HG12	1:33:A:GLY:HA3	11	0.14
(1,232)	1:27:A:VAL:HG13	1:33:A:GLY:HA3	11	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	2	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	2	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	2	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	7	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	7	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	7	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	10	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	10	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	10	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	11	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	11	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	11	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	12	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	12	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	12	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	13	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	13	0.14
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	16	0.14
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	14	0.14
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	14	0.14
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	14	0.14
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	16	0.14
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	16	0.14
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	16	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	1	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	1	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	1	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	2	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	2	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	2	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	6	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	6	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	6	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	8	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	8	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	8	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	9	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	9	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	9	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG21	19	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG22	19	0.14
(1,216)	1:52:A:THR:HB	1:93:A:THR:HG23	19	0.14
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG21	20	0.14
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG22	20	0.14
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG23	20	0.14
(1,214)	1:58:A:ILE:HG21	1:84:A:SER:HB3	16	0.14
(1,214)	1:58:A:ILE:HG22	1:84:A:SER:HB3	16	0.14
(1,214)	1:58:A:ILE:HG23	1:84:A:SER:HB3	16	0.14
(1,189)	1:119:A:MET:HA	1:124:A:LEU:HG	15	0.14
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD11	13	0.14
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD12	13	0.14
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD13	13	0.14
(1,180)	1:109:B:ASP:HA	1:112:B:LYS:HB3	4	0.14
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD21	1	0.14
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD22	1	0.14
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD23	1	0.14
(1,169)	1:27:A:VAL:HG11	1:33:A:GLY:HA2	3	0.14
(1,169)	1:27:A:VAL:HG12	1:33:A:GLY:HA2	3	0.14
(1,169)	1:27:A:VAL:HG13	1:33:A:GLY:HA2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD1	14	0.14
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD2	14	0.14
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD21	2	0.14
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD22	2	0.14
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD23	2	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	5	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	5	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	5	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	11	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	11	0.14
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	11	0.14
(1,94)	1:119:A:MET:HG3	1:124:A:LEU:HD11	11	0.14
(1,94)	1:119:A:MET:HG3	1:124:A:LEU:HD12	11	0.14
(1,94)	1:119:A:MET:HG3	1:124:A:LEU:HD13	11	0.14
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	10	0.14
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	10	0.14
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	10	0.14
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD11	5	0.14
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD12	5	0.14
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD13	5	0.14
(1,78)	1:71:A:VAL:HG21	1:113:A:GLU:HB3	17	0.14
(1,78)	1:71:A:VAL:HG22	1:113:A:GLU:HB3	17	0.14
(1,78)	1:71:A:VAL:HG23	1:113:A:GLU:HB3	17	0.14
(1,43)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	3	0.14
(1,43)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	3	0.14
(1,43)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	3	0.14
(1,41)	1:73:A:ILE:HG21	1:78:A:TYR:HB3	5	0.14
(1,41)	1:73:A:ILE:HG22	1:78:A:TYR:HB3	5	0.14
(1,41)	1:73:A:ILE:HG23	1:78:A:TYR:HB3	5	0.14
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	13	0.14
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	13	0.14
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	13	0.14
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	5	0.14
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	5	0.14
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	5	0.14
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	20	0.14
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	20	0.14
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	20	0.14
(1,3263)	1:126:B:ALA:HB1	1:127:B:VAL:HG11	14	0.13
(1,3263)	1:126:B:ALA:HB1	1:127:B:VAL:HG12	14	0.13
(1,3263)	1:126:B:ALA:HB1	1:127:B:VAL:HG13	14	0.13
(1,3263)	1:126:B:ALA:HB1	1:127:B:VAL:HG21	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3263)	1:126:B:ALA:HB1	1:127:B:VAL:HG22	14	0.13
(1,3263)	1:126:B:ALA:HB1	1:127:B:VAL:HG23	14	0.13
(1,3263)	1:126:B:ALA:HB2	1:127:B:VAL:HG11	14	0.13
(1,3263)	1:126:B:ALA:HB2	1:127:B:VAL:HG12	14	0.13
(1,3263)	1:126:B:ALA:HB2	1:127:B:VAL:HG13	14	0.13
(1,3263)	1:126:B:ALA:HB2	1:127:B:VAL:HG21	14	0.13
(1,3263)	1:126:B:ALA:HB2	1:127:B:VAL:HG22	14	0.13
(1,3263)	1:126:B:ALA:HB2	1:127:B:VAL:HG23	14	0.13
(1,3263)	1:126:B:ALA:HB3	1:127:B:VAL:HG11	14	0.13
(1,3263)	1:126:B:ALA:HB3	1:127:B:VAL:HG12	14	0.13
(1,3263)	1:126:B:ALA:HB3	1:127:B:VAL:HG13	14	0.13
(1,3263)	1:126:B:ALA:HB3	1:127:B:VAL:HG21	14	0.13
(1,3263)	1:126:B:ALA:HB3	1:127:B:VAL:HG22	14	0.13
(1,3263)	1:126:B:ALA:HB3	1:127:B:VAL:HG23	14	0.13
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	8	0.13
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	8	0.13
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	8	0.13
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	8	0.13
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	8	0.13
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	8	0.13
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	8	0.13
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	8	0.13
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	8	0.13
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	8	0.13
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	8	0.13
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	8	0.13
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	8	0.13
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	8	0.13
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	8	0.13
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	8	0.13
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	8	0.13
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	8	0.13
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	13	0.13
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	13	0.13
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB2	3	0.13
(1,3206)	1:113:B:GLU:HG2	1:116:B:ASN:HB3	3	0.13
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB2	3	0.13
(1,3206)	1:113:B:GLU:HG3	1:116:B:ASN:HB3	3	0.13
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	1	0.13
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	1	0.13
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	1	0.13
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	8	0.13
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	8	0.13
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	8	0.13
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	8	0.13
(1,3191)	1:112:B:LYS:H	1:112:B:LYS:HB2	5	0.13
(1,3191)	1:112:B:LYS:H	1:112:B:LYS:HB3	5	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD11	3	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD12	3	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD13	3	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD21	3	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD22	3	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD23	3	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD11	3	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD12	3	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD13	3	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD21	3	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD22	3	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD23	3	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD11	16	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD12	16	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD13	16	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD21	16	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD22	16	0.13
(1,3121)	1:91:B:ILE:HG12	1:118:B:LEU:HD23	16	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD11	16	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD12	16	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD13	16	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD21	16	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD22	16	0.13
(1,3121)	1:91:B:ILE:HG13	1:118:B:LEU:HD23	16	0.13
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	9	0.13
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	9	0.13
(1,3049)	1:74:B:GLU:HB2	1:77:B:LYS:HB2	9	0.13
(1,3049)	1:74:B:GLU:HB2	1:77:B:LYS:HB3	9	0.13
(1,3049)	1:74:B:GLU:HB3	1:77:B:LYS:HB2	9	0.13
(1,3049)	1:74:B:GLU:HB3	1:77:B:LYS:HB3	9	0.13
(1,3048)	1:74:B:GLU:HB2	1:77:B:LYS:H	8	0.13
(1,3048)	1:74:B:GLU:HB3	1:77:B:LYS:H	8	0.13
(1,3048)	1:74:B:GLU:HB2	1:77:B:LYS:H	17	0.13
(1,3048)	1:74:B:GLU:HB3	1:77:B:LYS:H	17	0.13
(1,3000)	1:62:B:ILE:HG21	1:85:B:VAL:HG11	19	0.13
(1,3000)	1:62:B:ILE:HG21	1:85:B:VAL:HG12	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3000)	1:62:B:ILE:HG21	1:85:B:VAL:HG13	19	0.13
(1,3000)	1:62:B:ILE:HG21	1:85:B:VAL:HG21	19	0.13
(1,3000)	1:62:B:ILE:HG21	1:85:B:VAL:HG22	19	0.13
(1,3000)	1:62:B:ILE:HG21	1:85:B:VAL:HG23	19	0.13
(1,3000)	1:62:B:ILE:HG22	1:85:B:VAL:HG11	19	0.13
(1,3000)	1:62:B:ILE:HG22	1:85:B:VAL:HG12	19	0.13
(1,3000)	1:62:B:ILE:HG22	1:85:B:VAL:HG13	19	0.13
(1,3000)	1:62:B:ILE:HG22	1:85:B:VAL:HG21	19	0.13
(1,3000)	1:62:B:ILE:HG22	1:85:B:VAL:HG22	19	0.13
(1,3000)	1:62:B:ILE:HG22	1:85:B:VAL:HG23	19	0.13
(1,3000)	1:62:B:ILE:HG23	1:85:B:VAL:HG11	19	0.13
(1,3000)	1:62:B:ILE:HG23	1:85:B:VAL:HG12	19	0.13
(1,3000)	1:62:B:ILE:HG23	1:85:B:VAL:HG13	19	0.13
(1,3000)	1:62:B:ILE:HG23	1:85:B:VAL:HG21	19	0.13
(1,3000)	1:62:B:ILE:HG23	1:85:B:VAL:HG22	19	0.13
(1,3000)	1:62:B:ILE:HG23	1:85:B:VAL:HG23	19	0.13
(1,2999)	1:62:B:ILE:HB	1:85:B:VAL:HG11	10	0.13
(1,2999)	1:62:B:ILE:HB	1:85:B:VAL:HG12	10	0.13
(1,2999)	1:62:B:ILE:HB	1:85:B:VAL:HG13	10	0.13
(1,2999)	1:62:B:ILE:HB	1:85:B:VAL:HG21	10	0.13
(1,2999)	1:62:B:ILE:HB	1:85:B:VAL:HG22	10	0.13
(1,2999)	1:62:B:ILE:HB	1:85:B:VAL:HG23	10	0.13
(1,2982)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	16	0.13
(1,2982)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	16	0.13
(1,2982)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	16	0.13
(1,2982)	1:53:B:VAL:HG21	1:94:B:LEU:HB2	16	0.13
(1,2982)	1:53:B:VAL:HG22	1:94:B:LEU:HB2	16	0.13
(1,2982)	1:53:B:VAL:HG23	1:94:B:LEU:HB2	16	0.13
(1,2972)	1:48:B:LYS:HE2	1:49:B:TYR:HE1	18	0.13
(1,2972)	1:48:B:LYS:HE2	1:49:B:TYR:HE2	18	0.13
(1,2972)	1:48:B:LYS:HE3	1:49:B:TYR:HE1	18	0.13
(1,2972)	1:48:B:LYS:HE3	1:49:B:TYR:HE2	18	0.13
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	11	0.13
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	11	0.13
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	4	0.13
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	4	0.13
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	4	0.13
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	4	0.13
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	4	0.13
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	4	0.13
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	6	0.13
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	6	0.13
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	6	0.13
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	6	0.13
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	6	0.13
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	11	0.13
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	11	0.13
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	11	0.13
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	11	0.13
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	11	0.13
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	11	0.13
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	12	0.13
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	12	0.13
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	12	0.13
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	12	0.13
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	12	0.13
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	12	0.13
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	4	0.13
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	4	0.13
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	4	0.13
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	4	0.13
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	4	0.13
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	4	0.13
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	6	0.13
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	6	0.13
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	6	0.13
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	6	0.13
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	6	0.13
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	6	0.13
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	15	0.13
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	15	0.13
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	15	0.13
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	15	0.13
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	15	0.13
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	15	0.13
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB2	6	0.13
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB3	6	0.13
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB2	6	0.13
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB3	6	0.13
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB2	6	0.13
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB3	6	0.13
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB2	6	0.13
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB2	6	0.13
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB3	6	0.13
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB2	6	0.13
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB3	6	0.13
(1,2884)	1:26:B:PRO:HD2	1:27:B:VAL:H	17	0.13
(1,2884)	1:26:B:PRO:HD3	1:27:B:VAL:H	17	0.13
(1,2874)	1:24:B:LEU:HD11	1:32:B:GLN:HE22	15	0.13
(1,2874)	1:24:B:LEU:HD12	1:32:B:GLN:HE22	15	0.13
(1,2874)	1:24:B:LEU:HD13	1:32:B:GLN:HE22	15	0.13
(1,2874)	1:24:B:LEU:HD21	1:32:B:GLN:HE22	15	0.13
(1,2874)	1:24:B:LEU:HD22	1:32:B:GLN:HE22	15	0.13
(1,2874)	1:24:B:LEU:HD23	1:32:B:GLN:HE22	15	0.13
(1,2869)	1:24:B:LEU:HD11	1:32:B:GLN:H	10	0.13
(1,2869)	1:24:B:LEU:HD12	1:32:B:GLN:H	10	0.13
(1,2869)	1:24:B:LEU:HD13	1:32:B:GLN:H	10	0.13
(1,2869)	1:24:B:LEU:HD21	1:32:B:GLN:H	10	0.13
(1,2869)	1:24:B:LEU:HD22	1:32:B:GLN:H	10	0.13
(1,2869)	1:24:B:LEU:HD23	1:32:B:GLN:H	10	0.13
(1,2849)	1:21:B:LEU:HD11	1:103:B:LEU:H	8	0.13
(1,2849)	1:21:B:LEU:HD12	1:103:B:LEU:H	8	0.13
(1,2849)	1:21:B:LEU:HD13	1:103:B:LEU:H	8	0.13
(1,2849)	1:21:B:LEU:HD21	1:103:B:LEU:H	8	0.13
(1,2849)	1:21:B:LEU:HD22	1:103:B:LEU:H	8	0.13
(1,2849)	1:21:B:LEU:HD23	1:103:B:LEU:H	8	0.13
(1,2769)	1:123:A:GLY:HA2	1:43:B:ASN:HD21	16	0.13
(1,2769)	1:123:A:GLY:HA2	1:43:B:ASN:HD22	16	0.13
(1,2769)	1:123:A:GLY:HA3	1:43:B:ASN:HD21	16	0.13
(1,2769)	1:123:A:GLY:HA3	1:43:B:ASN:HD22	16	0.13
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	7	0.13
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	7	0.13
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	7	0.13
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	7	0.13
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	7	0.13
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	7	0.13
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	7	0.13
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	7	0.13
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	7	0.13
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	7	0.13
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	7	0.13
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	7	0.13
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	7	0.13
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	7	0.13
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	7	0.13
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	7	0.13
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	7	0.13
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	13	0.13
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	13	0.13
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB2	7	0.13
(1,2708)	1:113:A:GLU:HG2	1:116:A:ASN:HB3	7	0.13
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB2	7	0.13
(1,2708)	1:113:A:GLU:HG3	1:116:A:ASN:HB3	7	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	4	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	4	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	4	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	4	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	6	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	6	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	6	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	6	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	8	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	8	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	8	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	8	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	18	0.13
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	18	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	18	0.13
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	18	0.13
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD11	16	0.13
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD12	16	0.13
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD13	16	0.13
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD21	16	0.13
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD22	16	0.13
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD23	16	0.13
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD11	16	0.13
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD12	16	0.13
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD13	16	0.13
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD21	16	0.13
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD22	16	0.13
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD23	16	0.13
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	2	0.13
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	2	0.13
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	2	0.13
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	2	0.13
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	2	0.13
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	2	0.13
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	2	0.13
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	2	0.13
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	2	0.13
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	2	0.13
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	2	0.13
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	1	0.13
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	1	0.13
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	5	0.13
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE3	5	0.13
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	5	0.13
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE3	5	0.13
(1,2560)	1:75:A:LYS:HD2	1:82:A:LYS:HB2	4	0.13
(1,2560)	1:75:A:LYS:HD2	1:82:A:LYS:HB3	4	0.13
(1,2560)	1:75:A:LYS:HD3	1:82:A:LYS:HB2	4	0.13
(1,2560)	1:75:A:LYS:HD3	1:82:A:LYS:HB3	4	0.13
(1,2555)	1:75:A:LYS:HA	1:80:A:LEU:HD11	4	0.13
(1,2555)	1:75:A:LYS:HA	1:80:A:LEU:HD12	4	0.13
(1,2555)	1:75:A:LYS:HA	1:80:A:LEU:HD13	4	0.13
(1,2555)	1:75:A:LYS:HA	1:80:A:LEU:HD21	4	0.13
(1,2555)	1:75:A:LYS:HA	1:80:A:LEU:HD22	4	0.13
(1,2555)	1:75:A:LYS:HA	1:80:A:LEU:HD23	4	0.13
(1,2548)	1:74:A:GLU:HB2	1:77:A:LYS:H	17	0.13
(1,2548)	1:74:A:GLU:HB3	1:77:A:LYS:H	17	0.13
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG11	1	0.13
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG12	1	0.13
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG13	1	0.13
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG21	1	0.13
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG22	1	0.13
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG23	1	0.13
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG11	7	0.13
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG12	7	0.13
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG13	7	0.13
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	7	0.13
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	7	0.13
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	7	0.13
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG11	7	0.13
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG12	7	0.13
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG13	7	0.13
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG21	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG22	7	0.13
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG23	7	0.13
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	1	0.13
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	1	0.13
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	1	0.13
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	1	0.13
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	1	0.13
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	1	0.13
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	16	0.13
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	16	0.13
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	16	0.13
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	16	0.13
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	16	0.13
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	16	0.13
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	18	0.13
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	18	0.13
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	18	0.13
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	18	0.13
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	18	0.13
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	18	0.13
(1,2463)	1:45:A:THR:HG21	1:48:A:LYS:HG2	19	0.13
(1,2463)	1:45:A:THR:HG21	1:48:A:LYS:HG3	19	0.13
(1,2463)	1:45:A:THR:HG22	1:48:A:LYS:HG2	19	0.13
(1,2463)	1:45:A:THR:HG22	1:48:A:LYS:HG3	19	0.13
(1,2463)	1:45:A:THR:HG23	1:48:A:LYS:HG2	19	0.13
(1,2463)	1:45:A:THR:HG23	1:48:A:LYS:HG3	19	0.13
(1,2448)	1:43:A:ASN:HB2	1:44:A:ASP:H	17	0.13
(1,2448)	1:43:A:ASN:HB3	1:44:A:ASP:H	17	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	2	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	2	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	2	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG21	2	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG22	2	0.13
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG23	2	0.13
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	6	0.13
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	6	0.13
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	6	0.13
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	6	0.13
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	6	0.13
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	6	0.13
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	11	0.13
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	11	0.13
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	11	0.13
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	11	0.13
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	11	0.13
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	12	0.13
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	12	0.13
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	12	0.13
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	12	0.13
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	12	0.13
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	12	0.13
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	16	0.13
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	16	0.13
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	16	0.13
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	16	0.13
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	16	0.13
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	16	0.13
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD2	7	0.13
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD3	7	0.13
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD2	7	0.13
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD3	7	0.13
(1,2370)	1:24:A:LEU:HD11	1:90:A:GLN:HE22	8	0.13
(1,2370)	1:24:A:LEU:HD12	1:90:A:GLN:HE22	8	0.13
(1,2370)	1:24:A:LEU:HD13	1:90:A:GLN:HE22	8	0.13
(1,2370)	1:24:A:LEU:HD21	1:90:A:GLN:HE22	8	0.13
(1,2370)	1:24:A:LEU:HD22	1:90:A:GLN:HE22	8	0.13
(1,2370)	1:24:A:LEU:HD23	1:90:A:GLN:HE22	8	0.13
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	18	0.13
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	18	0.13
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	18	0.13
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	18	0.13
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	18	0.13
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	18	0.13
(1,2365)	1:24:A:LEU:HD21	1:32:A:GLN:HG2	8	0.13
(1,2365)	1:24:A:LEU:HD22	1:32:A:GLN:HG2	8	0.13
(1,2365)	1:24:A:LEU:HD23	1:32:A:GLN:HG2	8	0.13
(1,2359)	1:24:A:LEU:HB2	1:25:A:SER:H	15	0.13
(1,2359)	1:24:A:LEU:HB3	1:25:A:SER:H	15	0.13
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD11	16	0.13
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD12	16	0.13
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD13	16	0.13
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD21	16	0.13
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD22	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2349)	1:23:A:ASP:H	1:24:A:LEU:HD23	16	0.13
(1,2274)	1:20:B:TYR:HE1	1:40:B:ILE:HG13	16	0.13
(1,2274)	1:20:B:TYR:HE2	1:40:B:ILE:HG13	16	0.13
(1,2269)	1:18:B:ASP:HA	1:105:B:TYR:HA	17	0.13
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	20	0.13
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	20	0.13
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	3	0.13
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	3	0.13
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	14	0.13
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	14	0.13
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	5	0.13
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	4	0.13
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	19	0.13
(1,2221)	1:116:B:ASN:HD21	1:118:B:LEU:H	7	0.13
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	11	0.13
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	11	0.13
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	11	0.13
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	17	0.13
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	17	0.13
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	17	0.13
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	1	0.13
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	9	0.13
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	17	0.13
(1,2200)	1:119:B:MET:HE1	1:125:B:ASN:HD22	1	0.13
(1,2200)	1:119:B:MET:HE2	1:125:B:ASN:HD22	1	0.13
(1,2200)	1:119:B:MET:HE3	1:125:B:ASN:HD22	1	0.13
(1,2200)	1:119:B:MET:HE1	1:125:B:ASN:HD22	19	0.13
(1,2200)	1:119:B:MET:HE2	1:125:B:ASN:HD22	19	0.13
(1,2200)	1:119:B:MET:HE3	1:125:B:ASN:HD22	19	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	4	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	4	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	4	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	14	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	14	0.13
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	14	0.13
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG21	14	0.13
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG22	14	0.13
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG23	14	0.13
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	18	0.13
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	18	0.13
(1,2165)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	18	0.13
(1,2152)	1:123:B:GLY:H	1:125:B:ASN:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2150)	1:119:B:MET:HE1	1:124:B:LEU:H	9	0.13
(1,2150)	1:119:B:MET:HE2	1:124:B:LEU:H	9	0.13
(1,2150)	1:119:B:MET:HE3	1:124:B:LEU:H	9	0.13
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	3	0.13
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	3	0.13
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	3	0.13
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	5	0.13
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	5	0.13
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	5	0.13
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	10	0.13
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	11	0.13
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	20	0.13
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	8	0.13
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	10	0.13
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	5	0.13
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	5	0.13
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	5	0.13
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE1	12	0.13
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE2	12	0.13
(1,2130)	1:119:B:MET:H	1:119:B:MET:HE3	12	0.13
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	1	0.13
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	12	0.13
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	15	0.13
(1,2103)	1:110:A:LYS:H	1:110:A:LYS:HE2	6	0.13
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	1	0.13
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	3	0.13
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	11	0.13
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	3	0.13
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	4	0.13
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	10	0.13
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	19	0.13
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	20	0.13
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	4	0.13
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	12	0.13
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	14	0.13
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	16	0.13
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	17	0.13
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	10	0.13
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	10	0.13
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	10	0.13
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	8	0.13
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	8	0.13
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	13	0.13
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	13	0.13
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	13	0.13
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	14	0.13
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	14	0.13
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	14	0.13
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	15	0.13
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	15	0.13
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	15	0.13
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	12	0.13
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	14	0.13
(1,2002)	1:74:B:GLU:H	1:78:B:TYR:HE1	19	0.13
(1,2002)	1:74:B:GLU:H	1:78:B:TYR:HE2	19	0.13
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	3	0.13
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	3	0.13
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	3	0.13
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	4	0.13
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	4	0.13
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	4	0.13
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	7	0.13
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	7	0.13
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	7	0.13
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	7	0.13
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	7	0.13
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	7	0.13
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	13	0.13
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	13	0.13
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	13	0.13
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	20	0.13
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	20	0.13
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	20	0.13
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	5	0.13
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	16	0.13
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	1	0.13
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	1	0.13
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	1	0.13
(1,1931)	1:42:A:GLN:H	1:54:A:ILE:HG21	13	0.13
(1,1931)	1:42:A:GLN:H	1:54:A:ILE:HG22	13	0.13
(1,1931)	1:42:A:GLN:H	1:54:A:ILE:HG23	13	0.13
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	9	0.13
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	13	0.13
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	19	0.13
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	20	0.13
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	16	0.13
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	16	0.13
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	16	0.13
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	3	0.13
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	4	0.13
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	7	0.13
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	8	0.13
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	16	0.13
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	1	0.13
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	1	0.13
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	1	0.13
(1,1878)	1:25:B:SER:H	1:27:B:VAL:H	5	0.13
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	12	0.13
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	15	0.13
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	20	0.13
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	2	0.13
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	19	0.13
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG21	16	0.13
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG22	16	0.13
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG23	16	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	3	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	3	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	3	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	12	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	12	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	12	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	14	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	14	0.13
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	14	0.13
(1,1742)	1:42:B:GLN:HE22	1:43:B:ASN:H	17	0.13
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	16	0.13
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	7	0.13
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	10	0.13
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	12	0.13
(1,1710)	1:127:B:VAL:HA	1:128:B:ALA:H	2	0.13
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	10	0.13
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	11	0.13
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	12	0.13
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	19	0.13
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG11	18	0.13
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG12	18	0.13
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG13	18	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	5	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	5	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	5	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	6	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	6	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	6	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	8	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	8	0.13
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	8	0.13
(1,1675)	1:124:B:LEU:H	1:124:B:LEU:HG	10	0.13
(1,1675)	1:124:B:LEU:H	1:124:B:LEU:HG	17	0.13
(1,1674)	1:76:A:LYS:H	1:76:A:LYS:HD3	16	0.13
(1,1631)	1:74:B:GLU:H	1:74:B:GLU:HG2	19	0.13
(1,1611)	1:90:B:GLN:HB3	1:90:B:GLN:HE21	15	0.13
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	7	0.13
(1,1585)	1:112:B:LYS:H	1:112:B:LYS:HB2	5	0.13
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	19	0.13
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	13	0.13
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	14	0.13
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	19	0.13
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	3	0.13
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	3	0.13
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	3	0.13
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	5	0.13
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	5	0.13
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	5	0.13
(1,1506)	1:20:B:TYR:H	1:21:B:LEU:H	9	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	4	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	4	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	6	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	6	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	12	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	12	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	15	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	15	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	17	0.13
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	17	0.13
(1,1498)	1:48:B:LYS:H	1:48:B:LYS:HD2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	5	0.13
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	7	0.13
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	17	0.13
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	17	0.13
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	17	0.13
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	8	0.13
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	15	0.13
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	16	0.13
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	1	0.13
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	14	0.13
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD11	14	0.13
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD12	14	0.13
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD13	14	0.13
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	1	0.13
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	1	0.13
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	1	0.13
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	1	0.13
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	1	0.13
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	1	0.13
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	1	0.13
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	1	0.13
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	1	0.13
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	18	0.13
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	18	0.13
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	18	0.13
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	18	0.13
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	18	0.13
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	18	0.13
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	18	0.13
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	18	0.13
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	18	0.13
(1,1359)	1:27:B:VAL:HG11	1:33:B:GLY:HA3	11	0.13
(1,1359)	1:27:B:VAL:HG12	1:33:B:GLY:HA3	11	0.13
(1,1359)	1:27:B:VAL:HG13	1:33:B:GLY:HA3	11	0.13
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	10	0.13
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	10	0.13
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	10	0.13
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	13	0.13
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	13	0.13
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	13	0.13
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	20	0.13
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	8	0.13
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	8	0.13
(1,1342)	1:91:A:ILE:HG21	1:93:B:THR:HB	5	0.13
(1,1342)	1:91:A:ILE:HG22	1:93:B:THR:HB	5	0.13
(1,1342)	1:91:A:ILE:HG23	1:93:B:THR:HB	5	0.13
(1,1318)	1:16:B:ARG:HA	1:40:B:ILE:HB	12	0.13
(1,1317)	1:75:A:LYS:HA	1:80:A:LEU:HD21	15	0.13
(1,1317)	1:75:A:LYS:HA	1:80:A:LEU:HD22	15	0.13
(1,1317)	1:75:A:LYS:HA	1:80:A:LEU:HD23	15	0.13
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD11	8	0.13
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD12	8	0.13
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD13	8	0.13
(1,1295)	1:27:B:VAL:HG11	1:33:B:GLY:HA2	3	0.13
(1,1295)	1:27:B:VAL:HG12	1:33:B:GLY:HA2	3	0.13
(1,1295)	1:27:B:VAL:HG13	1:33:B:GLY:HA2	3	0.13
(1,1295)	1:27:B:VAL:HG11	1:33:B:GLY:HA2	20	0.13
(1,1295)	1:27:B:VAL:HG12	1:33:B:GLY:HA2	20	0.13
(1,1295)	1:27:B:VAL:HG13	1:33:B:GLY:HA2	20	0.13
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD21	2	0.13
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD22	2	0.13
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD23	2	0.13
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	18	0.13
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	18	0.13
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	18	0.13
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	11	0.13
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	11	0.13
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	11	0.13
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD11	16	0.13
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD12	16	0.13
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD13	16	0.13
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	2	0.13
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	2	0.13
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	2	0.13
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	3	0.13
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	3	0.13
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	3	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	5	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	5	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	5	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	8	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	8	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	20	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	20	0.13
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	20	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	15	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	15	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	15	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	19	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	19	0.13
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	19	0.13
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG21	17	0.13
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG22	17	0.13
(1,1154)	1:103:B:LEU:HG	1:104:B:THR:HG23	17	0.13
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	5	0.13
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	5	0.13
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	5	0.13
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	7	0.13
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	7	0.13
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	7	0.13
(1,1116)	1:18:A:ASP:HA	1:105:A:TYR:HA	4	0.13
(1,1083)	1:76:A:LYS:H	1:80:A:LEU:H	4	0.13
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	14	0.13
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	17	0.13
(1,1048)	1:119:A:MET:HE1	1:125:A:ASN:HD22	8	0.13
(1,1048)	1:119:A:MET:HE2	1:125:A:ASN:HD22	8	0.13
(1,1048)	1:119:A:MET:HE3	1:125:A:ASN:HD22	8	0.13
(1,1045)	1:120:A:ILE:HG12	1:125:A:ASN:HD21	3	0.13
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	14	0.13
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	14	0.13
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	14	0.13
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG21	14	0.13
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG22	14	0.13
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG23	14	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG21	1	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG22	1	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG23	1	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG21	14	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG22	14	0.13
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG23	14	0.13
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	6	0.13
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	11	0.13
(1,1009)	1:119:A:MET:HE1	1:126:A:ALA:H	4	0.13
(1,1009)	1:119:A:MET:HE2	1:126:A:ALA:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	1:119:A:MET:HE3	1:126:A:ALA:H	4	0.13
(1,1006)	1:123:A:GLY:H	1:125:A:ASN:H	3	0.13
(1,1006)	1:123:A:GLY:H	1:125:A:ASN:H	9	0.13
(1,1006)	1:123:A:GLY:H	1:125:A:ASN:H	14	0.13
(1,1003)	1:119:A:MET:HA	1:124:A:LEU:H	17	0.13
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	3	0.13
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	3	0.13
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	3	0.13
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	6	0.13
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	6	0.13
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	6	0.13
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	10	0.13
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	10	0.13
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	10	0.13
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	11	0.13
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	11	0.13
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	11	0.13
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	20	0.13
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	20	0.13
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	20	0.13
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	12	0.13
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	12	0.13
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	12	0.13
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	3	0.13
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	1	0.13
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	2	0.13
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	9	0.13
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	15	0.13
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	4	0.13
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	14	0.13
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	16	0.13
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	19	0.13
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	4	0.13
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	12	0.13
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	14	0.13
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	20	0.13
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	10	0.13
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	10	0.13
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	10	0.13
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	9	0.13
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	9	0.13
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:75:A:LYS:H	1:83:A:ASP:H	20	0.13
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	4	0.13
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	4	0.13
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	4	0.13
(1,864)	1:80:A:LEU:HD11	1:81:A:ASP:H	13	0.13
(1,864)	1:80:A:LEU:HD12	1:81:A:ASP:H	13	0.13
(1,864)	1:80:A:LEU:HD13	1:81:A:ASP:H	13	0.13
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	10	0.13
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	12	0.13
(1,857)	1:73:A:ILE:HG21	1:74:A:GLU:H	20	0.13
(1,857)	1:73:A:ILE:HG22	1:74:A:GLU:H	20	0.13
(1,857)	1:73:A:ILE:HG23	1:74:A:GLU:H	20	0.13
(1,855)	1:74:A:GLU:H	1:78:A:TYR:HD1	20	0.13
(1,855)	1:74:A:GLU:H	1:78:A:TYR:HD2	20	0.13
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	3	0.13
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	3	0.13
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	3	0.13
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	7	0.13
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	7	0.13
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	7	0.13
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	13	0.13
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	13	0.13
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	13	0.13
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	20	0.13
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	20	0.13
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	20	0.13
(1,819)	1:53:A:VAL:HG21	1:54:A:ILE:H	11	0.13
(1,819)	1:53:A:VAL:HG22	1:54:A:ILE:H	11	0.13
(1,819)	1:53:A:VAL:HG23	1:54:A:ILE:H	11	0.13
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	16	0.13
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	1	0.13
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	1	0.13
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	1	0.13
(1,787)	1:43:A:ASN:H	1:122:B:LEU:HA	12	0.13
(1,785)	1:42:B:GLN:H	1:54:B:ILE:HG21	13	0.13
(1,785)	1:42:B:GLN:H	1:54:B:ILE:HG22	13	0.13
(1,785)	1:42:B:GLN:H	1:54:B:ILE:HG23	13	0.13
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	8	0.13
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	12	0.13
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	19	0.13
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	20	0.13
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	11	0.13
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	11	0.13
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	16	0.13
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	16	0.13
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	16	0.13
(1,757)	1:27:A:VAL:HG21	1:34:A:GLY:H	9	0.13
(1,757)	1:27:A:VAL:HG22	1:34:A:GLY:H	9	0.13
(1,757)	1:27:A:VAL:HG23	1:34:A:GLY:H	9	0.13
(1,742)	1:31:A:GLU:H	1:95:B:ASP:H	8	0.13
(1,737)	1:24:A:LEU:HD11	1:25:A:SER:H	1	0.13
(1,737)	1:24:A:LEU:HD12	1:25:A:SER:H	1	0.13
(1,737)	1:24:A:LEU:HD13	1:25:A:SER:H	1	0.13
(1,727)	1:22:A:ALA:H	1:35:A:VAL:HB	2	0.13
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	2	0.13
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	12	0.13
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	19	0.13
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	14	0.13
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	14	0.13
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	14	0.13
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	20	0.13
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	20	0.13
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	20	0.13
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	16	0.13
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	6	0.13
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	16	0.13
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	10	0.13
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	11	0.13
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	14	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	5	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	5	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	5	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	6	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	6	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	6	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	8	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	8	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	8	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	19	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	19	0.13
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	19	0.13
(1,533)	1:76:B:LYS:H	1:76:B:LYS:HD3	16	0.13
(1,495)	1:15:A:ARG:H	1:15:A:ARG:HG3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:105:A:TYR:H	1:106:A:LEU:H	6	0.13
(1,455)	1:105:A:TYR:H	1:106:A:LEU:H	12	0.13
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	19	0.13
(1,404)	1:32:A:GLN:H	1:32:A:GLN:HE21	10	0.13
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	2	0.13
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	3	0.13
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	12	0.13
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	15	0.13
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	17	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	3	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	3	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	6	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	6	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	11	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	11	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	12	0.13
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	12	0.13
(1,356)	1:115:B:ASP:HB2	1:116:B:ASN:H	19	0.13
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	15	0.13
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	17	0.13
(1,354)	1:125:A:ASN:HA	1:125:A:ASN:HD22	4	0.13
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	5	0.13
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	9	0.13
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	9	0.13
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	9	0.13
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	8	0.13
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	15	0.13
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	16	0.13
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	18	0.13
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	19	0.13
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	3	0.13
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	12	0.13
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	14	0.13
(1,261)	1:52:A:THR:HG21	1:95:A:ASP:HA	11	0.13
(1,261)	1:52:A:THR:HG22	1:95:A:ASP:HA	11	0.13
(1,261)	1:52:A:THR:HG23	1:95:A:ASP:HA	11	0.13
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	6	0.13
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	6	0.13
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	6	0.13
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	6	0.13
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	6	0.13
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	6	0.13
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	6	0.13
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	6	0.13
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	19	0.13
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	19	0.13
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	19	0.13
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	19	0.13
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	19	0.13
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	19	0.13
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	19	0.13
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	19	0.13
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	19	0.13
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	5	0.13
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	5	0.13
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	5	0.13
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	4	0.13
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	20	0.13
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG11	11	0.13
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG12	11	0.13
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG13	11	0.13
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	10	0.13
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	10	0.13
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	10	0.13
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	20	0.13
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	20	0.13
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	20	0.13
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG21	5	0.13
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG22	5	0.13
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG23	5	0.13
(1,214)	1:58:A:ILE:HG21	1:84:A:SER:HB3	20	0.13
(1,214)	1:58:A:ILE:HG22	1:84:A:SER:HB3	20	0.13
(1,214)	1:58:A:ILE:HG23	1:84:A:SER:HB3	20	0.13
(1,192)	1:16:A:ARG:HA	1:40:A:ILE:HB	11	0.13
(1,169)	1:27:A:VAL:HG11	1:33:A:GLY:HA2	20	0.13
(1,169)	1:27:A:VAL:HG12	1:33:A:GLY:HA2	20	0.13
(1,169)	1:27:A:VAL:HG13	1:33:A:GLY:HA2	20	0.13
(1,162)	1:80:A:LEU:HB3	1:81:A:ASP:HB2	15	0.13
(1,132)	1:96:A:LYS:HA	1:99:A:LEU:HG	18	0.13
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD21	15	0.13
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD22	15	0.13
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD23	15	0.13
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	17	0.13
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	17	0.13
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	13	0.13
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	13	0.13
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	13	0.13
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	2	0.13
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	2	0.13
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	2	0.13
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	13	0.13
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	13	0.13
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	13	0.13
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD11	19	0.13
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD12	19	0.13
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD13	19	0.13
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD11	20	0.13
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD12	20	0.13
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD13	20	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB1	9	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB2	9	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB3	9	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB1	9	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB2	9	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB3	9	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB1	9	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB2	9	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB3	9	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB1	13	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB2	13	0.13
(1,62)	1:69:A:THR:HG21	1:117:A:ALA:HB3	13	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB1	13	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB2	13	0.13
(1,62)	1:69:A:THR:HG22	1:117:A:ALA:HB3	13	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB1	13	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB2	13	0.13
(1,62)	1:69:A:THR:HG23	1:117:A:ALA:HB3	13	0.13
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	15	0.13
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	15	0.13
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	15	0.13
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	7	0.13
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	7	0.13
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	7	0.13
(1,19)	1:27:B:VAL:HG21	1:33:B:GLY:HA3	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:27:B:VAL:HG22	1:33:B:GLY:HA3	16	0.13
(1,19)	1:27:B:VAL:HG23	1:33:B:GLY:HA3	16	0.13
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG2	10	0.12
(1,3232)	1:119:B:MET:H	1:119:B:MET:HG3	10	0.12
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	18	0.12
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	18	0.12
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	18	0.12
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	18	0.12
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	19	0.12
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	19	0.12
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	19	0.12
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	19	0.12
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	16	0.12
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	16	0.12
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	6	0.12
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	6	0.12
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	6	0.12
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	6	0.12
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	6	0.12
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	6	0.12
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	6	0.12
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	6	0.12
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	6	0.12
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	6	0.12
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	6	0.12
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	6	0.12
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	1	0.12
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	1	0.12
(1,3110)	1:87:B:LEU:HD11	1:90:B:GLN:HB3	13	0.12
(1,3110)	1:87:B:LEU:HD12	1:90:B:GLN:HB3	13	0.12
(1,3110)	1:87:B:LEU:HD13	1:90:B:GLN:HB3	13	0.12
(1,3110)	1:87:B:LEU:HD21	1:90:B:GLN:HB3	13	0.12
(1,3110)	1:87:B:LEU:HD22	1:90:B:GLN:HB3	13	0.12
(1,3110)	1:87:B:LEU:HD23	1:90:B:GLN:HB3	13	0.12
(1,3110)	1:87:B:LEU:HD11	1:90:B:GLN:HB3	16	0.12
(1,3110)	1:87:B:LEU:HD12	1:90:B:GLN:HB3	16	0.12
(1,3110)	1:87:B:LEU:HD13	1:90:B:GLN:HB3	16	0.12
(1,3110)	1:87:B:LEU:HD21	1:90:B:GLN:HB3	16	0.12
(1,3110)	1:87:B:LEU:HD22	1:90:B:GLN:HB3	16	0.12
(1,3110)	1:87:B:LEU:HD23	1:90:B:GLN:HB3	16	0.12
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE2	5	0.12
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE3	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE2	5	0.12
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE3	5	0.12
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD2	1	0.12
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD3	1	0.12
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD2	7	0.12
(1,3054)	1:75:B:LYS:HA	1:75:B:LYS:HD3	7	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG11	1	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG12	1	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG13	1	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG21	1	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG22	1	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG23	1	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG11	10	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG12	10	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG13	10	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG21	10	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG22	10	0.12
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG23	10	0.12
(1,2989)	1:54:B:ILE:HG12	1:92:B:ARG:H	7	0.12
(1,2989)	1:54:B:ILE:HG13	1:92:B:ARG:H	7	0.12
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	2	0.12
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	2	0.12
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	2	0.12
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	2	0.12
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	2	0.12
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	2	0.12
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	9	0.12
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	9	0.12
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	9	0.12
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	9	0.12
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	9	0.12
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	9	0.12
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	15	0.12
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	15	0.12
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	15	0.12
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	15	0.12
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	15	0.12
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	15	0.12
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	16	0.12
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	16	0.12
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	16	0.12
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	16	0.12
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	16	0.12
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	3	0.12
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	3	0.12
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	3	0.12
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	3	0.12
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	3	0.12
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	3	0.12
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	9	0.12
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	9	0.12
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	9	0.12
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	9	0.12
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	9	0.12
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	9	0.12
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	12	0.12
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	12	0.12
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	12	0.12
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	12	0.12
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	12	0.12
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	12	0.12
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	19	0.12
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	19	0.12
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	19	0.12
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	19	0.12
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	19	0.12
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	19	0.12
(1,2884)	1:26:B:PRO:HD2	1:27:B:VAL:H	15	0.12
(1,2884)	1:26:B:PRO:HD3	1:27:B:VAL:H	15	0.12
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	1	0.12
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	1	0.12
(1,2882)	1:25:B:SER:HB2	1:27:B:VAL:H	20	0.12
(1,2882)	1:25:B:SER:HB3	1:27:B:VAL:H	20	0.12
(1,2877)	1:24:B:LEU:HD11	1:90:B:GLN:HE22	8	0.12
(1,2877)	1:24:B:LEU:HD12	1:90:B:GLN:HE22	8	0.12
(1,2877)	1:24:B:LEU:HD13	1:90:B:GLN:HE22	8	0.12
(1,2877)	1:24:B:LEU:HD21	1:90:B:GLN:HE22	8	0.12
(1,2877)	1:24:B:LEU:HD22	1:90:B:GLN:HE22	8	0.12
(1,2877)	1:24:B:LEU:HD23	1:90:B:GLN:HE22	8	0.12
(1,2872)	1:24:B:LEU:HD21	1:32:B:GLN:HG2	10	0.12
(1,2872)	1:24:B:LEU:HD22	1:32:B:GLN:HG2	10	0.12
(1,2872)	1:24:B:LEU:HD23	1:32:B:GLN:HG2	10	0.12
(1,2871)	1:24:B:LEU:HD11	1:32:B:GLN:HG2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2871)	1:24:B:LEU:HD11	1:32:B:GLN:HG3	4	0.12
(1,2871)	1:24:B:LEU:HD12	1:32:B:GLN:HG2	4	0.12
(1,2871)	1:24:B:LEU:HD12	1:32:B:GLN:HG3	4	0.12
(1,2871)	1:24:B:LEU:HD13	1:32:B:GLN:HG2	4	0.12
(1,2871)	1:24:B:LEU:HD13	1:32:B:GLN:HG3	4	0.12
(1,2871)	1:24:B:LEU:HD21	1:32:B:GLN:HG2	4	0.12
(1,2871)	1:24:B:LEU:HD21	1:32:B:GLN:HG3	4	0.12
(1,2871)	1:24:B:LEU:HD22	1:32:B:GLN:HG2	4	0.12
(1,2871)	1:24:B:LEU:HD22	1:32:B:GLN:HG3	4	0.12
(1,2871)	1:24:B:LEU:HD23	1:32:B:GLN:HG2	4	0.12
(1,2871)	1:24:B:LEU:HD23	1:32:B:GLN:HG3	4	0.12
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	20	0.12
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	20	0.12
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	20	0.12
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	20	0.12
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	20	0.12
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	20	0.12
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD11	16	0.12
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD12	16	0.12
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD13	16	0.12
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD21	16	0.12
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD22	16	0.12
(1,2856)	1:23:B:ASP:H	1:24:B:LEU:HD23	16	0.12
(1,2823)	1:19:B:VAL:HG11	1:106:B:LEU:H	3	0.12
(1,2823)	1:19:B:VAL:HG12	1:106:B:LEU:H	3	0.12
(1,2823)	1:19:B:VAL:HG13	1:106:B:LEU:H	3	0.12
(1,2823)	1:19:B:VAL:HG21	1:106:B:LEU:H	3	0.12
(1,2823)	1:19:B:VAL:HG22	1:106:B:LEU:H	3	0.12
(1,2823)	1:19:B:VAL:HG23	1:106:B:LEU:H	3	0.12
(1,2816)	1:19:B:VAL:HG11	1:103:B:LEU:HB2	5	0.12
(1,2816)	1:19:B:VAL:HG12	1:103:B:LEU:HB2	5	0.12
(1,2816)	1:19:B:VAL:HG13	1:103:B:LEU:HB2	5	0.12
(1,2816)	1:19:B:VAL:HG21	1:103:B:LEU:HB2	5	0.12
(1,2816)	1:19:B:VAL:HG22	1:103:B:LEU:HB2	5	0.12
(1,2816)	1:19:B:VAL:HG23	1:103:B:LEU:HB2	5	0.12
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB2	1	0.12
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB3	1	0.12
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB2	20	0.12
(1,2749)	1:119:A:MET:HE1	1:124:A:LEU:HB3	20	0.12
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB2	20	0.12
(1,2749)	1:119:A:MET:HE2	1:124:A:LEU:HB3	20	0.12
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB2	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2749)	1:119:A:MET:HE3	1:124:A:LEU:HB3	20	0.12
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD11	1	0.12
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD12	1	0.12
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD13	1	0.12
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD21	1	0.12
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD22	1	0.12
(1,2747)	1:119:A:MET:HG2	1:124:A:LEU:HD23	1	0.12
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD11	1	0.12
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD12	1	0.12
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD13	1	0.12
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD21	1	0.12
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD22	1	0.12
(1,2747)	1:119:A:MET:HG3	1:124:A:LEU:HD23	1	0.12
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG2	10	0.12
(1,2740)	1:119:A:MET:H	1:119:A:MET:HG3	10	0.12
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	3	0.12
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	3	0.12
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	11	0.12
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	11	0.12
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	18	0.12
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	18	0.12
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	3	0.12
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	3	0.12
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD21	7	0.12
(1,2709)	1:113:A:GLU:HG2	1:116:A:ASN:HD22	7	0.12
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD21	7	0.12
(1,2709)	1:113:A:GLU:HG3	1:116:A:ASN:HD22	7	0.12
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	15	0.12
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	15	0.12
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	15	0.12
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	15	0.12
(1,2633)	1:95:A:ASP:HB2	1:30:B:SER:H	8	0.12
(1,2633)	1:95:A:ASP:HB3	1:30:B:SER:H	8	0.12
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	16	0.12
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	16	0.12
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	16	0.12
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	16	0.12
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	16	0.12
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	16	0.12
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	16	0.12
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	16	0.12
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	16	0.12
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	16	0.12
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	16	0.12
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	3	0.12
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	3	0.12
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	9	0.12
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	9	0.12
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	15	0.12
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	15	0.12
(1,2587)	1:80:A:LEU:HD11	1:84:A:SER:HB2	15	0.12
(1,2587)	1:80:A:LEU:HD11	1:84:A:SER:HB3	15	0.12
(1,2587)	1:80:A:LEU:HD12	1:84:A:SER:HB2	15	0.12
(1,2587)	1:80:A:LEU:HD12	1:84:A:SER:HB3	15	0.12
(1,2587)	1:80:A:LEU:HD13	1:84:A:SER:HB2	15	0.12
(1,2587)	1:80:A:LEU:HD13	1:84:A:SER:HB3	15	0.12
(1,2587)	1:80:A:LEU:HD21	1:84:A:SER:HB2	15	0.12
(1,2587)	1:80:A:LEU:HD21	1:84:A:SER:HB3	15	0.12
(1,2587)	1:80:A:LEU:HD22	1:84:A:SER:HB2	15	0.12
(1,2587)	1:80:A:LEU:HD22	1:84:A:SER:HB3	15	0.12
(1,2587)	1:80:A:LEU:HD23	1:84:A:SER:HB2	15	0.12
(1,2587)	1:80:A:LEU:HD23	1:84:A:SER:HB3	15	0.12
(1,2556)	1:75:A:LYS:HB2	1:83:A:ASP:H	14	0.12
(1,2556)	1:75:A:LYS:HB3	1:83:A:ASP:H	14	0.12
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD2	1	0.12
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD3	1	0.12
(1,2550)	1:74:A:GLU:HG2	1:76:A:LYS:H	11	0.12
(1,2550)	1:74:A:GLU:HG3	1:76:A:LYS:H	11	0.12
(1,2549)	1:74:A:GLU:HB2	1:77:A:LYS:HB2	9	0.12
(1,2549)	1:74:A:GLU:HB2	1:77:A:LYS:HB3	9	0.12
(1,2549)	1:74:A:GLU:HB3	1:77:A:LYS:HB2	9	0.12
(1,2549)	1:74:A:GLU:HB3	1:77:A:LYS:HB3	9	0.12
(1,2548)	1:74:A:GLU:HB2	1:77:A:LYS:H	8	0.12
(1,2548)	1:74:A:GLU:HB3	1:77:A:LYS:H	8	0.12
(1,2548)	1:74:A:GLU:HB2	1:77:A:LYS:H	16	0.12
(1,2548)	1:74:A:GLU:HB3	1:77:A:LYS:H	16	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG11	10	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG12	10	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG13	10	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG21	10	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG22	10	0.12
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG23	10	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG11	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG12	1	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG13	1	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	1	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	1	0.12
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	1	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG11	1	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG12	1	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG13	1	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG21	1	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG22	1	0.12
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG23	1	0.12
(1,2504)	1:62:A:ILE:HG21	1:85:A:VAL:HG11	19	0.12
(1,2504)	1:62:A:ILE:HG21	1:85:A:VAL:HG12	19	0.12
(1,2504)	1:62:A:ILE:HG21	1:85:A:VAL:HG13	19	0.12
(1,2504)	1:62:A:ILE:HG21	1:85:A:VAL:HG21	19	0.12
(1,2504)	1:62:A:ILE:HG21	1:85:A:VAL:HG22	19	0.12
(1,2504)	1:62:A:ILE:HG21	1:85:A:VAL:HG23	19	0.12
(1,2504)	1:62:A:ILE:HG22	1:85:A:VAL:HG11	19	0.12
(1,2504)	1:62:A:ILE:HG22	1:85:A:VAL:HG12	19	0.12
(1,2504)	1:62:A:ILE:HG22	1:85:A:VAL:HG13	19	0.12
(1,2504)	1:62:A:ILE:HG22	1:85:A:VAL:HG21	19	0.12
(1,2504)	1:62:A:ILE:HG22	1:85:A:VAL:HG22	19	0.12
(1,2504)	1:62:A:ILE:HG22	1:85:A:VAL:HG23	19	0.12
(1,2504)	1:62:A:ILE:HG23	1:85:A:VAL:HG11	19	0.12
(1,2504)	1:62:A:ILE:HG23	1:85:A:VAL:HG12	19	0.12
(1,2504)	1:62:A:ILE:HG23	1:85:A:VAL:HG13	19	0.12
(1,2504)	1:62:A:ILE:HG23	1:85:A:VAL:HG21	19	0.12
(1,2504)	1:62:A:ILE:HG23	1:85:A:VAL:HG22	19	0.12
(1,2504)	1:62:A:ILE:HG23	1:85:A:VAL:HG23	19	0.12
(1,2493)	1:54:A:ILE:HG12	1:92:A:ARG:H	7	0.12
(1,2493)	1:54:A:ILE:HG13	1:92:A:ARG:H	7	0.12
(1,2464)	1:45:A:THR:HG21	1:49:A:TYR:HB2	18	0.12
(1,2464)	1:45:A:THR:HG21	1:49:A:TYR:HB3	18	0.12
(1,2464)	1:45:A:THR:HG22	1:49:A:TYR:HB2	18	0.12
(1,2464)	1:45:A:THR:HG22	1:49:A:TYR:HB3	18	0.12
(1,2464)	1:45:A:THR:HG23	1:49:A:TYR:HB2	18	0.12
(1,2464)	1:45:A:THR:HG23	1:49:A:TYR:HB3	18	0.12
(1,2459)	1:43:A:ASN:HD21	1:123:B:GLY:HA2	20	0.12
(1,2459)	1:43:A:ASN:HD21	1:123:B:GLY:HA3	20	0.12
(1,2459)	1:43:A:ASN:HD22	1:123:B:GLY:HA2	20	0.12
(1,2459)	1:43:A:ASN:HD22	1:123:B:GLY:HA3	20	0.12
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	1	0.12
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	4	0.12
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	4	0.12
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	4	0.12
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	4	0.12
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	4	0.12
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	4	0.12
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	15	0.12
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	15	0.12
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	15	0.12
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	15	0.12
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	15	0.12
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	15	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	3	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	3	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	3	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	3	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	3	0.12
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	3	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	4	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	4	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	4	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	4	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	4	0.12
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	4	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	9	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	9	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	9	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	9	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	9	0.12
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	9	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	12	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	12	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	12	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	12	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	12	0.12
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	12	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	15	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	15	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	15	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	15	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	15	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	17	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	17	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	17	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	17	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	17	0.12
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	17	0.12
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	19	0.12
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	19	0.12
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	19	0.12
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	19	0.12
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	19	0.12
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	19	0.12
(1,2410)	1:36:A:ARG:H	1:36:A:ARG:HG2	5	0.12
(1,2410)	1:36:A:ARG:H	1:36:A:ARG:HG3	5	0.12
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB2	8	0.12
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB3	8	0.12
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD2	5	0.12
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD3	5	0.12
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD2	5	0.12
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD3	5	0.12
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD2	9	0.12
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD3	9	0.12
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD2	9	0.12
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD3	9	0.12
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB2	6	0.12
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB3	6	0.12
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB2	6	0.12
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB3	6	0.12
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB2	6	0.12
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB3	6	0.12
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB2	6	0.12
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB3	6	0.12
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB2	6	0.12
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB3	6	0.12
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB2	6	0.12
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB3	6	0.12
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB2	14	0.12
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB3	14	0.12
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB2	14	0.12
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB3	14	0.12
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB3	14	0.12
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB2	14	0.12
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB3	14	0.12
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB2	14	0.12
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB3	14	0.12
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB2	14	0.12
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB3	14	0.12
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE21	13	0.12
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE22	13	0.12
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE21	13	0.12
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE22	13	0.12
(1,2377)	1:26:A:PRO:HD2	1:27:A:VAL:H	17	0.12
(1,2377)	1:26:A:PRO:HD3	1:27:A:VAL:H	17	0.12
(1,2375)	1:25:A:SER:HB2	1:27:A:VAL:H	7	0.12
(1,2375)	1:25:A:SER:HB3	1:27:A:VAL:H	7	0.12
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	6	0.12
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	6	0.12
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	6	0.12
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	6	0.12
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	6	0.12
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	6	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	16	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	16	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	16	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	16	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	16	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	16	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	20	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	20	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	20	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	20	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	20	0.12
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	20	0.12
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	19	0.12
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	19	0.12
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	19	0.12
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	19	0.12
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	19	0.12
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	19	0.12
(1,2309)	1:19:A:VAL:HG11	1:103:A:LEU:HB2	5	0.12
(1,2309)	1:19:A:VAL:HG12	1:103:A:LEU:HB2	5	0.12
(1,2309)	1:19:A:VAL:HG13	1:103:A:LEU:HB2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2309)	1:19:A:VAL:HG21	1:103:A:LEU:HB2	5	0.12
(1,2309)	1:19:A:VAL:HG22	1:103:A:LEU:HB2	5	0.12
(1,2309)	1:19:A:VAL:HG23	1:103:A:LEU:HB2	5	0.12
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB2	1	0.12
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB3	1	0.12
(1,2295)	1:15:A:ARG:HB2	1:16:A:ARG:H	1	0.12
(1,2295)	1:15:A:ARG:HB3	1:16:A:ARG:H	1	0.12
(1,2290)	1:14:A:ILE:HD11	1:99:A:LEU:HB2	11	0.12
(1,2290)	1:14:A:ILE:HD11	1:99:A:LEU:HB3	11	0.12
(1,2290)	1:14:A:ILE:HD12	1:99:A:LEU:HB2	11	0.12
(1,2290)	1:14:A:ILE:HD12	1:99:A:LEU:HB3	11	0.12
(1,2290)	1:14:A:ILE:HD13	1:99:A:LEU:HB2	11	0.12
(1,2290)	1:14:A:ILE:HD13	1:99:A:LEU:HB3	11	0.12
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD1	12	0.12
(1,2280)	1:73:A:ILE:HG12	1:78:A:TYR:HD2	12	0.12
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE1	12	0.12
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE2	12	0.12
(1,2269)	1:18:B:ASP:HA	1:105:B:TYR:HA	11	0.12
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE1	17	0.12
(1,2267)	1:73:B:ILE:HA	1:78:B:TYR:HE2	17	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	6	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	6	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	17	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	17	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	18	0.12
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	18	0.12
(1,2257)	1:104:B:THR:HA	1:105:B:TYR:HD1	11	0.12
(1,2257)	1:104:B:THR:HA	1:105:B:TYR:HD2	11	0.12
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE1	9	0.12
(1,2254)	1:73:B:ILE:HG21	1:78:B:TYR:HE2	9	0.12
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE1	9	0.12
(1,2254)	1:73:B:ILE:HG22	1:78:B:TYR:HE2	9	0.12
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE1	9	0.12
(1,2254)	1:73:B:ILE:HG23	1:78:B:TYR:HE2	9	0.12
(1,2243)	1:113:B:GLU:HA	1:116:B:ASN:H	1	0.12
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	6	0.12
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	6	0.12
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	6	0.12
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB1	19	0.12
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB2	19	0.12
(1,2219)	1:116:B:ASN:HD22	1:117:B:ALA:HB3	19	0.12
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2214)	1:43:A:ASN:H	1:122:B:LEU:HG	12	0.12
(1,2203)	1:120:B:ILE:HG13	1:125:B:ASN:HD22	18	0.12
(1,2200)	1:119:B:MET:HE1	1:125:B:ASN:HD22	12	0.12
(1,2200)	1:119:B:MET:HE2	1:125:B:ASN:HD22	12	0.12
(1,2200)	1:119:B:MET:HE3	1:125:B:ASN:HD22	12	0.12
(1,2199)	1:120:B:ILE:HG13	1:125:B:ASN:HD21	14	0.12
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG11	11	0.12
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG12	11	0.12
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG13	11	0.12
(1,2180)	1:23:B:ASP:H	1:100:B:LYS:H	7	0.12
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	9	0.12
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	9	0.12
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	9	0.12
(1,2152)	1:123:B:GLY:H	1:125:B:ASN:H	3	0.12
(1,2150)	1:119:B:MET:HE1	1:124:B:LEU:H	3	0.12
(1,2150)	1:119:B:MET:HE2	1:124:B:LEU:H	3	0.12
(1,2150)	1:119:B:MET:HE3	1:124:B:LEU:H	3	0.12
(1,2150)	1:119:B:MET:HE1	1:124:B:LEU:H	7	0.12
(1,2150)	1:119:B:MET:HE2	1:124:B:LEU:H	7	0.12
(1,2150)	1:119:B:MET:HE3	1:124:B:LEU:H	7	0.12
(1,2150)	1:119:B:MET:HE1	1:124:B:LEU:H	16	0.12
(1,2150)	1:119:B:MET:HE2	1:124:B:LEU:H	16	0.12
(1,2150)	1:119:B:MET:HE3	1:124:B:LEU:H	16	0.12
(1,2150)	1:119:B:MET:HE1	1:124:B:LEU:H	19	0.12
(1,2150)	1:119:B:MET:HE2	1:124:B:LEU:H	19	0.12
(1,2150)	1:119:B:MET:HE3	1:124:B:LEU:H	19	0.12
(1,2149)	1:119:B:MET:HA	1:124:B:LEU:H	17	0.12
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	6	0.12
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	6	0.12
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	6	0.12
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	17	0.12
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	17	0.12
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	17	0.12
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	14	0.12
(1,2142)	1:44:A:ASP:H	1:123:B:GLY:H	20	0.12
(1,2111)	1:111:B:MET:HG3	1:112:B:LYS:H	2	0.12
(1,2107)	1:112:B:LYS:H	1:115:B:ASP:H	5	0.12
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	8	0.12
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	4	0.12
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	6	0.12
(1,2088)	1:103:B:LEU:HD11	1:104:B:THR:H	1	0.12
(1,2088)	1:103:B:LEU:HD12	1:104:B:THR:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2088)	1:103:B:LEU:HD13	1:104:B:THR:H	1	0.12
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	1	0.12
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	14	0.12
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	16	0.12
(1,2072)	1:99:A:LEU:HD21	1:100:A:LYS:H	3	0.12
(1,2072)	1:99:A:LEU:HD22	1:100:A:LYS:H	3	0.12
(1,2072)	1:99:A:LEU:HD23	1:100:A:LYS:H	3	0.12
(1,2072)	1:99:A:LEU:HD21	1:100:A:LYS:H	7	0.12
(1,2072)	1:99:A:LEU:HD22	1:100:A:LYS:H	7	0.12
(1,2072)	1:99:A:LEU:HD23	1:100:A:LYS:H	7	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	2	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	2	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	2	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	5	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	5	0.12
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	5	0.12
(1,2043)	1:93:A:THR:HG1	1:91:B:ILE:H	20	0.12
(1,2030)	1:58:B:ILE:H	1:87:B:LEU:H	8	0.12
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	7	0.12
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	7	0.12
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	7	0.12
(1,2011)	1:80:B:LEU:HD11	1:82:B:LYS:H	3	0.12
(1,2011)	1:80:B:LEU:HD12	1:82:B:LYS:H	3	0.12
(1,2011)	1:80:B:LEU:HD13	1:82:B:LYS:H	3	0.12
(1,2010)	1:80:B:LEU:HD11	1:81:B:ASP:H	4	0.12
(1,2010)	1:80:B:LEU:HD12	1:81:B:ASP:H	4	0.12
(1,2010)	1:80:B:LEU:HD13	1:81:B:ASP:H	4	0.12
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	1	0.12
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	1	0.12
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	1	0.12
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	10	0.12
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	10	0.12
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	10	0.12
(1,1988)	1:61:A:ARG:H	1:61:A:ARG:HG2	19	0.12
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	10	0.12
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	10	0.12
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	10	0.12
(1,1966)	1:53:B:VAL:HG11	1:54:B:ILE:H	17	0.12
(1,1966)	1:53:B:VAL:HG12	1:54:B:ILE:H	17	0.12
(1,1966)	1:53:B:VAL:HG13	1:54:B:ILE:H	17	0.12
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	8	0.12
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	7	0.12
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	8	0.12
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	16	0.12
(1,1903)	1:27:B:VAL:HG21	1:34:B:GLY:H	9	0.12
(1,1903)	1:27:B:VAL:HG22	1:34:B:GLY:H	9	0.12
(1,1903)	1:27:B:VAL:HG23	1:34:B:GLY:H	9	0.12
(1,1900)	1:27:B:VAL:HG11	1:33:B:GLY:H	5	0.12
(1,1900)	1:27:B:VAL:HG12	1:33:B:GLY:H	5	0.12
(1,1900)	1:27:B:VAL:HG13	1:33:B:GLY:H	5	0.12
(1,1898)	1:32:B:GLN:HG2	1:33:B:GLY:H	4	0.12
(1,1897)	1:24:B:LEU:HD21	1:32:B:GLN:H	19	0.12
(1,1897)	1:24:B:LEU:HD22	1:32:B:GLN:H	19	0.12
(1,1897)	1:24:B:LEU:HD23	1:32:B:GLN:H	19	0.12
(1,1891)	1:28:B:GLN:HA	1:31:B:GLU:H	2	0.12
(1,1888)	1:95:A:ASP:H	1:31:B:GLU:H	8	0.12
(1,1825)	1:18:B:ASP:H	1:19:B:VAL:H	14	0.12
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	16	0.12
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	17	0.12
(1,1814)	1:87:B:LEU:HD11	1:88:B:LEU:H	18	0.12
(1,1814)	1:87:B:LEU:HD12	1:88:B:LEU:H	18	0.12
(1,1814)	1:87:B:LEU:HD13	1:88:B:LEU:H	18	0.12
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG21	3	0.12
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG22	3	0.12
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG23	3	0.12
(1,1767)	1:96:A:LYS:HB2	1:97:A:LYS:H	17	0.12
(1,1764)	1:96:A:LYS:HB3	1:97:A:LYS:H	20	0.12
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	6	0.12
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	6	0.12
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	6	0.12
(1,1742)	1:42:B:GLN:HE22	1:43:B:ASN:H	11	0.12
(1,1742)	1:42:B:GLN:HE22	1:43:B:ASN:H	16	0.12
(1,1741)	1:24:B:LEU:H	1:24:B:LEU:HD21	11	0.12
(1,1741)	1:24:B:LEU:H	1:24:B:LEU:HD22	11	0.12
(1,1741)	1:24:B:LEU:H	1:24:B:LEU:HD23	11	0.12
(1,1734)	1:90:A:GLN:HB3	1:90:A:GLN:HE22	3	0.12
(1,1729)	1:91:B:ILE:H	1:91:B:ILE:HG13	14	0.12
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	13	0.12
(1,1710)	1:127:B:VAL:HA	1:128:B:ALA:H	4	0.12
(1,1710)	1:127:B:VAL:HA	1:128:B:ALA:H	7	0.12
(1,1707)	1:127:B:VAL:HB	1:128:B:ALA:H	16	0.12
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	2	0.12
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	14	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	4	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	4	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	4	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	19	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	19	0.12
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	19	0.12
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD21	16	0.12
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD22	16	0.12
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD23	16	0.12
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	2	0.12
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	11	0.12
(1,1594)	1:94:B:LEU:HB3	1:95:B:ASP:H	18	0.12
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	12	0.12
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	20	0.12
(1,1553)	1:126:B:ALA:HB1	1:127:B:VAL:H	9	0.12
(1,1553)	1:126:B:ALA:HB2	1:127:B:VAL:H	9	0.12
(1,1553)	1:126:B:ALA:HB3	1:127:B:VAL:H	9	0.12
(1,1553)	1:126:B:ALA:HB1	1:127:B:VAL:H	12	0.12
(1,1553)	1:126:B:ALA:HB2	1:127:B:VAL:H	12	0.12
(1,1553)	1:126:B:ALA:HB3	1:127:B:VAL:H	12	0.12
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	7	0.12
(1,1552)	1:126:B:ALA:HA	1:127:B:VAL:H	10	0.12
(1,1537)	1:103:B:LEU:H	1:103:B:LEU:HG	11	0.12
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	1	0.12
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	2	0.12
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	9	0.12
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	10	0.12
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	12	0.12
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	15	0.12
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	17	0.12
(1,1508)	1:19:B:VAL:H	1:20:B:TYR:H	10	0.12
(1,1506)	1:20:B:TYR:H	1:21:B:LEU:H	11	0.12
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	11	0.12
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	11	0.12
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	14	0.12
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	14	0.12
(1,1497)	1:47:B:ASN:HA	1:48:B:LYS:H	19	0.12
(1,1489)	1:115:B:ASP:HB3	1:116:B:ASN:H	17	0.12
(1,1489)	1:115:B:ASP:HB3	1:116:B:ASN:H	18	0.12
(1,1486)	1:120:B:ILE:H	1:120:B:ILE:HG21	1	0.12
(1,1486)	1:120:B:ILE:H	1:120:B:ILE:HG22	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1486)	1:120:B:ILE:H	1:120:B:ILE:HG23	1	0.12
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	6	0.12
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	2	0.12
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	2	0.12
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	2	0.12
(1,1462)	1:82:B:LYS:H	1:82:B:LYS:HB2	16	0.12
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	18	0.12
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	8	0.12
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	10	0.12
(1,1423)	1:28:B:GLN:HB2	1:28:B:GLN:HE22	12	0.12
(1,1395)	1:119:B:MET:HB2	1:119:B:MET:HE1	9	0.12
(1,1395)	1:119:B:MET:HB2	1:119:B:MET:HE2	9	0.12
(1,1395)	1:119:B:MET:HB2	1:119:B:MET:HE3	9	0.12
(1,1388)	1:52:B:THR:HG21	1:95:B:ASP:HA	4	0.12
(1,1388)	1:52:B:THR:HG22	1:95:B:ASP:HA	4	0.12
(1,1388)	1:52:B:THR:HG23	1:95:B:ASP:HA	4	0.12
(1,1388)	1:52:B:THR:HG21	1:95:B:ASP:HA	11	0.12
(1,1388)	1:52:B:THR:HG22	1:95:B:ASP:HA	11	0.12
(1,1388)	1:52:B:THR:HG23	1:95:B:ASP:HA	11	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	4	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	4	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	4	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	4	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	4	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	4	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	4	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	4	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	4	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	15	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	15	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	15	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	15	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	15	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	15	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	15	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	15	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	15	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	17	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	17	0.12
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	17	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	17	0.12
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	17	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	17	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	17	0.12
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	17	0.12
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD21	11	0.12
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD22	11	0.12
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD23	11	0.12
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD21	11	0.12
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD22	11	0.12
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD23	11	0.12
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD21	11	0.12
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD22	11	0.12
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD23	11	0.12
(1,1362)	1:91:A:ILE:HD11	1:93:B:THR:HG21	8	0.12
(1,1362)	1:91:A:ILE:HD11	1:93:B:THR:HG22	8	0.12
(1,1362)	1:91:A:ILE:HD11	1:93:B:THR:HG23	8	0.12
(1,1362)	1:91:A:ILE:HD12	1:93:B:THR:HG21	8	0.12
(1,1362)	1:91:A:ILE:HD12	1:93:B:THR:HG22	8	0.12
(1,1362)	1:91:A:ILE:HD12	1:93:B:THR:HG23	8	0.12
(1,1362)	1:91:A:ILE:HD13	1:93:B:THR:HG21	8	0.12
(1,1362)	1:91:A:ILE:HD13	1:93:B:THR:HG22	8	0.12
(1,1362)	1:91:A:ILE:HD13	1:93:B:THR:HG23	8	0.12
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	4	0.12
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	6	0.12
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG11	1	0.12
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG12	1	0.12
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG13	1	0.12
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG11	11	0.12
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG12	11	0.12
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG13	11	0.12
(1,1350)	1:19:B:VAL:HG21	1:105:B:TYR:HA	10	0.12
(1,1350)	1:19:B:VAL:HG22	1:105:B:TYR:HA	10	0.12
(1,1350)	1:19:B:VAL:HG23	1:105:B:TYR:HA	10	0.12
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG21	4	0.12
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG22	4	0.12
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG23	4	0.12
(1,1342)	1:91:A:ILE:HG21	1:93:B:THR:HB	13	0.12
(1,1342)	1:91:A:ILE:HG22	1:93:B:THR:HB	13	0.12
(1,1342)	1:91:A:ILE:HG23	1:93:B:THR:HB	13	0.12
(1,1312)	1:112:A:LYS:HA	1:115:A:ASP:HB2	10	0.12
(1,1295)	1:27:B:VAL:HG11	1:33:B:GLY:HA2	7	0.12
(1,1295)	1:27:B:VAL:HG12	1:33:B:GLY:HA2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:27:B:VAL:HG13	1:33:B:GLY:HA2	7	0.12
(1,1273)	1:24:B:LEU:HD11	1:32:B:GLN:HG3	10	0.12
(1,1273)	1:24:B:LEU:HD12	1:32:B:GLN:HG3	10	0.12
(1,1273)	1:24:B:LEU:HD13	1:32:B:GLN:HG3	10	0.12
(1,1266)	1:19:A:VAL:HG11	1:37:A:PRO:HB3	7	0.12
(1,1266)	1:19:A:VAL:HG12	1:37:A:PRO:HB3	7	0.12
(1,1266)	1:19:A:VAL:HG13	1:37:A:PRO:HB3	7	0.12
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD21	20	0.12
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD22	20	0.12
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD23	20	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD21	15	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD22	15	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD23	15	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD21	19	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD22	19	0.12
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD23	19	0.12
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD21	10	0.12
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD22	10	0.12
(1,1251)	1:119:B:MET:HA	1:124:B:LEU:HD23	10	0.12
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	13	0.12
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	13	0.12
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	13	0.12
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD11	17	0.12
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD12	17	0.12
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD13	17	0.12
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	6	0.12
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	6	0.12
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	6	0.12
(1,1217)	1:45:B:THR:HG21	1:49:B:TYR:HA	7	0.12
(1,1217)	1:45:B:THR:HG22	1:49:B:TYR:HA	7	0.12
(1,1217)	1:45:B:THR:HG23	1:49:B:TYR:HA	7	0.12
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	13	0.12
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	13	0.12
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	13	0.12
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	19	0.12
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	19	0.12
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	19	0.12
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	1	0.12
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	1	0.12
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	1	0.12
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB1	17	0.12
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB2	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1188)	1:69:B:THR:HG21	1:117:B:ALA:HB3	17	0.12
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB1	17	0.12
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB2	17	0.12
(1,1188)	1:69:B:THR:HG22	1:117:B:ALA:HB3	17	0.12
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB1	17	0.12
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB2	17	0.12
(1,1188)	1:69:B:THR:HG23	1:117:B:ALA:HB3	17	0.12
(1,1169)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	8	0.12
(1,1169)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	8	0.12
(1,1169)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	8	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	6	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	6	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	6	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	12	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	12	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	12	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	18	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	18	0.12
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	18	0.12
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	4	0.12
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	4	0.12
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	4	0.12
(1,1145)	1:27:A:VAL:HG21	1:33:A:GLY:HA3	10	0.12
(1,1145)	1:27:A:VAL:HG22	1:33:A:GLY:HA3	10	0.12
(1,1145)	1:27:A:VAL:HG23	1:33:A:GLY:HA3	10	0.12
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	12	0.12
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	12	0.12
(1,1119)	1:18:A:ASP:HB3	1:20:A:TYR:HE1	12	0.12
(1,1119)	1:18:A:ASP:HB3	1:20:A:TYR:HE2	12	0.12
(1,1118)	1:18:A:ASP:H	1:20:A:TYR:HE1	14	0.12
(1,1118)	1:18:A:ASP:H	1:20:A:TYR:HE2	14	0.12
(1,1118)	1:18:A:ASP:H	1:20:A:TYR:HE1	20	0.12
(1,1118)	1:18:A:ASP:H	1:20:A:TYR:HE2	20	0.12
(1,1116)	1:18:A:ASP:HA	1:105:A:TYR:HA	11	0.12
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE1	17	0.12
(1,1114)	1:73:A:ILE:HA	1:78:A:TYR:HE2	17	0.12
(1,1104)	1:104:A:THR:HA	1:105:A:TYR:HD1	11	0.12
(1,1104)	1:104:A:THR:HA	1:105:A:TYR:HD2	11	0.12
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	5	0.12
(1,1083)	1:76:A:LYS:H	1:80:A:LEU:H	9	0.12
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	4	0.12
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB1	3	0.12
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB2	3	0.12
(1,1067)	1:116:A:ASN:HD22	1:117:A:ALA:HB3	3	0.12
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	7	0.12
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	12	0.12
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	13	0.12
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	13	0.12
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	13	0.12
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG11	11	0.12
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG12	11	0.12
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG13	11	0.12
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG11	18	0.12
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG12	18	0.12
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG13	18	0.12
(1,1034)	1:23:A:ASP:H	1:100:A:LYS:H	7	0.12
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG21	9	0.12
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG22	9	0.12
(1,1029)	1:42:A:GLN:HE21	1:54:A:ILE:HG23	9	0.12
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	18	0.12
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	18	0.12
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	18	0.12
(1,1004)	1:119:A:MET:HE1	1:124:A:LEU:H	16	0.12
(1,1004)	1:119:A:MET:HE2	1:124:A:LEU:H	16	0.12
(1,1004)	1:119:A:MET:HE3	1:124:A:LEU:H	16	0.12
(1,1003)	1:119:A:MET:HA	1:124:A:LEU:H	18	0.12
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	6	0.12
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	6	0.12
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	6	0.12
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	9	0.12
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	9	0.12
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	9	0.12
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	10	0.12
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	13	0.12
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	20	0.12
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	2	0.12
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	2	0.12
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	2	0.12
(1,990)	1:117:A:ALA:HA	1:120:A:ILE:H	14	0.12
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	2	0.12
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	8	0.12
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	12	0.12
(1,958)	1:110:B:LYS:H	1:110:B:LYS:HE3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	3	0.12
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	11	0.12
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	14	0.12
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	6	0.12
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	12	0.12
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	3	0.12
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	15	0.12
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	16	0.12
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	18	0.12
(1,926)	1:99:B:LEU:HD21	1:100:B:LYS:H	3	0.12
(1,926)	1:99:B:LEU:HD22	1:100:B:LYS:H	3	0.12
(1,926)	1:99:B:LEU:HD23	1:100:B:LYS:H	3	0.12
(1,926)	1:99:B:LEU:HD21	1:100:B:LYS:H	16	0.12
(1,926)	1:99:B:LEU:HD22	1:100:B:LYS:H	16	0.12
(1,926)	1:99:B:LEU:HD23	1:100:B:LYS:H	16	0.12
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	2	0.12
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	2	0.12
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	2	0.12
(1,897)	1:91:A:ILE:H	1:93:B:THR:HG1	20	0.12
(1,884)	1:58:A:ILE:H	1:87:A:LEU:H	8	0.12
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	7	0.12
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	7	0.12
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	7	0.12
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	8	0.12
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	8	0.12
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	8	0.12
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	11	0.12
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	11	0.12
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	11	0.12
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	14	0.12
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	14	0.12
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	14	0.12
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	20	0.12
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	20	0.12
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	20	0.12
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	9	0.12
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	14	0.12
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	18	0.12
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	17	0.12
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	17	0.12
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	17	0.12
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	7	0.12
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	8	0.12
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	18	0.12
(1,765)	1:35:A:VAL:HG11	1:36:A:ARG:H	1	0.12
(1,765)	1:35:A:VAL:HG12	1:36:A:ARG:H	1	0.12
(1,765)	1:35:A:VAL:HG13	1:36:A:ARG:H	1	0.12
(1,751)	1:24:A:LEU:HD21	1:32:A:GLN:H	19	0.12
(1,751)	1:24:A:LEU:HD22	1:32:A:GLN:H	19	0.12
(1,751)	1:24:A:LEU:HD23	1:32:A:GLN:H	19	0.12
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	8	0.12
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	10	0.12
(1,704)	1:16:A:ARG:H	1:47:A:ASN:HD21	6	0.12
(1,681)	1:18:A:ASP:H	1:19:A:VAL:H	14	0.12
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	17	0.12
(1,672)	1:87:A:LEU:HD11	1:88:A:LEU:H	18	0.12
(1,672)	1:87:A:LEU:HD12	1:88:A:LEU:H	18	0.12
(1,672)	1:87:A:LEU:HD13	1:88:A:LEU:H	18	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG21	3	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG22	3	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG23	3	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG21	16	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG22	16	0.12
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG23	16	0.12
(1,625)	1:96:B:LYS:HB2	1:97:B:LYS:H	3	0.12
(1,625)	1:96:B:LYS:HB2	1:97:B:LYS:H	17	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	3	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	3	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	3	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	11	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	11	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	11	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	12	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	12	0.12
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	12	0.12
(1,600)	1:42:A:GLN:HE22	1:43:A:ASN:H	11	0.12
(1,600)	1:42:A:GLN:HE22	1:43:A:ASN:H	17	0.12
(1,599)	1:24:A:LEU:H	1:24:A:LEU:HD21	11	0.12
(1,599)	1:24:A:LEU:H	1:24:A:LEU:HD22	11	0.12
(1,599)	1:24:A:LEU:H	1:24:A:LEU:HD23	11	0.12
(1,582)	1:116:A:ASN:HA	1:116:A:ASN:HD21	15	0.12
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	1	0.12
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,567)	1:127:A:VAL:HA	1:128:A:ALA:H	4	0.12
(1,567)	1:127:A:VAL:HA	1:128:A:ALA:H	7	0.12
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	2	0.12
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	6	0.12
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	13	0.12
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	20	0.12
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG11	2	0.12
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG12	2	0.12
(1,539)	1:35:A:VAL:H	1:35:A:VAL:HG13	2	0.12
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	4	0.12
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	4	0.12
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	4	0.12
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	7	0.12
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	7	0.12
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	7	0.12
(1,534)	1:124:A:LEU:H	1:124:A:LEU:HG	10	0.12
(1,534)	1:124:A:LEU:H	1:124:A:LEU:HG	17	0.12
(1,530)	1:76:A:LYS:H	1:76:A:LYS:HB2	15	0.12
(1,478)	1:111:A:MET:H	1:111:A:MET:HE1	13	0.12
(1,478)	1:111:A:MET:H	1:111:A:MET:HE2	13	0.12
(1,478)	1:111:A:MET:H	1:111:A:MET:HE3	13	0.12
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	2	0.12
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	11	0.12
(1,457)	1:94:A:LEU:HB3	1:95:A:ASP:H	18	0.12
(1,455)	1:105:A:TYR:H	1:106:A:LEU:H	3	0.12
(1,455)	1:105:A:TYR:H	1:106:A:LEU:H	4	0.12
(1,418)	1:126:A:ALA:HB1	1:127:A:VAL:H	9	0.12
(1,418)	1:126:A:ALA:HB2	1:127:A:VAL:H	9	0.12
(1,418)	1:126:A:ALA:HB3	1:127:A:VAL:H	9	0.12
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	1	0.12
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	8	0.12
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	13	0.12
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	19	0.12
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	12	0.12
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	12	0.12
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	12	0.12
(1,371)	1:20:A:TYR:H	1:21:A:LEU:H	5	0.12
(1,371)	1:20:A:TYR:H	1:21:A:LEU:H	9	0.12
(1,371)	1:20:A:TYR:H	1:21:A:LEU:H	11	0.12
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	14	0.12
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	14	0.12
(1,363)	1:48:A:LYS:H	1:48:A:LYS:HD2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,362)	1:47:A:ASN:HA	1:48:A:LYS:H	19	0.12
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	11	0.12
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	14	0.12
(1,355)	1:115:A:ASP:HB3	1:116:A:ASN:H	18	0.12
(1,353)	1:125:A:ASN:H	1:125:A:ASN:HD22	9	0.12
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	2	0.12
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	6	0.12
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	7	0.12
(1,338)	1:80:A:LEU:H	1:80:A:LEU:HB3	4	0.12
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	19	0.12
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	19	0.12
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	19	0.12
(1,329)	1:82:A:LYS:H	1:82:A:LYS:HB2	16	0.12
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	9	0.12
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	1	0.12
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	2	0.12
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	7	0.12
(1,294)	1:28:A:GLN:HB2	1:28:A:GLN:HE22	8	0.12
(1,274)	1:27:A:VAL:HG11	1:28:A:GLN:HG2	5	0.12
(1,274)	1:27:A:VAL:HG12	1:28:A:GLN:HG2	5	0.12
(1,274)	1:27:A:VAL:HG13	1:28:A:GLN:HG2	5	0.12
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB1	17	0.12
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB2	17	0.12
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB3	17	0.12
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB1	17	0.12
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB2	17	0.12
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB3	17	0.12
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB1	17	0.12
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB2	17	0.12
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB3	17	0.12
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	2	0.12
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	2	0.12
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	2	0.12
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	2	0.12
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	2	0.12
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	2	0.12
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	2	0.12
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	2	0.12
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	2	0.12
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	6	0.12
(1,230)	1:20:A:TYR:HA	1:102:A:LYS:HA	19	0.12
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG11	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG12	1	0.12
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG13	1	0.12
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG11	19	0.12
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG12	19	0.12
(1,219)	1:25:B:SER:HA	1:27:B:VAL:HG13	19	0.12
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG21	13	0.12
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG22	13	0.12
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG23	13	0.12
(1,214)	1:58:A:ILE:HG21	1:84:A:SER:HB3	3	0.12
(1,214)	1:58:A:ILE:HG22	1:84:A:SER:HB3	3	0.12
(1,214)	1:58:A:ILE:HG23	1:84:A:SER:HB3	3	0.12
(1,186)	1:112:B:LYS:HA	1:115:B:ASP:HB2	10	0.12
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD11	8	0.12
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD12	8	0.12
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD13	8	0.12
(1,169)	1:27:A:VAL:HG11	1:33:A:GLY:HA2	7	0.12
(1,169)	1:27:A:VAL:HG12	1:33:A:GLY:HA2	7	0.12
(1,169)	1:27:A:VAL:HG13	1:33:A:GLY:HA2	7	0.12
(1,140)	1:19:B:VAL:HG11	1:37:B:PRO:HB3	7	0.12
(1,140)	1:19:B:VAL:HG12	1:37:B:PRO:HB3	7	0.12
(1,140)	1:19:B:VAL:HG13	1:37:B:PRO:HB3	7	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD21	16	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD22	16	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD23	16	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD21	19	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD22	19	0.12
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD23	19	0.12
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	10	0.12
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	10	0.12
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	10	0.12
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD21	18	0.12
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD22	18	0.12
(1,126)	1:119:A:MET:HA	1:124:A:LEU:HD23	18	0.12
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	19	0.12
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	19	0.12
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	19	0.12
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG21	9	0.12
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG22	9	0.12
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG23	9	0.12
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG21	9	0.12
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG22	9	0.12
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG23	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG21	9	0.12
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG22	9	0.12
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG23	9	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD11	16	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD12	16	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD13	16	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD11	17	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD12	17	0.12
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD13	17	0.12
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	13	0.12
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	13	0.12
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	13	0.12
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	14	0.12
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	14	0.12
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	14	0.12
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	18	0.12
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	18	0.12
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	18	0.12
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD11	13	0.12
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD12	13	0.12
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD13	13	0.12
(1,43)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	8	0.12
(1,43)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	8	0.12
(1,43)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	8	0.12
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	6	0.12
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	6	0.12
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	6	0.12
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	19	0.12
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	19	0.12
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	19	0.12
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG21	17	0.12
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG22	17	0.12
(1,28)	1:103:A:LEU:HG	1:104:A:THR:HG23	17	0.12
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG11	4	0.12
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG12	4	0.12
(1,21)	1:40:A:ILE:HG13	1:55:A:VAL:HG13	4	0.12
(1,19)	1:27:B:VAL:HG21	1:33:B:GLY:HA3	7	0.12
(1,19)	1:27:B:VAL:HG22	1:33:B:GLY:HA3	7	0.12
(1,19)	1:27:B:VAL:HG23	1:33:B:GLY:HA3	7	0.12
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD11	7	0.11
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD12	7	0.11
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD13	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD21	7	0.11
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD22	7	0.11
(1,3241)	1:119:B:MET:HE1	1:124:B:LEU:HD23	7	0.11
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD11	7	0.11
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD12	7	0.11
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD13	7	0.11
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD21	7	0.11
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD22	7	0.11
(1,3241)	1:119:B:MET:HE2	1:124:B:LEU:HD23	7	0.11
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD11	7	0.11
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD12	7	0.11
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD13	7	0.11
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD21	7	0.11
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD22	7	0.11
(1,3241)	1:119:B:MET:HE3	1:124:B:LEU:HD23	7	0.11
(1,3240)	1:119:B:MET:HE1	1:124:B:LEU:HB2	20	0.11
(1,3240)	1:119:B:MET:HE1	1:124:B:LEU:HB3	20	0.11
(1,3240)	1:119:B:MET:HE2	1:124:B:LEU:HB2	20	0.11
(1,3240)	1:119:B:MET:HE2	1:124:B:LEU:HB3	20	0.11
(1,3240)	1:119:B:MET:HE3	1:124:B:LEU:HB2	20	0.11
(1,3240)	1:119:B:MET:HE3	1:124:B:LEU:HB3	20	0.11
(1,3234)	1:119:B:MET:HA	1:124:B:LEU:HB2	8	0.11
(1,3234)	1:119:B:MET:HA	1:124:B:LEU:HB3	8	0.11
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	20	0.11
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	20	0.11
(1,3141)	1:98:B:ARG:HB2	1:99:B:LEU:H	18	0.11
(1,3141)	1:98:B:ARG:HB3	1:99:B:LEU:H	18	0.11
(1,3124)	1:93:B:THR:H	1:94:B:LEU:HD11	17	0.11
(1,3124)	1:93:B:THR:H	1:94:B:LEU:HD12	17	0.11
(1,3124)	1:93:B:THR:H	1:94:B:LEU:HD13	17	0.11
(1,3124)	1:93:B:THR:H	1:94:B:LEU:HD21	17	0.11
(1,3124)	1:93:B:THR:H	1:94:B:LEU:HD22	17	0.11
(1,3124)	1:93:B:THR:H	1:94:B:LEU:HD23	17	0.11
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	16	0.11
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	16	0.11
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	16	0.11
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	16	0.11
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	16	0.11
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	16	0.11
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	16	0.11
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	16	0.11
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	16	0.11
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	16	0.11
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	16	0.11
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	3	0.11
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	3	0.11
(1,3110)	1:87:B:LEU:HD11	1:90:B:GLN:HB3	3	0.11
(1,3110)	1:87:B:LEU:HD12	1:90:B:GLN:HB3	3	0.11
(1,3110)	1:87:B:LEU:HD13	1:90:B:GLN:HB3	3	0.11
(1,3110)	1:87:B:LEU:HD21	1:90:B:GLN:HB3	3	0.11
(1,3110)	1:87:B:LEU:HD22	1:90:B:GLN:HB3	3	0.11
(1,3110)	1:87:B:LEU:HD23	1:90:B:GLN:HB3	3	0.11
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE2	14	0.11
(1,3094)	1:82:B:LYS:HB2	1:82:B:LYS:HE3	14	0.11
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE2	14	0.11
(1,3094)	1:82:B:LYS:HB3	1:82:B:LYS:HE3	14	0.11
(1,3070)	1:77:B:LYS:H	1:77:B:LYS:HG2	10	0.11
(1,3070)	1:77:B:LYS:H	1:77:B:LYS:HG3	10	0.11
(1,3039)	1:73:B:ILE:HG21	1:78:B:TYR:HB2	14	0.11
(1,3039)	1:73:B:ILE:HG21	1:78:B:TYR:HB3	14	0.11
(1,3039)	1:73:B:ILE:HG22	1:78:B:TYR:HB2	14	0.11
(1,3039)	1:73:B:ILE:HG22	1:78:B:TYR:HB3	14	0.11
(1,3039)	1:73:B:ILE:HG23	1:78:B:TYR:HB2	14	0.11
(1,3039)	1:73:B:ILE:HG23	1:78:B:TYR:HB3	14	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG11	6	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG12	6	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG13	6	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG21	6	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG22	6	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG23	6	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG11	15	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG12	15	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG13	15	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG21	15	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG22	15	0.11
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG23	15	0.11
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG11	7	0.11
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG12	7	0.11
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG13	7	0.11
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG21	7	0.11
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG22	7	0.11
(1,3035)	1:72:B:GLU:HG2	1:85:B:VAL:HG23	7	0.11
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG11	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG12	7	0.11
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG13	7	0.11
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG21	7	0.11
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG22	7	0.11
(1,3035)	1:72:B:GLU:HG3	1:85:B:VAL:HG23	7	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG12	5	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	5	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG12	5	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	5	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG12	5	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	5	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG12	9	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	9	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG12	9	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	9	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG12	9	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	9	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG12	20	0.11
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	20	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG12	20	0.11
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	20	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG12	20	0.11
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	20	0.11
(1,2984)	1:53:B:VAL:HG11	1:98:B:ARG:H	11	0.11
(1,2984)	1:53:B:VAL:HG12	1:98:B:ARG:H	11	0.11
(1,2984)	1:53:B:VAL:HG13	1:98:B:ARG:H	11	0.11
(1,2984)	1:53:B:VAL:HG21	1:98:B:ARG:H	11	0.11
(1,2984)	1:53:B:VAL:HG22	1:98:B:ARG:H	11	0.11
(1,2984)	1:53:B:VAL:HG23	1:98:B:ARG:H	11	0.11
(1,2982)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	7	0.11
(1,2982)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	7	0.11
(1,2982)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	7	0.11
(1,2982)	1:53:B:VAL:HG21	1:94:B:LEU:HB2	7	0.11
(1,2982)	1:53:B:VAL:HG22	1:94:B:LEU:HB2	7	0.11
(1,2982)	1:53:B:VAL:HG23	1:94:B:LEU:HB2	7	0.11
(1,2982)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	10	0.11
(1,2982)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	10	0.11
(1,2982)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	10	0.11
(1,2982)	1:53:B:VAL:HG21	1:94:B:LEU:HB2	10	0.11
(1,2982)	1:53:B:VAL:HG22	1:94:B:LEU:HB2	10	0.11
(1,2982)	1:53:B:VAL:HG23	1:94:B:LEU:HB2	10	0.11
(1,2982)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2982)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	13	0.11
(1,2982)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	13	0.11
(1,2982)	1:53:B:VAL:HG21	1:94:B:LEU:HB2	13	0.11
(1,2982)	1:53:B:VAL:HG22	1:94:B:LEU:HB2	13	0.11
(1,2982)	1:53:B:VAL:HG23	1:94:B:LEU:HB2	13	0.11
(1,2960)	1:45:B:THR:HG21	1:48:B:LYS:HG2	19	0.11
(1,2960)	1:45:B:THR:HG21	1:48:B:LYS:HG3	19	0.11
(1,2960)	1:45:B:THR:HG22	1:48:B:LYS:HG2	19	0.11
(1,2960)	1:45:B:THR:HG22	1:48:B:LYS:HG3	19	0.11
(1,2960)	1:45:B:THR:HG23	1:48:B:LYS:HG2	19	0.11
(1,2960)	1:45:B:THR:HG23	1:48:B:LYS:HG3	19	0.11
(1,2949)	1:43:B:ASN:HB2	1:44:B:ASP:H	17	0.11
(1,2949)	1:43:B:ASN:HB3	1:44:B:ASP:H	17	0.11
(1,2949)	1:43:B:ASN:HB2	1:44:B:ASP:H	19	0.11
(1,2949)	1:43:B:ASN:HB3	1:44:B:ASP:H	19	0.11
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	13	0.11
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	13	0.11
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	13	0.11
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	13	0.11
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	13	0.11
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	13	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD11	10	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD12	10	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD13	10	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD21	10	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD22	10	0.11
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD23	10	0.11
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	2	0.11
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	2	0.11
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	2	0.11
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	2	0.11
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	2	0.11
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	2	0.11
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	7	0.11
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	7	0.11
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	7	0.11
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	7	0.11
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	7	0.11
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	7	0.11
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	11	0.11
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	11	0.11
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	11	0.11
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	11	0.11
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	11	0.11
(1,2918)	1:38:B:VAL:HG11	1:57:B:ALA:H	17	0.11
(1,2918)	1:38:B:VAL:HG12	1:57:B:ALA:H	17	0.11
(1,2918)	1:38:B:VAL:HG13	1:57:B:ALA:H	17	0.11
(1,2918)	1:38:B:VAL:HG21	1:57:B:ALA:H	17	0.11
(1,2918)	1:38:B:VAL:HG22	1:57:B:ALA:H	17	0.11
(1,2918)	1:38:B:VAL:HG23	1:57:B:ALA:H	17	0.11
(1,2912)	1:36:B:ARG:H	1:36:B:ARG:HG2	5	0.11
(1,2912)	1:36:B:ARG:H	1:36:B:ARG:HG3	5	0.11
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB2	14	0.11
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB3	14	0.11
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB2	14	0.11
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB3	14	0.11
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB2	14	0.11
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB3	14	0.11
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB2	14	0.11
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB3	14	0.11
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB2	14	0.11
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB3	14	0.11
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB2	14	0.11
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB3	14	0.11
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	18	0.11
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	18	0.11
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	18	0.11
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	18	0.11
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	18	0.11
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	18	0.11
(1,2879)	1:25:B:SER:H	1:33:B:GLY:HA2	15	0.11
(1,2879)	1:25:B:SER:H	1:33:B:GLY:HA3	15	0.11
(1,2875)	1:24:B:LEU:HD11	1:34:B:GLY:H	4	0.11
(1,2875)	1:24:B:LEU:HD12	1:34:B:GLY:H	4	0.11
(1,2875)	1:24:B:LEU:HD13	1:34:B:GLY:H	4	0.11
(1,2875)	1:24:B:LEU:HD21	1:34:B:GLY:H	4	0.11
(1,2875)	1:24:B:LEU:HD22	1:34:B:GLY:H	4	0.11
(1,2875)	1:24:B:LEU:HD23	1:34:B:GLY:H	4	0.11
(1,2866)	1:24:B:LEU:HB2	1:25:B:SER:H	19	0.11
(1,2866)	1:24:B:LEU:HB3	1:25:B:SER:H	19	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	4	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	4	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	4	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	4	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	4	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	13	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	13	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	13	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	13	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	13	0.11
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	13	0.11
(1,2849)	1:21:B:LEU:HD11	1:103:B:LEU:H	5	0.11
(1,2849)	1:21:B:LEU:HD12	1:103:B:LEU:H	5	0.11
(1,2849)	1:21:B:LEU:HD13	1:103:B:LEU:H	5	0.11
(1,2849)	1:21:B:LEU:HD21	1:103:B:LEU:H	5	0.11
(1,2849)	1:21:B:LEU:HD22	1:103:B:LEU:H	5	0.11
(1,2849)	1:21:B:LEU:HD23	1:103:B:LEU:H	5	0.11
(1,2839)	1:21:B:LEU:HD11	1:22:B:ALA:H	10	0.11
(1,2839)	1:21:B:LEU:HD12	1:22:B:ALA:H	10	0.11
(1,2839)	1:21:B:LEU:HD13	1:22:B:ALA:H	10	0.11
(1,2839)	1:21:B:LEU:HD21	1:22:B:ALA:H	10	0.11
(1,2839)	1:21:B:LEU:HD22	1:22:B:ALA:H	10	0.11
(1,2839)	1:21:B:LEU:HD23	1:22:B:ALA:H	10	0.11
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB2	6	0.11
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB3	6	0.11
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB2	7	0.11
(1,2808)	1:19:B:VAL:H	1:105:B:TYR:HB3	7	0.11
(1,2782)	1:126:A:ALA:HB1	1:127:A:VAL:HG11	14	0.11
(1,2782)	1:126:A:ALA:HB1	1:127:A:VAL:HG12	14	0.11
(1,2782)	1:126:A:ALA:HB1	1:127:A:VAL:HG13	14	0.11
(1,2782)	1:126:A:ALA:HB1	1:127:A:VAL:HG21	14	0.11
(1,2782)	1:126:A:ALA:HB1	1:127:A:VAL:HG22	14	0.11
(1,2782)	1:126:A:ALA:HB1	1:127:A:VAL:HG23	14	0.11
(1,2782)	1:126:A:ALA:HB2	1:127:A:VAL:HG11	14	0.11
(1,2782)	1:126:A:ALA:HB2	1:127:A:VAL:HG12	14	0.11
(1,2782)	1:126:A:ALA:HB2	1:127:A:VAL:HG13	14	0.11
(1,2782)	1:126:A:ALA:HB2	1:127:A:VAL:HG21	14	0.11
(1,2782)	1:126:A:ALA:HB2	1:127:A:VAL:HG22	14	0.11
(1,2782)	1:126:A:ALA:HB2	1:127:A:VAL:HG23	14	0.11
(1,2782)	1:126:A:ALA:HB3	1:127:A:VAL:HG11	14	0.11
(1,2782)	1:126:A:ALA:HB3	1:127:A:VAL:HG12	14	0.11
(1,2782)	1:126:A:ALA:HB3	1:127:A:VAL:HG13	14	0.11
(1,2782)	1:126:A:ALA:HB3	1:127:A:VAL:HG21	14	0.11
(1,2782)	1:126:A:ALA:HB3	1:127:A:VAL:HG22	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2782)	1:126:A:ALA:HB3	1:127:A:VAL:HG23	14	0.11
(1,2779)	1:125:A:ASN:HB2	1:127:A:VAL:H	5	0.11
(1,2779)	1:125:A:ASN:HB3	1:127:A:VAL:H	5	0.11
(1,2769)	1:123:A:GLY:HA2	1:43:B:ASN:HD21	20	0.11
(1,2769)	1:123:A:GLY:HA2	1:43:B:ASN:HD22	20	0.11
(1,2769)	1:123:A:GLY:HA3	1:43:B:ASN:HD21	20	0.11
(1,2769)	1:123:A:GLY:HA3	1:43:B:ASN:HD22	20	0.11
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD11	12	0.11
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD12	12	0.11
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD13	12	0.11
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD21	12	0.11
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD22	12	0.11
(1,2750)	1:119:A:MET:HE1	1:124:A:LEU:HD23	12	0.11
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD11	12	0.11
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD12	12	0.11
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD13	12	0.11
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD21	12	0.11
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD22	12	0.11
(1,2750)	1:119:A:MET:HE2	1:124:A:LEU:HD23	12	0.11
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD11	12	0.11
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD12	12	0.11
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD13	12	0.11
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD21	12	0.11
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD22	12	0.11
(1,2750)	1:119:A:MET:HE3	1:124:A:LEU:HD23	12	0.11
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG12	20	0.11
(1,2731)	1:117:A:ALA:HA	1:120:A:ILE:HG13	20	0.11
(1,2728)	1:116:A:ASN:HD21	1:118:A:LEU:H	9	0.11
(1,2728)	1:116:A:ASN:HD22	1:118:A:LEU:H	9	0.11
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	2	0.11
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	2	0.11
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	2	0.11
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	2	0.11
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB2	11	0.11
(1,2707)	1:113:A:GLU:HB2	1:116:A:ASN:HB3	11	0.11
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB2	11	0.11
(1,2707)	1:113:A:GLU:HB3	1:116:A:ASN:HB3	11	0.11
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD21	6	0.11
(1,2703)	1:112:A:LYS:HD2	1:116:A:ASN:HD22	6	0.11
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD21	6	0.11
(1,2703)	1:112:A:LYS:HD3	1:116:A:ASN:HD22	6	0.11
(1,2645)	1:98:A:ARG:HB2	1:99:A:LEU:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2645)	1:98:A:ARG:HB3	1:99:A:LEU:H	18	0.11
(1,2625)	1:93:A:THR:H	1:94:A:LEU:HD11	17	0.11
(1,2625)	1:93:A:THR:H	1:94:A:LEU:HD12	17	0.11
(1,2625)	1:93:A:THR:H	1:94:A:LEU:HD13	17	0.11
(1,2625)	1:93:A:THR:H	1:94:A:LEU:HD21	17	0.11
(1,2625)	1:93:A:THR:H	1:94:A:LEU:HD22	17	0.11
(1,2625)	1:93:A:THR:H	1:94:A:LEU:HD23	17	0.11
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD11	3	0.11
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD12	3	0.11
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD13	3	0.11
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD21	3	0.11
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD22	3	0.11
(1,2622)	1:91:A:ILE:HG12	1:118:A:LEU:HD23	3	0.11
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD11	3	0.11
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD12	3	0.11
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD13	3	0.11
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD21	3	0.11
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD22	3	0.11
(1,2622)	1:91:A:ILE:HG13	1:118:A:LEU:HD23	3	0.11
(1,2610)	1:87:A:LEU:HD11	1:90:A:GLN:HB3	3	0.11
(1,2610)	1:87:A:LEU:HD12	1:90:A:GLN:HB3	3	0.11
(1,2610)	1:87:A:LEU:HD13	1:90:A:GLN:HB3	3	0.11
(1,2610)	1:87:A:LEU:HD21	1:90:A:GLN:HB3	3	0.11
(1,2610)	1:87:A:LEU:HD22	1:90:A:GLN:HB3	3	0.11
(1,2610)	1:87:A:LEU:HD23	1:90:A:GLN:HB3	3	0.11
(1,2610)	1:87:A:LEU:HD11	1:90:A:GLN:HB3	5	0.11
(1,2610)	1:87:A:LEU:HD12	1:90:A:GLN:HB3	5	0.11
(1,2610)	1:87:A:LEU:HD13	1:90:A:GLN:HB3	5	0.11
(1,2610)	1:87:A:LEU:HD21	1:90:A:GLN:HB3	5	0.11
(1,2610)	1:87:A:LEU:HD22	1:90:A:GLN:HB3	5	0.11
(1,2610)	1:87:A:LEU:HD23	1:90:A:GLN:HB3	5	0.11
(1,2610)	1:87:A:LEU:HD11	1:90:A:GLN:HB3	16	0.11
(1,2610)	1:87:A:LEU:HD12	1:90:A:GLN:HB3	16	0.11
(1,2610)	1:87:A:LEU:HD13	1:90:A:GLN:HB3	16	0.11
(1,2610)	1:87:A:LEU:HD21	1:90:A:GLN:HB3	16	0.11
(1,2610)	1:87:A:LEU:HD22	1:90:A:GLN:HB3	16	0.11
(1,2610)	1:87:A:LEU:HD23	1:90:A:GLN:HB3	16	0.11
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE2	14	0.11
(1,2594)	1:82:A:LYS:HB2	1:82:A:LYS:HE3	14	0.11
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE2	14	0.11
(1,2594)	1:82:A:LYS:HB3	1:82:A:LYS:HE3	14	0.11
(1,2571)	1:77:A:LYS:HA	1:77:A:LYS:HD2	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2571)	1:77:A:LYS:HA	1:77:A:LYS:HD3	17	0.11
(1,2570)	1:77:A:LYS:H	1:77:A:LYS:HG2	10	0.11
(1,2570)	1:77:A:LYS:H	1:77:A:LYS:HG3	10	0.11
(1,2566)	1:76:A:LYS:HA	1:76:A:LYS:HD2	11	0.11
(1,2566)	1:76:A:LYS:HA	1:76:A:LYS:HD3	11	0.11
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD2	3	0.11
(1,2554)	1:75:A:LYS:HA	1:75:A:LYS:HD3	3	0.11
(1,2550)	1:74:A:GLU:HG2	1:76:A:LYS:H	20	0.11
(1,2550)	1:74:A:GLU:HG3	1:76:A:LYS:H	20	0.11
(1,2548)	1:74:A:GLU:HB2	1:77:A:LYS:H	9	0.11
(1,2548)	1:74:A:GLU:HB3	1:77:A:LYS:H	9	0.11
(1,2543)	1:73:A:ILE:HG12	1:84:A:SER:H	16	0.11
(1,2543)	1:73:A:ILE:HG13	1:84:A:SER:H	16	0.11
(1,2539)	1:73:A:ILE:HG21	1:78:A:TYR:HB2	14	0.11
(1,2539)	1:73:A:ILE:HG21	1:78:A:TYR:HB3	14	0.11
(1,2539)	1:73:A:ILE:HG22	1:78:A:TYR:HB2	14	0.11
(1,2539)	1:73:A:ILE:HG22	1:78:A:TYR:HB3	14	0.11
(1,2539)	1:73:A:ILE:HG23	1:78:A:TYR:HB2	14	0.11
(1,2539)	1:73:A:ILE:HG23	1:78:A:TYR:HB3	14	0.11
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG11	15	0.11
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG12	15	0.11
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG13	15	0.11
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG21	15	0.11
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG22	15	0.11
(1,2537)	1:73:A:ILE:H	1:85:A:VAL:HG23	15	0.11
(1,2518)	1:70:A:HIS:H	1:71:A:VAL:HG11	4	0.11
(1,2518)	1:70:A:HIS:H	1:71:A:VAL:HG12	4	0.11
(1,2518)	1:70:A:HIS:H	1:71:A:VAL:HG13	4	0.11
(1,2518)	1:70:A:HIS:H	1:71:A:VAL:HG21	4	0.11
(1,2518)	1:70:A:HIS:H	1:71:A:VAL:HG22	4	0.11
(1,2518)	1:70:A:HIS:H	1:71:A:VAL:HG23	4	0.11
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG12	5	0.11
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	5	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG12	5	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	5	0.11
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG12	5	0.11
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	5	0.11
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG12	9	0.11
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	9	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG12	9	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	9	0.11
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	9	0.11
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG12	20	0.11
(1,2496)	1:56:A:ALA:HB1	1:91:A:ILE:HG13	20	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG12	20	0.11
(1,2496)	1:56:A:ALA:HB2	1:91:A:ILE:HG13	20	0.11
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG12	20	0.11
(1,2496)	1:56:A:ALA:HB3	1:91:A:ILE:HG13	20	0.11
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	10	0.11
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	10	0.11
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	10	0.11
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	10	0.11
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	10	0.11
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	10	0.11
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG11	8	0.11
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG12	8	0.11
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG13	8	0.11
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG21	8	0.11
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG22	8	0.11
(1,2445)	1:42:A:GLN:HE21	1:53:A:VAL:HG23	8	0.11
(1,2438)	1:42:A:GLN:HB2	1:42:A:GLN:HE21	20	0.11
(1,2438)	1:42:A:GLN:HB3	1:42:A:GLN:HE21	20	0.11
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	9	0.11
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	9	0.11
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	9	0.11
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	9	0.11
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	9	0.11
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	9	0.11
(1,2428)	1:39:A:VAL:HG11	1:86:A:ILE:HB	13	0.11
(1,2428)	1:39:A:VAL:HG12	1:86:A:ILE:HB	13	0.11
(1,2428)	1:39:A:VAL:HG13	1:86:A:ILE:HB	13	0.11
(1,2428)	1:39:A:VAL:HG21	1:86:A:ILE:HB	13	0.11
(1,2428)	1:39:A:VAL:HG22	1:86:A:ILE:HB	13	0.11
(1,2428)	1:39:A:VAL:HG23	1:86:A:ILE:HB	13	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD11	10	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD12	10	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD13	10	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD21	10	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD22	10	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD23	10	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD11	11	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD12	11	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD13	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD21	11	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD22	11	0.11
(1,2422)	1:39:A:VAL:HB	1:106:A:LEU:HD23	11	0.11
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	7	0.11
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	7	0.11
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	7	0.11
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	7	0.11
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	7	0.11
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	7	0.11
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	11	0.11
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	11	0.11
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	11	0.11
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	11	0.11
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	11	0.11
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	11	0.11
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB2	4	0.11
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB3	4	0.11
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB2	10	0.11
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB3	10	0.11
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD2	1	0.11
(1,2390)	1:28:A:GLN:HE21	1:26:B:PRO:HD3	1	0.11
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD2	1	0.11
(1,2390)	1:28:A:GLN:HE22	1:26:B:PRO:HD3	1	0.11
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE21	1	0.11
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE22	1	0.11
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE21	1	0.11
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE22	1	0.11
(1,2377)	1:26:A:PRO:HD2	1:27:A:VAL:H	15	0.11
(1,2377)	1:26:A:PRO:HD3	1:27:A:VAL:H	15	0.11
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG11	10	0.11
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG12	10	0.11
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG13	10	0.11
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG21	10	0.11
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG22	10	0.11
(1,2373)	1:25:A:SER:H	1:35:A:VAL:HG23	10	0.11
(1,2372)	1:25:A:SER:H	1:33:A:GLY:HA2	15	0.11
(1,2372)	1:25:A:SER:H	1:33:A:GLY:HA3	15	0.11
(1,2367)	1:24:A:LEU:HD11	1:32:A:GLN:HE22	1	0.11
(1,2367)	1:24:A:LEU:HD12	1:32:A:GLN:HE22	1	0.11
(1,2367)	1:24:A:LEU:HD13	1:32:A:GLN:HE22	1	0.11
(1,2367)	1:24:A:LEU:HD21	1:32:A:GLN:HE22	1	0.11
(1,2367)	1:24:A:LEU:HD22	1:32:A:GLN:HE22	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2367)	1:24:A:LEU:HD23	1:32:A:GLN:HE22	1	0.11
(1,2365)	1:24:A:LEU:HD21	1:32:A:GLN:HG2	9	0.11
(1,2365)	1:24:A:LEU:HD22	1:32:A:GLN:HG2	9	0.11
(1,2365)	1:24:A:LEU:HD23	1:32:A:GLN:HG2	9	0.11
(1,2342)	1:21:A:LEU:HD11	1:103:A:LEU:H	5	0.11
(1,2342)	1:21:A:LEU:HD12	1:103:A:LEU:H	5	0.11
(1,2342)	1:21:A:LEU:HD13	1:103:A:LEU:H	5	0.11
(1,2342)	1:21:A:LEU:HD21	1:103:A:LEU:H	5	0.11
(1,2342)	1:21:A:LEU:HD22	1:103:A:LEU:H	5	0.11
(1,2342)	1:21:A:LEU:HD23	1:103:A:LEU:H	5	0.11
(1,2332)	1:21:A:LEU:HD11	1:22:A:ALA:H	10	0.11
(1,2332)	1:21:A:LEU:HD12	1:22:A:ALA:H	10	0.11
(1,2332)	1:21:A:LEU:HD13	1:22:A:ALA:H	10	0.11
(1,2332)	1:21:A:LEU:HD21	1:22:A:ALA:H	10	0.11
(1,2332)	1:21:A:LEU:HD22	1:22:A:ALA:H	10	0.11
(1,2332)	1:21:A:LEU:HD23	1:22:A:ALA:H	10	0.11
(1,2316)	1:19:A:VAL:HG11	1:106:A:LEU:H	18	0.11
(1,2316)	1:19:A:VAL:HG12	1:106:A:LEU:H	18	0.11
(1,2316)	1:19:A:VAL:HG13	1:106:A:LEU:H	18	0.11
(1,2316)	1:19:A:VAL:HG21	1:106:A:LEU:H	18	0.11
(1,2316)	1:19:A:VAL:HG22	1:106:A:LEU:H	18	0.11
(1,2316)	1:19:A:VAL:HG23	1:106:A:LEU:H	18	0.11
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB2	7	0.11
(1,2301)	1:19:A:VAL:H	1:105:A:TYR:HB3	7	0.11
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE1	14	0.11
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE2	14	0.11
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE1	19	0.11
(1,2272)	1:18:B:ASP:HB3	1:20:B:TYR:HE2	19	0.11
(1,2271)	1:18:B:ASP:H	1:20:B:TYR:HE1	14	0.11
(1,2271)	1:18:B:ASP:H	1:20:B:TYR:HE2	14	0.11
(1,2271)	1:18:B:ASP:H	1:20:B:TYR:HE1	20	0.11
(1,2271)	1:18:B:ASP:H	1:20:B:TYR:HE2	20	0.11
(1,2269)	1:18:B:ASP:HA	1:105:B:TYR:HA	4	0.11
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	9	0.11
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	9	0.11
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	13	0.11
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	13	0.11
(1,2236)	1:76:B:LYS:H	1:80:B:LEU:H	2	0.11
(1,2236)	1:76:B:LYS:H	1:80:B:LEU:H	4	0.11
(1,2231)	1:56:B:ALA:H	1:91:B:ILE:HA	15	0.11
(1,2194)	1:119:A:MET:HG3	1:124:A:LEU:H	7	0.11
(1,2194)	1:119:A:MET:HG3	1:124:A:LEU:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG11	6	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG12	6	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG13	6	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG11	18	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG12	18	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG13	18	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG11	19	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG12	19	0.11
(1,2191)	1:112:B:LYS:H	1:114:B:VAL:HG13	19	0.11
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD11	10	0.11
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD12	10	0.11
(1,2160)	1:116:B:ASN:HD21	1:120:B:ILE:HD13	10	0.11
(1,2152)	1:123:B:GLY:H	1:125:B:ASN:H	11	0.11
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	10	0.11
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	10	0.11
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	10	0.11
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	18	0.11
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	18	0.11
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	18	0.11
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	16	0.11
(1,2138)	1:120:B:ILE:HD11	1:121:B:SER:H	13	0.11
(1,2138)	1:120:B:ILE:HD12	1:121:B:SER:H	13	0.11
(1,2138)	1:120:B:ILE:HD13	1:121:B:SER:H	13	0.11
(1,2111)	1:111:B:MET:HG3	1:112:B:LYS:H	19	0.11
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	7	0.11
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	10	0.11
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	13	0.11
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	16	0.11
(1,2097)	1:78:B:TYR:HD1	1:107:B:SER:H	5	0.11
(1,2097)	1:78:B:TYR:HD2	1:107:B:SER:H	5	0.11
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	2	0.11
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	14	0.11
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	16	0.11
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	6	0.11
(1,2082)	1:20:B:TYR:H	1:104:B:THR:H	8	0.11
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	13	0.11
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	15	0.11
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	18	0.11
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	20	0.11
(1,2072)	1:99:A:LEU:HD21	1:100:A:LYS:H	16	0.11
(1,2072)	1:99:A:LEU:HD22	1:100:A:LYS:H	16	0.11
(1,2072)	1:99:A:LEU:HD23	1:100:A:LYS:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	1	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	1	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	1	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	3	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	3	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	3	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	9	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	9	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	9	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	13	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	13	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	13	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	14	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	14	0.11
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	14	0.11
(1,2050)	1:92:A:ARG:HG3	1:93:A:THR:H	8	0.11
(1,2039)	1:87:B:LEU:H	1:90:B:GLN:H	16	0.11
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	6	0.11
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	6	0.11
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	6	0.11
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	11	0.11
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	11	0.11
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	11	0.11
(1,2028)	1:86:B:ILE:HD11	1:87:B:LEU:H	20	0.11
(1,2028)	1:86:B:ILE:HD12	1:87:B:LEU:H	20	0.11
(1,2028)	1:86:B:ILE:HD13	1:87:B:LEU:H	20	0.11
(1,2018)	1:75:B:LYS:H	1:84:B:SER:H	7	0.11
(1,2011)	1:80:B:LEU:HD11	1:82:B:LYS:H	11	0.11
(1,2011)	1:80:B:LEU:HD12	1:82:B:LYS:H	11	0.11
(1,2011)	1:80:B:LEU:HD13	1:82:B:LYS:H	11	0.11
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	9	0.11
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	17	0.11
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	18	0.11
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	17	0.11
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	17	0.11
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	17	0.11
(1,1955)	1:31:B:GLU:HA	1:90:B:GLN:HE22	12	0.11
(1,1952)	1:50:B:SER:H	1:52:B:THR:H	19	0.11
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	13	0.11
(1,1938)	1:42:B:GLN:HE21	1:45:B:THR:H	15	0.11
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	4	0.11
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	7	0.11
(1,1928)	1:42:B:GLN:H	1:54:B:ILE:H	14	0.11
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	5	0.11
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	9	0.11
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	14	0.11
(1,1926)	1:40:B:ILE:H	1:42:B:GLN:H	15	0.11
(1,1920)	1:38:B:VAL:HG11	1:39:B:VAL:H	8	0.11
(1,1920)	1:38:B:VAL:HG12	1:39:B:VAL:H	8	0.11
(1,1920)	1:38:B:VAL:HG13	1:39:B:VAL:H	8	0.11
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	6	0.11
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	6	0.11
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	6	0.11
(1,1911)	1:35:B:VAL:HG11	1:36:B:ARG:H	11	0.11
(1,1911)	1:35:B:VAL:HG12	1:36:B:ARG:H	11	0.11
(1,1911)	1:35:B:VAL:HG13	1:36:B:ARG:H	11	0.11
(1,1900)	1:27:B:VAL:HG11	1:33:B:GLY:H	13	0.11
(1,1900)	1:27:B:VAL:HG12	1:33:B:GLY:H	13	0.11
(1,1900)	1:27:B:VAL:HG13	1:33:B:GLY:H	13	0.11
(1,1900)	1:27:B:VAL:HG11	1:33:B:GLY:H	19	0.11
(1,1900)	1:27:B:VAL:HG12	1:33:B:GLY:H	19	0.11
(1,1900)	1:27:B:VAL:HG13	1:33:B:GLY:H	19	0.11
(1,1893)	1:27:B:VAL:HG11	1:31:B:GLU:H	17	0.11
(1,1893)	1:27:B:VAL:HG12	1:31:B:GLU:H	17	0.11
(1,1893)	1:27:B:VAL:HG13	1:31:B:GLU:H	17	0.11
(1,1873)	1:22:B:ALA:H	1:35:B:VAL:HB	2	0.11
(1,1848)	1:16:B:ARG:H	1:47:B:ASN:HD21	6	0.11
(1,1840)	1:92:B:ARG:H	1:92:B:ARG:HG2	5	0.11
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	3	0.11
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	10	0.11
(1,1767)	1:96:A:LYS:HB2	1:97:A:LYS:H	3	0.11
(1,1767)	1:96:A:LYS:HB2	1:97:A:LYS:H	14	0.11
(1,1764)	1:96:A:LYS:HB3	1:97:A:LYS:H	18	0.11
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	11	0.11
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	11	0.11
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	11	0.11
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	15	0.11
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	15	0.11
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	15	0.11
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	1	0.11
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	9	0.11
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	16	0.11
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	1	0.11
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	9	0.11
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	16	0.11
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	17	0.11
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	18	0.11
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	20	0.11
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG11	2	0.11
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG12	2	0.11
(1,1680)	1:35:B:VAL:H	1:35:B:VAL:HG13	2	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	7	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	7	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	7	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	12	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	12	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	12	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	14	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	14	0.11
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	14	0.11
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD21	7	0.11
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD22	7	0.11
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD23	7	0.11
(1,1675)	1:124:B:LEU:H	1:124:B:LEU:HG	6	0.11
(1,1675)	1:124:B:LEU:H	1:124:B:LEU:HG	18	0.11
(1,1672)	1:75:B:LYS:HB2	1:76:B:LYS:H	5	0.11
(1,1632)	1:80:A:LEU:HB2	1:81:A:ASP:H	4	0.11
(1,1630)	1:74:B:GLU:H	1:74:B:GLU:HG3	15	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE1	10	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE2	10	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE3	10	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE1	13	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE2	13	0.11
(1,1617)	1:111:B:MET:H	1:111:B:MET:HE3	13	0.11
(1,1610)	1:90:B:GLN:H	1:90:B:GLN:HE21	9	0.11
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	8	0.11
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	20	0.11
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	4	0.11
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	13	0.11
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	14	0.11
(1,1586)	1:112:A:LYS:H	1:112:A:LYS:HB3	10	0.11
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	5	0.11
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	6	0.11
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	4	0.11
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	4	0.11
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	4	0.11
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD11	7	0.11
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD12	7	0.11
(1,1528)	1:118:B:LEU:H	1:118:B:LEU:HD13	7	0.11
(1,1506)	1:20:B:TYR:H	1:21:B:LEU:H	5	0.11
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE1	1	0.11
(1,1505)	1:20:B:TYR:H	1:20:B:TYR:HE2	1	0.11
(1,1489)	1:115:B:ASP:HB3	1:116:B:ASN:H	11	0.11
(1,1484)	1:120:B:ILE:H	1:120:B:ILE:HG13	7	0.11
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	2	0.11
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	8	0.11
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	16	0.11
(1,1480)	1:124:B:LEU:HA	1:125:B:ASN:H	17	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	1	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	1	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	1	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	8	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	8	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	8	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD21	19	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD22	19	0.11
(1,1467)	1:80:B:LEU:H	1:80:B:LEU:HD23	19	0.11
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	6	0.11
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	9	0.11
(1,1405)	1:99:B:LEU:HA	1:100:B:LYS:HG2	19	0.11
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD11	13	0.11
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD12	13	0.11
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD13	13	0.11
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD11	15	0.11
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD12	15	0.11
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD13	15	0.11
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB1	13	0.11
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB2	13	0.11
(1,1380)	1:88:B:LEU:HD11	1:117:B:ALA:HB3	13	0.11
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB1	13	0.11
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB2	13	0.11
(1,1380)	1:88:B:LEU:HD12	1:117:B:ALA:HB3	13	0.11
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB1	13	0.11
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB2	13	0.11
(1,1380)	1:88:B:LEU:HD13	1:117:B:ALA:HB3	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD21	8	0.11
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD22	8	0.11
(1,1371)	1:56:B:ALA:HB1	1:88:B:LEU:HD23	8	0.11
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD21	8	0.11
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD22	8	0.11
(1,1371)	1:56:B:ALA:HB2	1:88:B:LEU:HD23	8	0.11
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD21	8	0.11
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD22	8	0.11
(1,1371)	1:56:B:ALA:HB3	1:88:B:LEU:HD23	8	0.11
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD11	16	0.11
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD12	16	0.11
(1,1358)	1:56:A:ALA:HA	1:91:A:ILE:HD13	16	0.11
(1,1357)	1:20:B:TYR:HA	1:102:B:LYS:HA	19	0.11
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG11	20	0.11
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG12	20	0.11
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG13	20	0.11
(1,1342)	1:91:A:ILE:HG21	1:93:B:THR:HB	2	0.11
(1,1342)	1:91:A:ILE:HG22	1:93:B:THR:HB	2	0.11
(1,1342)	1:91:A:ILE:HG23	1:93:B:THR:HB	2	0.11
(1,1342)	1:91:A:ILE:HG21	1:93:B:THR:HB	7	0.11
(1,1342)	1:91:A:ILE:HG22	1:93:B:THR:HB	7	0.11
(1,1342)	1:91:A:ILE:HG23	1:93:B:THR:HB	7	0.11
(1,1341)	1:58:B:ILE:HG21	1:84:B:SER:HB3	20	0.11
(1,1341)	1:58:B:ILE:HG22	1:84:B:SER:HB3	20	0.11
(1,1341)	1:58:B:ILE:HG23	1:84:B:SER:HB3	20	0.11
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD11	3	0.11
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD12	3	0.11
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD13	3	0.11
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD11	4	0.11
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD12	4	0.11
(1,1310)	1:119:B:MET:HA	1:124:B:LEU:HD13	4	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD11	14	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD12	14	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD13	14	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD11	16	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD12	16	0.11
(1,1309)	1:115:B:ASP:HA	1:118:B:LEU:HD13	16	0.11
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	10	0.11
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	14	0.11
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	19	0.11
(1,1304)	1:116:B:ASN:HA	1:119:B:MET:HE1	15	0.11
(1,1304)	1:116:B:ASN:HA	1:119:B:MET:HE2	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:116:B:ASN:HA	1:119:B:MET:HE3	15	0.11
(1,1295)	1:27:B:VAL:HG11	1:33:B:GLY:HA2	13	0.11
(1,1295)	1:27:B:VAL:HG12	1:33:B:GLY:HA2	13	0.11
(1,1295)	1:27:B:VAL:HG13	1:33:B:GLY:HA2	13	0.11
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD1	6	0.11
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD2	6	0.11
(1,1266)	1:19:A:VAL:HG11	1:37:A:PRO:HB3	19	0.11
(1,1266)	1:19:A:VAL:HG12	1:37:A:PRO:HB3	19	0.11
(1,1266)	1:19:A:VAL:HG13	1:37:A:PRO:HB3	19	0.11
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD21	1	0.11
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD22	1	0.11
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD23	1	0.11
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD21	16	0.11
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD22	16	0.11
(1,1252)	1:119:B:MET:HG2	1:124:B:LEU:HD23	16	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	3	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	3	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	3	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	7	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	7	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	7	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	16	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	16	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	16	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD11	19	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD12	19	0.11
(1,1244)	1:118:B:LEU:HA	1:118:B:LEU:HD13	19	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG21	2	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG22	2	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG23	2	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG21	2	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG22	2	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG23	2	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG21	2	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG22	2	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG23	2	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG21	6	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG22	6	0.11
(1,1242)	1:111:B:MET:HE1	1:114:B:VAL:HG23	6	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG21	6	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG22	6	0.11
(1,1242)	1:111:B:MET:HE2	1:114:B:VAL:HG23	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG21	6	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG22	6	0.11
(1,1242)	1:111:B:MET:HE3	1:114:B:VAL:HG23	6	0.11
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD11	18	0.11
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD12	18	0.11
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD13	18	0.11
(1,1226)	1:56:B:ALA:HB1	1:91:B:ILE:HB	12	0.11
(1,1226)	1:56:B:ALA:HB2	1:91:B:ILE:HB	12	0.11
(1,1226)	1:56:B:ALA:HB3	1:91:B:ILE:HB	12	0.11
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	12	0.11
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	12	0.11
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	12	0.11
(1,1220)	1:27:B:VAL:HG21	1:33:B:GLY:HA2	19	0.11
(1,1220)	1:27:B:VAL:HG22	1:33:B:GLY:HA2	19	0.11
(1,1220)	1:27:B:VAL:HG23	1:33:B:GLY:HA2	19	0.11
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	5	0.11
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	5	0.11
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	5	0.11
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	14	0.11
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	14	0.11
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	14	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	4	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	4	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	4	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	15	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	15	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	15	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	16	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	16	0.11
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	16	0.11
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG11	15	0.11
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG12	15	0.11
(1,1147)	1:40:B:ILE:HG13	1:55:B:VAL:HG13	15	0.11
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD1	19	0.11
(1,1127)	1:73:B:ILE:HG12	1:78:B:TYR:HD2	19	0.11
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD1	4	0.11
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD2	4	0.11
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD1	15	0.11
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD2	15	0.11
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD1	19	0.11
(1,1105)	1:18:A:ASP:HA	1:105:A:TYR:HD2	19	0.11
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE1	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1101)	1:73:A:ILE:HG21	1:78:A:TYR:HE2	9	0.11
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE1	9	0.11
(1,1101)	1:73:A:ILE:HG22	1:78:A:TYR:HE2	9	0.11
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE1	9	0.11
(1,1101)	1:73:A:ILE:HG23	1:78:A:TYR:HE2	9	0.11
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	12	0.11
(1,1083)	1:76:A:LYS:H	1:80:A:LEU:H	8	0.11
(1,1083)	1:76:A:LYS:H	1:80:A:LEU:H	16	0.11
(1,1078)	1:56:A:ALA:H	1:91:A:ILE:HA	15	0.11
(1,1071)	1:24:A:LEU:HD11	1:32:A:GLN:H	15	0.11
(1,1071)	1:24:A:LEU:HD12	1:32:A:GLN:H	15	0.11
(1,1071)	1:24:A:LEU:HD13	1:32:A:GLN:H	15	0.11
(1,1056)	1:43:A:ASN:HD22	1:45:A:THR:HB	15	0.11
(1,1048)	1:119:A:MET:HE1	1:125:A:ASN:HD22	14	0.11
(1,1048)	1:119:A:MET:HE2	1:125:A:ASN:HD22	14	0.11
(1,1048)	1:119:A:MET:HE3	1:125:A:ASN:HD22	14	0.11
(1,1042)	1:119:B:MET:HG3	1:124:B:LEU:H	16	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG11	6	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG12	6	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG13	6	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG11	19	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG12	19	0.11
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG13	19	0.11
(1,1016)	1:112:B:LYS:HB2	1:116:B:ASN:HD22	7	0.11
(1,1015)	1:112:A:LYS:HB3	1:116:A:ASN:HD22	8	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	10	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	10	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	10	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	20	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	20	0.11
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	20	0.11
(1,1004)	1:119:A:MET:HE1	1:124:A:LEU:H	3	0.11
(1,1004)	1:119:A:MET:HE2	1:124:A:LEU:H	3	0.11
(1,1004)	1:119:A:MET:HE3	1:124:A:LEU:H	3	0.11
(1,1004)	1:119:A:MET:HE1	1:124:A:LEU:H	9	0.11
(1,1004)	1:119:A:MET:HE2	1:124:A:LEU:H	9	0.11
(1,1004)	1:119:A:MET:HE3	1:124:A:LEU:H	9	0.11
(1,1003)	1:119:A:MET:HA	1:124:A:LEU:H	10	0.11
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	5	0.11
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	5	0.11
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	5	0.11
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	10	0.11
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	10	0.11
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	14	0.11
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	14	0.11
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	14	0.11
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	14	0.11
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	20	0.11
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	6	0.11
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	10	0.11
(1,998)	1:123:A:GLY:H	1:42:B:GLN:HA	14	0.11
(1,996)	1:123:A:GLY:H	1:44:B:ASP:H	10	0.11
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	3	0.11
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	3	0.11
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	3	0.11
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	7	0.11
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	7	0.11
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	7	0.11
(1,992)	1:120:A:ILE:HD11	1:121:A:SER:H	17	0.11
(1,992)	1:120:A:ILE:HD12	1:121:A:SER:H	17	0.11
(1,992)	1:120:A:ILE:HD13	1:121:A:SER:H	17	0.11
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	17	0.11
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	17	0.11
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	17	0.11
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	5	0.11
(1,961)	1:112:A:LYS:H	1:115:A:ASP:H	5	0.11
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	7	0.11
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	10	0.11
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	13	0.11
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	15	0.11
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	16	0.11
(1,951)	1:78:A:TYR:HD1	1:107:A:SER:H	5	0.11
(1,951)	1:78:A:TYR:HD2	1:107:A:SER:H	5	0.11
(1,946)	1:78:A:TYR:HA	1:105:A:TYR:H	4	0.11
(1,942)	1:103:A:LEU:HD11	1:104:A:THR:H	1	0.11
(1,942)	1:103:A:LEU:HD12	1:104:A:THR:H	1	0.11
(1,942)	1:103:A:LEU:HD13	1:104:A:THR:H	1	0.11
(1,942)	1:103:A:LEU:HD11	1:104:A:THR:H	9	0.11
(1,942)	1:103:A:LEU:HD12	1:104:A:THR:H	9	0.11
(1,942)	1:103:A:LEU:HD13	1:104:A:THR:H	9	0.11
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	1	0.11
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	2	0.11
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	19	0.11
(1,926)	1:99:B:LEU:HD21	1:100:B:LYS:H	7	0.11
(1,926)	1:99:B:LEU:HD22	1:100:B:LYS:H	7	0.11
(1,926)	1:99:B:LEU:HD23	1:100:B:LYS:H	7	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	1	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	1	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	1	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	3	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	3	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	3	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	9	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	9	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	9	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	12	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	12	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	12	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	14	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	14	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	14	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	18	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	18	0.11
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	18	0.11
(1,904)	1:92:B:ARG:HG3	1:93:B:THR:H	8	0.11
(1,893)	1:87:A:LEU:H	1:90:A:GLN:H	16	0.11
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	6	0.11
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	6	0.11
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	6	0.11
(1,872)	1:75:A:LYS:H	1:84:A:SER:H	7	0.11
(1,865)	1:80:A:LEU:HD11	1:82:A:LYS:H	3	0.11
(1,865)	1:80:A:LEU:HD12	1:82:A:LYS:H	3	0.11
(1,865)	1:80:A:LEU:HD13	1:82:A:LYS:H	3	0.11
(1,865)	1:80:A:LEU:HD11	1:82:A:LYS:H	13	0.11
(1,865)	1:80:A:LEU:HD12	1:82:A:LYS:H	13	0.11
(1,865)	1:80:A:LEU:HD13	1:82:A:LYS:H	13	0.11
(1,859)	1:74:A:GLU:HG3	1:77:A:LYS:H	1	0.11
(1,857)	1:73:A:ILE:HG21	1:74:A:GLU:H	9	0.11
(1,857)	1:73:A:ILE:HG22	1:74:A:GLU:H	9	0.11
(1,857)	1:73:A:ILE:HG23	1:74:A:GLU:H	9	0.11
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	1	0.11
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	1	0.11
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	1	0.11
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	10	0.11
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	10	0.11
(1,846)	1:65:A:ALA:HB1	1:70:A:HIS:H	9	0.11
(1,846)	1:65:A:ALA:HB2	1:70:A:HIS:H	9	0.11
(1,846)	1:65:A:ALA:HB3	1:70:A:HIS:H	9	0.11
(1,820)	1:53:A:VAL:HG11	1:54:A:ILE:H	10	0.11
(1,820)	1:53:A:VAL:HG12	1:54:A:ILE:H	10	0.11
(1,820)	1:53:A:VAL:HG13	1:54:A:ILE:H	10	0.11
(1,806)	1:50:A:SER:H	1:52:A:THR:H	19	0.11
(1,793)	1:42:B:GLN:HE22	1:45:B:THR:H	13	0.11
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	3	0.11
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	3	0.11
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	3	0.11
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	10	0.11
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	10	0.11
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	10	0.11
(1,790)	1:41:A:ILE:HD11	1:43:A:ASN:H	13	0.11
(1,790)	1:41:A:ILE:HD12	1:43:A:ASN:H	13	0.11
(1,790)	1:41:A:ILE:HD13	1:43:A:ASN:H	13	0.11
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	4	0.11
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	7	0.11
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	14	0.11
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	5	0.11
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	16	0.11
(1,781)	1:42:B:GLN:H	1:42:B:GLN:HE21	17	0.11
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	9	0.11
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	14	0.11
(1,754)	1:27:A:VAL:HG11	1:33:A:GLY:H	2	0.11
(1,754)	1:27:A:VAL:HG12	1:33:A:GLY:H	2	0.11
(1,754)	1:27:A:VAL:HG13	1:33:A:GLY:H	2	0.11
(1,754)	1:27:A:VAL:HG11	1:33:A:GLY:H	7	0.11
(1,754)	1:27:A:VAL:HG12	1:33:A:GLY:H	7	0.11
(1,754)	1:27:A:VAL:HG13	1:33:A:GLY:H	7	0.11
(1,754)	1:27:A:VAL:HG11	1:33:A:GLY:H	13	0.11
(1,754)	1:27:A:VAL:HG12	1:33:A:GLY:H	13	0.11
(1,754)	1:27:A:VAL:HG13	1:33:A:GLY:H	13	0.11
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	2	0.11
(1,727)	1:22:A:ALA:H	1:35:A:VAL:HB	18	0.11
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	10	0.11
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	6	0.11
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	6	0.11
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD11	15	0.11
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD12	15	0.11
(1,613)	1:41:A:ILE:H	1:41:A:ILE:HD13	15	0.11
(1,600)	1:42:A:GLN:HE22	1:43:A:ASN:H	16	0.11
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	2	0.11
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	4	0.11
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	8	0.11
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	17	0.11
(1,567)	1:127:A:VAL:HA	1:128:A:ALA:H	2	0.11
(1,564)	1:127:A:VAL:HB	1:128:A:ALA:H	16	0.11
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	4	0.11
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	5	0.11
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	16	0.11
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	19	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	3	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	3	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	3	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	12	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	12	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	12	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	14	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	14	0.11
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	14	0.11
(1,536)	1:124:B:LEU:H	1:124:B:LEU:HD11	20	0.11
(1,536)	1:124:B:LEU:H	1:124:B:LEU:HD12	20	0.11
(1,536)	1:124:B:LEU:H	1:124:B:LEU:HD13	20	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD21	7	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD22	7	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD23	7	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD21	16	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD22	16	0.11
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD23	16	0.11
(1,534)	1:124:A:LEU:H	1:124:A:LEU:HG	6	0.11
(1,534)	1:124:A:LEU:H	1:124:A:LEU:HG	18	0.11
(1,531)	1:75:A:LYS:HB2	1:76:A:LYS:H	5	0.11
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG21	18	0.11
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG22	18	0.11
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG23	18	0.11
(1,478)	1:111:A:MET:H	1:111:A:MET:HE1	10	0.11
(1,478)	1:111:A:MET:H	1:111:A:MET:HE2	10	0.11
(1,478)	1:111:A:MET:H	1:111:A:MET:HE3	10	0.11
(1,471)	1:90:A:GLN:H	1:90:A:GLN:HE21	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	20	0.11
(1,457)	1:94:A:LEU:HB3	1:95:A:ASP:H	4	0.11
(1,449)	1:112:B:LYS:H	1:112:B:LYS:HB3	10	0.11
(1,418)	1:126:A:ALA:HB1	1:127:A:VAL:H	13	0.11
(1,418)	1:126:A:ALA:HB2	1:127:A:VAL:H	13	0.11
(1,418)	1:126:A:ALA:HB3	1:127:A:VAL:H	13	0.11
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	7	0.11
(1,404)	1:32:A:GLN:H	1:32:A:GLN:HE21	6	0.11
(1,402)	1:103:A:LEU:H	1:103:A:LEU:HG	11	0.11
(1,399)	1:102:A:LYS:H	1:103:A:LEU:H	9	0.11
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	5	0.11
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	5	0.11
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	5	0.11
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD11	13	0.11
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD12	13	0.11
(1,393)	1:118:A:LEU:H	1:118:A:LEU:HD13	13	0.11
(1,371)	1:20:A:TYR:H	1:21:A:LEU:H	1	0.11
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	1	0.11
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	1	0.11
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE1	10	0.11
(1,370)	1:20:A:TYR:H	1:20:A:TYR:HE2	10	0.11
(1,364)	1:48:A:LYS:H	1:48:A:LYS:HD3	9	0.11
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	8	0.11
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	16	0.11
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	1	0.11
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	1	0.11
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	1	0.11
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	17	0.11
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	17	0.11
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	17	0.11
(1,323)	1:14:B:ILE:H	1:14:B:ILE:HG13	14	0.11
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	3	0.11
(1,278)	1:99:A:LEU:HA	1:100:A:LYS:HG2	19	0.11
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB1	4	0.11
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB2	4	0.11
(1,270)	1:119:A:MET:HE1	1:126:A:ALA:HB3	4	0.11
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB1	4	0.11
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB2	4	0.11
(1,270)	1:119:A:MET:HE2	1:126:A:ALA:HB3	4	0.11
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB1	4	0.11
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB2	4	0.11
(1,270)	1:119:A:MET:HE3	1:126:A:ALA:HB3	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:52:A:THR:HG21	1:95:A:ASP:HA	4	0.11
(1,261)	1:52:A:THR:HG22	1:95:A:ASP:HA	4	0.11
(1,261)	1:52:A:THR:HG23	1:95:A:ASP:HA	4	0.11
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD11	15	0.11
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD12	15	0.11
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD13	15	0.11
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD11	16	0.11
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD12	16	0.11
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD13	16	0.11
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	4	0.11
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	4	0.11
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	4	0.11
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	4	0.11
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	4	0.11
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	4	0.11
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	4	0.11
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	4	0.11
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	4	0.11
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	18	0.11
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	18	0.11
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	18	0.11
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	18	0.11
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	18	0.11
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	18	0.11
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	18	0.11
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	18	0.11
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	18	0.11
(1,235)	1:93:A:THR:HG21	1:91:B:ILE:HD11	8	0.11
(1,235)	1:93:A:THR:HG21	1:91:B:ILE:HD12	8	0.11
(1,235)	1:93:A:THR:HG21	1:91:B:ILE:HD13	8	0.11
(1,235)	1:93:A:THR:HG22	1:91:B:ILE:HD11	8	0.11
(1,235)	1:93:A:THR:HG22	1:91:B:ILE:HD12	8	0.11
(1,235)	1:93:A:THR:HG22	1:91:B:ILE:HD13	8	0.11
(1,235)	1:93:A:THR:HG23	1:91:B:ILE:HD11	8	0.11
(1,235)	1:93:A:THR:HG23	1:91:B:ILE:HD12	8	0.11
(1,235)	1:93:A:THR:HG23	1:91:B:ILE:HD13	8	0.11
(1,234)	1:24:A:LEU:HD21	1:32:A:GLN:HG3	4	0.11
(1,234)	1:24:A:LEU:HD22	1:32:A:GLN:HG3	4	0.11
(1,234)	1:24:A:LEU:HD23	1:32:A:GLN:HG3	4	0.11
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG11	12	0.11
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG12	12	0.11
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG13	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG11	20	0.11
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG12	20	0.11
(1,228)	1:111:B:MET:HA	1:114:B:VAL:HG13	20	0.11
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG21	2	0.11
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG22	2	0.11
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG23	2	0.11
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG21	7	0.11
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG22	7	0.11
(1,215)	1:93:A:THR:HB	1:91:B:ILE:HG23	7	0.11
(1,192)	1:16:A:ARG:HA	1:40:A:ILE:HB	12	0.11
(1,191)	1:75:B:LYS:HA	1:80:B:LEU:HD21	15	0.11
(1,191)	1:75:B:LYS:HA	1:80:B:LEU:HD22	15	0.11
(1,191)	1:75:B:LYS:HA	1:80:B:LEU:HD23	15	0.11
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD11	4	0.11
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD12	4	0.11
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD13	4	0.11
(1,183)	1:115:A:ASP:HA	1:118:A:LEU:HD11	16	0.11
(1,183)	1:115:A:ASP:HA	1:118:A:LEU:HD12	16	0.11
(1,183)	1:115:A:ASP:HA	1:118:A:LEU:HD13	16	0.11
(1,179)	1:109:A:ASP:HA	1:112:A:LYS:HB2	5	0.11
(1,174)	1:117:A:ALA:HA	1:120:A:ILE:HD11	1	0.11
(1,174)	1:117:A:ALA:HA	1:120:A:ILE:HD12	1	0.11
(1,174)	1:117:A:ALA:HA	1:120:A:ILE:HD13	1	0.11
(1,169)	1:27:A:VAL:HG11	1:33:A:GLY:HA2	10	0.11
(1,169)	1:27:A:VAL:HG12	1:33:A:GLY:HA2	10	0.11
(1,169)	1:27:A:VAL:HG13	1:33:A:GLY:HA2	10	0.11
(1,169)	1:27:A:VAL:HG11	1:33:A:GLY:HA2	13	0.11
(1,169)	1:27:A:VAL:HG12	1:33:A:GLY:HA2	13	0.11
(1,169)	1:27:A:VAL:HG13	1:33:A:GLY:HA2	13	0.11
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD1	12	0.11
(1,160)	1:73:A:ILE:HB	1:78:A:TYR:HD2	12	0.11
(1,147)	1:24:A:LEU:HD11	1:32:A:GLN:HG3	8	0.11
(1,147)	1:24:A:LEU:HD12	1:32:A:GLN:HG3	8	0.11
(1,147)	1:24:A:LEU:HD13	1:32:A:GLN:HG3	8	0.11
(1,140)	1:19:B:VAL:HG11	1:37:B:PRO:HB3	19	0.11
(1,140)	1:19:B:VAL:HG12	1:37:B:PRO:HB3	19	0.11
(1,140)	1:19:B:VAL:HG13	1:37:B:PRO:HB3	19	0.11
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD21	8	0.11
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD22	8	0.11
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD23	8	0.11
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD21	20	0.11
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD22	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:119:B:MET:HG3	1:124:B:LEU:HD23	20	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG21	2	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG22	2	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG23	2	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG21	2	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG22	2	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG23	2	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG21	2	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG22	2	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG23	2	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG21	6	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG22	6	0.11
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG23	6	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG21	6	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG22	6	0.11
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG23	6	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG21	6	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG22	6	0.11
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG23	6	0.11
(1,108)	1:22:A:ALA:HB1	1:24:A:LEU:HA	15	0.11
(1,108)	1:22:A:ALA:HB2	1:24:A:LEU:HA	15	0.11
(1,108)	1:22:A:ALA:HB3	1:24:A:LEU:HA	15	0.11
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	19	0.11
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	19	0.11
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	19	0.11
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	15	0.11
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	15	0.11
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	15	0.11
(1,89)	1:71:A:VAL:HG11	1:113:A:GLU:HB3	2	0.11
(1,89)	1:71:A:VAL:HG12	1:113:A:GLU:HB3	2	0.11
(1,89)	1:71:A:VAL:HG13	1:113:A:GLU:HB3	2	0.11
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD11	8	0.11
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD12	8	0.11
(1,82)	1:80:B:LEU:HA	1:80:B:LEU:HD13	8	0.11
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	1	0.11
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	1	0.11
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	1	0.11
(1,71)	1:19:A:VAL:HG21	1:103:A:LEU:HG	9	0.11
(1,71)	1:19:A:VAL:HG22	1:103:A:LEU:HG	9	0.11
(1,71)	1:19:A:VAL:HG23	1:103:A:LEU:HG	9	0.11
(1,41)	1:73:A:ILE:HG21	1:78:A:TYR:HB3	17	0.11
(1,41)	1:73:A:ILE:HG22	1:78:A:TYR:HB3	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:73:A:ILE:HG23	1:78:A:TYR:HB3	17	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	5	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	5	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	5	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	12	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	12	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	12	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	14	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	14	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	14	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	18	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	18	0.11
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	18	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	2	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	2	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	2	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	4	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	4	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	4	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	16	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	16	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	16	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	20	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	20	0.11
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	20	0.11
(1,3259)	1:125:B:ASN:HB2	1:126:B:ALA:H	17	0.1
(1,3259)	1:125:B:ASN:HB3	1:126:B:ALA:H	17	0.1
(1,3222)	1:116:B:ASN:HB2	1:118:B:LEU:H	7	0.1
(1,3222)	1:116:B:ASN:HB3	1:118:B:LEU:H	7	0.1
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB2	5	0.1
(1,3205)	1:113:B:GLU:HB2	1:116:B:ASN:HB3	5	0.1
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB2	5	0.1
(1,3205)	1:113:B:GLU:HB3	1:116:B:ASN:HB3	5	0.1
(1,3201)	1:112:B:LYS:HD2	1:116:B:ASN:HD22	5	0.1
(1,3201)	1:112:B:LYS:HD3	1:116:B:ASN:HD22	5	0.1
(1,3200)	1:112:B:LYS:HD2	1:116:B:ASN:HD21	18	0.1
(1,3200)	1:112:B:LYS:HD3	1:116:B:ASN:HD21	18	0.1
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD11	7	0.1
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD12	7	0.1
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD13	7	0.1
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD21	7	0.1
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD22	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3118)	1:89:B:GLU:HB2	1:122:B:LEU:HD23	7	0.1
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD11	7	0.1
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD12	7	0.1
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD13	7	0.1
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD21	7	0.1
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD22	7	0.1
(1,3118)	1:89:B:GLU:HB3	1:122:B:LEU:HD23	7	0.1
(1,3117)	1:89:B:GLU:HB2	1:90:B:GLN:H	4	0.1
(1,3117)	1:89:B:GLU:HB3	1:90:B:GLN:H	4	0.1
(1,3110)	1:87:B:LEU:HD11	1:90:B:GLN:HB3	5	0.1
(1,3110)	1:87:B:LEU:HD12	1:90:B:GLN:HB3	5	0.1
(1,3110)	1:87:B:LEU:HD13	1:90:B:GLN:HB3	5	0.1
(1,3110)	1:87:B:LEU:HD21	1:90:B:GLN:HB3	5	0.1
(1,3110)	1:87:B:LEU:HD22	1:90:B:GLN:HB3	5	0.1
(1,3110)	1:87:B:LEU:HD23	1:90:B:GLN:HB3	5	0.1
(1,3110)	1:87:B:LEU:HD11	1:90:B:GLN:HB3	17	0.1
(1,3110)	1:87:B:LEU:HD12	1:90:B:GLN:HB3	17	0.1
(1,3110)	1:87:B:LEU:HD13	1:90:B:GLN:HB3	17	0.1
(1,3110)	1:87:B:LEU:HD21	1:90:B:GLN:HB3	17	0.1
(1,3110)	1:87:B:LEU:HD22	1:90:B:GLN:HB3	17	0.1
(1,3110)	1:87:B:LEU:HD23	1:90:B:GLN:HB3	17	0.1
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB2	2	0.1
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB3	2	0.1
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB2	2	0.1
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB3	2	0.1
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB2	2	0.1
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB3	2	0.1
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB2	2	0.1
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB3	2	0.1
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB2	2	0.1
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB3	2	0.1
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB2	2	0.1
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB3	2	0.1
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB2	10	0.1
(1,3087)	1:80:B:LEU:HD11	1:84:B:SER:HB3	10	0.1
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB2	10	0.1
(1,3087)	1:80:B:LEU:HD12	1:84:B:SER:HB3	10	0.1
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB2	10	0.1
(1,3087)	1:80:B:LEU:HD13	1:84:B:SER:HB3	10	0.1
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB2	10	0.1
(1,3087)	1:80:B:LEU:HD21	1:84:B:SER:HB3	10	0.1
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB2	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3087)	1:80:B:LEU:HD22	1:84:B:SER:HB3	10	0.1
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB2	10	0.1
(1,3087)	1:80:B:LEU:HD23	1:84:B:SER:HB3	10	0.1
(1,3071)	1:77:B:LYS:HA	1:77:B:LYS:HD2	17	0.1
(1,3071)	1:77:B:LYS:HA	1:77:B:LYS:HD3	17	0.1
(1,3049)	1:74:B:GLU:HB2	1:77:B:LYS:HB2	18	0.1
(1,3049)	1:74:B:GLU:HB2	1:77:B:LYS:HB3	18	0.1
(1,3049)	1:74:B:GLU:HB3	1:77:B:LYS:HB2	18	0.1
(1,3049)	1:74:B:GLU:HB3	1:77:B:LYS:HB3	18	0.1
(1,3048)	1:74:B:GLU:HB2	1:77:B:LYS:H	9	0.1
(1,3048)	1:74:B:GLU:HB3	1:77:B:LYS:H	9	0.1
(1,3043)	1:73:B:ILE:HG12	1:84:B:SER:H	20	0.1
(1,3043)	1:73:B:ILE:HG13	1:84:B:SER:H	20	0.1
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG11	7	0.1
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG12	7	0.1
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG13	7	0.1
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG21	7	0.1
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG22	7	0.1
(1,3037)	1:73:B:ILE:H	1:85:B:VAL:HG23	7	0.1
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG12	6	0.1
(1,2992)	1:56:B:ALA:HB1	1:91:B:ILE:HG13	6	0.1
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG12	6	0.1
(1,2992)	1:56:B:ALA:HB2	1:91:B:ILE:HG13	6	0.1
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG12	6	0.1
(1,2992)	1:56:B:ALA:HB3	1:91:B:ILE:HG13	6	0.1
(1,2982)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	17	0.1
(1,2982)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	17	0.1
(1,2982)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	17	0.1
(1,2982)	1:53:B:VAL:HG21	1:94:B:LEU:HB2	17	0.1
(1,2982)	1:53:B:VAL:HG22	1:94:B:LEU:HB2	17	0.1
(1,2982)	1:53:B:VAL:HG23	1:94:B:LEU:HB2	17	0.1
(1,2961)	1:45:B:THR:HG21	1:49:B:TYR:HB2	18	0.1
(1,2961)	1:45:B:THR:HG21	1:49:B:TYR:HB3	18	0.1
(1,2961)	1:45:B:THR:HG22	1:49:B:TYR:HB2	18	0.1
(1,2961)	1:45:B:THR:HG22	1:49:B:TYR:HB3	18	0.1
(1,2961)	1:45:B:THR:HG23	1:49:B:TYR:HB2	18	0.1
(1,2961)	1:45:B:THR:HG23	1:49:B:TYR:HB3	18	0.1
(1,2949)	1:43:B:ASN:HB2	1:44:B:ASP:H	15	0.1
(1,2949)	1:43:B:ASN:HB3	1:44:B:ASP:H	15	0.1
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG11	8	0.1
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG12	8	0.1
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG13	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	8	0.1
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	8	0.1
(1,2947)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	8	0.1
(1,2940)	1:42:B:GLN:HB2	1:42:B:GLN:HE21	20	0.1
(1,2940)	1:42:B:GLN:HB3	1:42:B:GLN:HE21	20	0.1
(1,2930)	1:39:B:VAL:HG11	1:86:B:ILE:HB	8	0.1
(1,2930)	1:39:B:VAL:HG12	1:86:B:ILE:HB	8	0.1
(1,2930)	1:39:B:VAL:HG13	1:86:B:ILE:HB	8	0.1
(1,2930)	1:39:B:VAL:HG21	1:86:B:ILE:HB	8	0.1
(1,2930)	1:39:B:VAL:HG22	1:86:B:ILE:HB	8	0.1
(1,2930)	1:39:B:VAL:HG23	1:86:B:ILE:HB	8	0.1
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD11	11	0.1
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD12	11	0.1
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD13	11	0.1
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD21	11	0.1
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD22	11	0.1
(1,2924)	1:39:B:VAL:HB	1:106:B:LEU:HD23	11	0.1
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB2	3	0.1
(1,2887)	1:27:B:VAL:HG11	1:31:B:GLU:HB3	3	0.1
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB2	3	0.1
(1,2887)	1:27:B:VAL:HG12	1:31:B:GLU:HB3	3	0.1
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB2	3	0.1
(1,2887)	1:27:B:VAL:HG13	1:31:B:GLU:HB3	3	0.1
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB2	3	0.1
(1,2887)	1:27:B:VAL:HG21	1:31:B:GLU:HB3	3	0.1
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB2	3	0.1
(1,2887)	1:27:B:VAL:HG22	1:31:B:GLU:HB3	3	0.1
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB2	3	0.1
(1,2887)	1:27:B:VAL:HG23	1:31:B:GLU:HB3	3	0.1
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG11	6	0.1
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG12	6	0.1
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG13	6	0.1
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG21	6	0.1
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG22	6	0.1
(1,2880)	1:25:B:SER:H	1:35:B:VAL:HG23	6	0.1
(1,2876)	1:24:B:LEU:HD11	1:90:B:GLN:HE21	2	0.1
(1,2876)	1:24:B:LEU:HD12	1:90:B:GLN:HE21	2	0.1
(1,2876)	1:24:B:LEU:HD13	1:90:B:GLN:HE21	2	0.1
(1,2876)	1:24:B:LEU:HD21	1:90:B:GLN:HE21	2	0.1
(1,2876)	1:24:B:LEU:HD22	1:90:B:GLN:HE21	2	0.1
(1,2876)	1:24:B:LEU:HD23	1:90:B:GLN:HE21	2	0.1
(1,2874)	1:24:B:LEU:HD11	1:32:B:GLN:HE22	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2874)	1:24:B:LEU:HD12	1:32:B:GLN:HE22	18	0.1
(1,2874)	1:24:B:LEU:HD13	1:32:B:GLN:HE22	18	0.1
(1,2874)	1:24:B:LEU:HD21	1:32:B:GLN:HE22	18	0.1
(1,2874)	1:24:B:LEU:HD22	1:32:B:GLN:HE22	18	0.1
(1,2874)	1:24:B:LEU:HD23	1:32:B:GLN:HE22	18	0.1
(1,2872)	1:24:B:LEU:HD21	1:32:B:GLN:HG2	9	0.1
(1,2872)	1:24:B:LEU:HD22	1:32:B:GLN:HG2	9	0.1
(1,2872)	1:24:B:LEU:HD23	1:32:B:GLN:HG2	9	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	7	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	7	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	7	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	7	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	7	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	7	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG11	14	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG12	14	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG13	14	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG21	14	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG22	14	0.1
(1,2859)	1:23:B:ASP:HA	1:35:B:VAL:HG23	14	0.1
(1,2797)	1:14:B:ILE:HD11	1:99:B:LEU:HB2	11	0.1
(1,2797)	1:14:B:ILE:HD11	1:99:B:LEU:HB3	11	0.1
(1,2797)	1:14:B:ILE:HD12	1:99:B:LEU:HB2	11	0.1
(1,2797)	1:14:B:ILE:HD12	1:99:B:LEU:HB3	11	0.1
(1,2797)	1:14:B:ILE:HD13	1:99:B:LEU:HB2	11	0.1
(1,2797)	1:14:B:ILE:HD13	1:99:B:LEU:HB3	11	0.1
(1,2753)	1:120:A:ILE:H	1:120:A:ILE:HG12	19	0.1
(1,2753)	1:120:A:ILE:H	1:120:A:ILE:HG13	19	0.1
(1,2742)	1:119:A:MET:HA	1:124:A:LEU:HB2	8	0.1
(1,2742)	1:119:A:MET:HA	1:124:A:LEU:HB3	8	0.1
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD11	6	0.1
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD12	6	0.1
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD13	6	0.1
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD21	6	0.1
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD22	6	0.1
(1,2734)	1:118:A:LEU:H	1:118:A:LEU:HD23	6	0.1
(1,2633)	1:95:A:ASP:HB2	1:30:B:SER:H	12	0.1
(1,2633)	1:95:A:ASP:HB3	1:30:B:SER:H	12	0.1
(1,2627)	1:94:A:LEU:H	1:94:A:LEU:HD11	12	0.1
(1,2627)	1:94:A:LEU:H	1:94:A:LEU:HD12	12	0.1
(1,2627)	1:94:A:LEU:H	1:94:A:LEU:HD13	12	0.1
(1,2627)	1:94:A:LEU:H	1:94:A:LEU:HD21	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2627)	1:94:A:LEU:H	1:94:A:LEU:HD22	12	0.1
(1,2627)	1:94:A:LEU:H	1:94:A:LEU:HD23	12	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	6	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	6	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	6	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	6	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	6	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	6	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	6	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	6	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	6	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	6	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	6	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	6	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD11	7	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD12	7	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD13	7	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD21	7	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD22	7	0.1
(1,2618)	1:89:A:GLU:HB2	1:122:A:LEU:HD23	7	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD11	7	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD12	7	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD13	7	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD21	7	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD22	7	0.1
(1,2618)	1:89:A:GLU:HB3	1:122:A:LEU:HD23	7	0.1
(1,2617)	1:89:A:GLU:HB2	1:90:A:GLN:H	10	0.1
(1,2617)	1:89:A:GLU:HB3	1:90:A:GLN:H	10	0.1
(1,2605)	1:87:A:LEU:HB2	1:90:A:GLN:H	4	0.1
(1,2605)	1:87:A:LEU:HB3	1:90:A:GLN:H	4	0.1
(1,2566)	1:76:A:LYS:HA	1:76:A:LYS:HD2	20	0.1
(1,2566)	1:76:A:LYS:HA	1:76:A:LYS:HD3	20	0.1
(1,2560)	1:75:A:LYS:HD2	1:82:A:LYS:HB2	12	0.1
(1,2560)	1:75:A:LYS:HD2	1:82:A:LYS:HB3	12	0.1
(1,2560)	1:75:A:LYS:HD3	1:82:A:LYS:HB2	12	0.1
(1,2560)	1:75:A:LYS:HD3	1:82:A:LYS:HB3	12	0.1
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD11	17	0.1
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD12	17	0.1
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD13	17	0.1
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD21	17	0.1
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD22	17	0.1
(1,2544)	1:73:A:ILE:HD11	1:106:A:LEU:HD23	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD11	17	0.1
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD12	17	0.1
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD13	17	0.1
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD21	17	0.1
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD22	17	0.1
(1,2544)	1:73:A:ILE:HD12	1:106:A:LEU:HD23	17	0.1
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD11	17	0.1
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD12	17	0.1
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD13	17	0.1
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD21	17	0.1
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD22	17	0.1
(1,2544)	1:73:A:ILE:HD13	1:106:A:LEU:HD23	17	0.1
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG11	20	0.1
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG12	20	0.1
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG13	20	0.1
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG21	20	0.1
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG22	20	0.1
(1,2535)	1:72:A:GLU:HG2	1:85:A:VAL:HG23	20	0.1
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG11	20	0.1
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG12	20	0.1
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG13	20	0.1
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG21	20	0.1
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG22	20	0.1
(1,2535)	1:72:A:GLU:HG3	1:85:A:VAL:HG23	20	0.1
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG11	6	0.1
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG12	6	0.1
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG13	6	0.1
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG21	6	0.1
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG22	6	0.1
(1,2503)	1:62:A:ILE:HB	1:85:A:VAL:HG23	6	0.1
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	5	0.1
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	5	0.1
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	5	0.1
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	5	0.1
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	5	0.1
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	5	0.1
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	7	0.1
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	7	0.1
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	7	0.1
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	7	0.1
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	7	0.1
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2486)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	17	0.1
(1,2486)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	17	0.1
(1,2486)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	17	0.1
(1,2486)	1:53:A:VAL:HG21	1:94:A:LEU:HB2	17	0.1
(1,2486)	1:53:A:VAL:HG22	1:94:A:LEU:HB2	17	0.1
(1,2486)	1:53:A:VAL:HG23	1:94:A:LEU:HB2	17	0.1
(1,2448)	1:43:A:ASN:HB2	1:44:A:ASP:H	15	0.1
(1,2448)	1:43:A:ASN:HB3	1:44:A:ASP:H	15	0.1
(1,2436)	1:41:A:ILE:HB	1:114:A:VAL:HG11	12	0.1
(1,2436)	1:41:A:ILE:HB	1:114:A:VAL:HG12	12	0.1
(1,2436)	1:41:A:ILE:HB	1:114:A:VAL:HG13	12	0.1
(1,2436)	1:41:A:ILE:HB	1:114:A:VAL:HG21	12	0.1
(1,2436)	1:41:A:ILE:HB	1:114:A:VAL:HG22	12	0.1
(1,2436)	1:41:A:ILE:HB	1:114:A:VAL:HG23	12	0.1
(1,2416)	1:38:A:VAL:HG11	1:57:A:ALA:H	18	0.1
(1,2416)	1:38:A:VAL:HG12	1:57:A:ALA:H	18	0.1
(1,2416)	1:38:A:VAL:HG13	1:57:A:ALA:H	18	0.1
(1,2416)	1:38:A:VAL:HG21	1:57:A:ALA:H	18	0.1
(1,2416)	1:38:A:VAL:HG22	1:57:A:ALA:H	18	0.1
(1,2416)	1:38:A:VAL:HG23	1:57:A:ALA:H	18	0.1
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB2	11	0.1
(1,2391)	1:30:A:SER:H	1:95:B:ASP:HB3	11	0.1
(1,2384)	1:27:A:VAL:HG11	1:34:A:GLY:H	12	0.1
(1,2384)	1:27:A:VAL:HG12	1:34:A:GLY:H	12	0.1
(1,2384)	1:27:A:VAL:HG13	1:34:A:GLY:H	12	0.1
(1,2384)	1:27:A:VAL:HG21	1:34:A:GLY:H	12	0.1
(1,2384)	1:27:A:VAL:HG22	1:34:A:GLY:H	12	0.1
(1,2384)	1:27:A:VAL:HG23	1:34:A:GLY:H	12	0.1
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB2	3	0.1
(1,2381)	1:27:A:VAL:HG11	1:31:A:GLU:HB3	3	0.1
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB2	3	0.1
(1,2381)	1:27:A:VAL:HG12	1:31:A:GLU:HB3	3	0.1
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB2	3	0.1
(1,2381)	1:27:A:VAL:HG13	1:31:A:GLU:HB3	3	0.1
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB2	3	0.1
(1,2381)	1:27:A:VAL:HG21	1:31:A:GLU:HB3	3	0.1
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB2	3	0.1
(1,2381)	1:27:A:VAL:HG22	1:31:A:GLU:HB3	3	0.1
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB2	3	0.1
(1,2381)	1:27:A:VAL:HG23	1:31:A:GLU:HB3	3	0.1
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE21	9	0.1
(1,2378)	1:26:A:PRO:HD2	1:28:B:GLN:HE22	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE21	9	0.1
(1,2378)	1:26:A:PRO:HD3	1:28:B:GLN:HE22	9	0.1
(1,2377)	1:26:A:PRO:HD2	1:27:A:VAL:H	16	0.1
(1,2377)	1:26:A:PRO:HD3	1:27:A:VAL:H	16	0.1
(1,2361)	1:24:A:LEU:HB2	1:34:A:GLY:H	4	0.1
(1,2361)	1:24:A:LEU:HB3	1:34:A:GLY:H	4	0.1
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG11	4	0.1
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG12	4	0.1
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG13	4	0.1
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG21	4	0.1
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG22	4	0.1
(1,2352)	1:23:A:ASP:HA	1:35:A:VAL:HG23	4	0.1
(1,2344)	1:22:A:ALA:HB1	1:24:A:LEU:HB2	9	0.1
(1,2344)	1:22:A:ALA:HB1	1:24:A:LEU:HB3	9	0.1
(1,2344)	1:22:A:ALA:HB2	1:24:A:LEU:HB2	9	0.1
(1,2344)	1:22:A:ALA:HB2	1:24:A:LEU:HB3	9	0.1
(1,2344)	1:22:A:ALA:HB3	1:24:A:LEU:HB2	9	0.1
(1,2344)	1:22:A:ALA:HB3	1:24:A:LEU:HB3	9	0.1
(1,2316)	1:19:A:VAL:HG11	1:106:A:LEU:H	3	0.1
(1,2316)	1:19:A:VAL:HG12	1:106:A:LEU:H	3	0.1
(1,2316)	1:19:A:VAL:HG13	1:106:A:LEU:H	3	0.1
(1,2316)	1:19:A:VAL:HG21	1:106:A:LEU:H	3	0.1
(1,2316)	1:19:A:VAL:HG22	1:106:A:LEU:H	3	0.1
(1,2316)	1:19:A:VAL:HG23	1:106:A:LEU:H	3	0.1
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD1	15	0.1
(1,2258)	1:18:B:ASP:HA	1:105:B:TYR:HD2	15	0.1
(1,2236)	1:76:B:LYS:H	1:80:B:LEU:H	16	0.1
(1,2236)	1:76:B:LYS:H	1:80:B:LEU:H	17	0.1
(1,2200)	1:119:B:MET:HE1	1:125:B:ASN:HD22	8	0.1
(1,2200)	1:119:B:MET:HE2	1:125:B:ASN:HD22	8	0.1
(1,2200)	1:119:B:MET:HE3	1:125:B:ASN:HD22	8	0.1
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD11	4	0.1
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD12	4	0.1
(1,2195)	1:116:B:ASN:HD22	1:120:B:ILE:HD13	4	0.1
(1,2180)	1:23:B:ASP:H	1:100:B:LYS:H	16	0.1
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG21	1	0.1
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG22	1	0.1
(1,2175)	1:42:B:GLN:HE21	1:54:B:ILE:HG23	1	0.1
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG21	7	0.1
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG22	7	0.1
(1,2173)	1:42:B:GLN:HE21	1:53:B:VAL:HG23	7	0.1
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG21	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG22	9	0.1
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG23	9	0.1
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG21	18	0.1
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG22	18	0.1
(1,2166)	1:42:B:GLN:HE22	1:54:B:ILE:HG23	18	0.1
(1,2159)	1:112:A:LYS:HB2	1:116:A:ASN:HD21	8	0.1
(1,2149)	1:119:B:MET:HA	1:124:B:LEU:H	10	0.1
(1,2149)	1:119:B:MET:HA	1:124:B:LEU:H	13	0.1
(1,2149)	1:119:B:MET:HA	1:124:B:LEU:H	18	0.1
(1,2147)	1:120:A:ILE:HG21	1:123:A:GLY:H	4	0.1
(1,2147)	1:120:A:ILE:HG22	1:123:A:GLY:H	4	0.1
(1,2147)	1:120:A:ILE:HG23	1:123:A:GLY:H	4	0.1
(1,2145)	1:43:A:ASN:HB3	1:123:B:GLY:H	2	0.1
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	10	0.1
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	12	0.1
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	14	0.1
(1,2144)	1:42:A:GLN:HA	1:123:B:GLY:H	18	0.1
(1,2140)	1:69:B:THR:HB	1:121:B:SER:H	6	0.1
(1,2107)	1:112:B:LYS:H	1:115:B:ASP:H	20	0.1
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	17	0.1
(1,2106)	1:111:B:MET:H	1:111:B:MET:HG2	20	0.1
(1,2092)	1:78:B:TYR:HA	1:105:B:TYR:H	15	0.1
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	7	0.1
(1,2077)	1:99:B:LEU:HA	1:101:B:GLU:H	19	0.1
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	12	0.1
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	12	0.1
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	12	0.1
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD11	18	0.1
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD12	18	0.1
(1,2051)	1:93:B:THR:H	1:94:B:LEU:HD13	18	0.1
(1,2039)	1:87:B:LEU:H	1:90:B:GLN:H	15	0.1
(1,2019)	1:73:B:ILE:HB	1:84:B:SER:H	6	0.1
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	3	0.1
(1,2005)	1:74:B:GLU:HG3	1:77:B:LYS:H	10	0.1
(1,1994)	1:67:B:ILE:HD11	1:70:B:HIS:H	19	0.1
(1,1994)	1:67:B:ILE:HD12	1:70:B:HIS:H	19	0.1
(1,1994)	1:67:B:ILE:HD13	1:70:B:HIS:H	19	0.1
(1,1939)	1:42:A:GLN:HE22	1:45:A:THR:H	17	0.1
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	3	0.1
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	3	0.1
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	3	0.1
(1,1936)	1:41:B:ILE:HD11	1:43:B:ASN:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1936)	1:41:B:ILE:HD12	1:43:B:ASN:H	10	0.1
(1,1936)	1:41:B:ILE:HD13	1:43:B:ASN:H	10	0.1
(1,1933)	1:122:A:LEU:HA	1:43:B:ASN:H	1	0.1
(1,1927)	1:42:A:GLN:H	1:42:A:GLN:HE21	17	0.1
(1,1900)	1:27:B:VAL:HG11	1:33:B:GLY:H	6	0.1
(1,1900)	1:27:B:VAL:HG12	1:33:B:GLY:H	6	0.1
(1,1900)	1:27:B:VAL:HG13	1:33:B:GLY:H	6	0.1
(1,1883)	1:24:B:LEU:HD11	1:25:B:SER:H	8	0.1
(1,1883)	1:24:B:LEU:HD12	1:25:B:SER:H	8	0.1
(1,1883)	1:24:B:LEU:HD13	1:25:B:SER:H	8	0.1
(1,1873)	1:22:B:ALA:H	1:35:B:VAL:HB	18	0.1
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	4	0.1
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	6	0.1
(1,1820)	1:99:B:LEU:H	1:99:B:LEU:HG	9	0.1
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG21	19	0.1
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG22	19	0.1
(1,1780)	1:73:B:ILE:H	1:73:B:ILE:HG23	19	0.1
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	1	0.1
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	1	0.1
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	1	0.1
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD11	18	0.1
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD12	18	0.1
(1,1755)	1:41:B:ILE:H	1:41:B:ILE:HD13	18	0.1
(1,1746)	1:24:A:LEU:HB3	1:25:A:SER:H	17	0.1
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	2	0.1
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	4	0.1
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	11	0.1
(1,1721)	1:100:B:LYS:HB3	1:101:B:GLU:H	20	0.1
(1,1707)	1:127:B:VAL:HB	1:128:B:ALA:H	11	0.1
(1,1683)	1:27:B:VAL:H	1:28:B:GLN:H	4	0.1
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	3	0.1
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	3	0.1
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	3	0.1
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG21	15	0.1
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG22	15	0.1
(1,1679)	1:35:B:VAL:H	1:35:B:VAL:HG23	15	0.1
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD21	5	0.1
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD22	5	0.1
(1,1676)	1:124:A:LEU:H	1:124:A:LEU:HD23	5	0.1
(1,1671)	1:76:B:LYS:H	1:76:B:LYS:HB2	15	0.1
(1,1650)	1:84:B:SER:HB3	1:85:B:VAL:H	16	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG21	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG22	7	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG23	7	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG21	10	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG22	10	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG23	10	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG21	18	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG22	18	0.1
(1,1642)	1:54:B:ILE:H	1:54:B:ILE:HG23	18	0.1
(1,1609)	1:85:B:VAL:HB	1:86:B:ILE:H	4	0.1
(1,1594)	1:94:B:LEU:HB3	1:95:B:ASP:H	4	0.1
(1,1592)	1:105:B:TYR:H	1:106:B:LEU:H	3	0.1
(1,1534)	1:102:B:LYS:H	1:103:B:LEU:H	11	0.1
(1,1506)	1:20:B:TYR:H	1:21:B:LEU:H	1	0.1
(1,1499)	1:48:B:LYS:H	1:48:B:LYS:HD3	9	0.1
(1,1498)	1:48:B:LYS:H	1:48:B:LYS:HD2	4	0.1
(1,1498)	1:48:B:LYS:H	1:48:B:LYS:HD2	14	0.1
(1,1471)	1:80:B:LEU:H	1:80:B:LEU:HB3	4	0.1
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	3	0.1
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	4	0.1
(1,1436)	1:89:B:GLU:HB3	1:90:B:GLN:H	17	0.1
(1,1396)	1:119:B:MET:HB3	1:119:B:MET:HE1	5	0.1
(1,1396)	1:119:B:MET:HB3	1:119:B:MET:HE2	5	0.1
(1,1396)	1:119:B:MET:HB3	1:119:B:MET:HE3	5	0.1
(1,1384)	1:62:B:ILE:HA	1:62:B:ILE:HD11	1	0.1
(1,1384)	1:62:B:ILE:HA	1:62:B:ILE:HD12	1	0.1
(1,1384)	1:62:B:ILE:HA	1:62:B:ILE:HD13	1	0.1
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD11	16	0.1
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD12	16	0.1
(1,1383)	1:116:B:ASN:HB3	1:120:B:ILE:HD13	16	0.1
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG11	4	0.1
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG12	4	0.1
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG13	4	0.1
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG11	12	0.1
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG12	12	0.1
(1,1355)	1:111:A:MET:HA	1:114:A:VAL:HG13	12	0.1
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG11	19	0.1
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG12	19	0.1
(1,1346)	1:25:A:SER:HA	1:27:A:VAL:HG13	19	0.1
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG21	17	0.1
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG22	17	0.1
(1,1345)	1:25:B:SER:HA	1:27:B:VAL:HG23	17	0.1
(1,1330)	1:40:B:ILE:HA	1:55:B:VAL:HA	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1314)	1:75:A:LYS:HA	1:75:A:LYS:HD2	14	0.1
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	1	0.1
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	2	0.1
(1,1306)	1:109:A:ASP:HA	1:112:A:LYS:HB3	12	0.1
(1,1288)	1:80:B:LEU:HB3	1:81:B:ASP:HB2	15	0.1
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD1	12	0.1
(1,1286)	1:73:B:ILE:HB	1:78:B:TYR:HD2	12	0.1
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD21	8	0.1
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD22	8	0.1
(1,1253)	1:119:A:MET:HG3	1:124:A:LEU:HD23	8	0.1
(1,1245)	1:88:B:LEU:HD11	1:114:B:VAL:HA	2	0.1
(1,1245)	1:88:B:LEU:HD12	1:114:B:VAL:HA	2	0.1
(1,1245)	1:88:B:LEU:HD13	1:114:B:VAL:HA	2	0.1
(1,1233)	1:22:B:ALA:HB1	1:24:B:LEU:HA	15	0.1
(1,1233)	1:22:B:ALA:HB2	1:24:B:LEU:HA	15	0.1
(1,1233)	1:22:B:ALA:HB3	1:24:B:LEU:HA	15	0.1
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD11	1	0.1
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD12	1	0.1
(1,1227)	1:21:B:LEU:HB2	1:21:B:LEU:HD13	1	0.1
(1,1214)	1:71:B:VAL:HG11	1:113:B:GLU:HB3	2	0.1
(1,1214)	1:71:B:VAL:HG12	1:113:B:GLU:HB3	2	0.1
(1,1214)	1:71:B:VAL:HG13	1:113:B:GLU:HB3	2	0.1
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD11	16	0.1
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD12	16	0.1
(1,1207)	1:80:A:LEU:HA	1:80:A:LEU:HD13	16	0.1
(1,1196)	1:19:B:VAL:HG21	1:103:B:LEU:HG	9	0.1
(1,1196)	1:19:B:VAL:HG22	1:103:B:LEU:HG	9	0.1
(1,1196)	1:19:B:VAL:HG23	1:103:B:LEU:HG	9	0.1
(1,1169)	1:53:B:VAL:HG11	1:94:B:LEU:HB2	19	0.1
(1,1169)	1:53:B:VAL:HG12	1:94:B:LEU:HB2	19	0.1
(1,1169)	1:53:B:VAL:HG13	1:94:B:LEU:HB2	19	0.1
(1,1167)	1:73:B:ILE:HG21	1:78:B:TYR:HB3	17	0.1
(1,1167)	1:73:B:ILE:HG22	1:78:B:TYR:HB3	17	0.1
(1,1167)	1:73:B:ILE:HG23	1:78:B:TYR:HB3	17	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG21	9	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG22	9	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG23	9	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG21	12	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG22	12	0.1
(1,1163)	1:42:B:GLN:HB2	1:54:B:ILE:HG23	12	0.1
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG21	18	0.1
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG22	18	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1162)	1:42:B:GLN:HB3	1:54:B:ILE:HG23	18	0.1
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG21	2	0.1
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG22	2	0.1
(1,1156)	1:78:B:TYR:HB3	1:104:B:THR:HG23	2	0.1
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	2	0.1
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	2	0.1
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	2	0.1
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG21	20	0.1
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG22	20	0.1
(1,1153)	1:103:B:LEU:HB2	1:104:B:THR:HG23	20	0.1
(1,1119)	1:18:A:ASP:HB3	1:20:A:TYR:HE1	19	0.1
(1,1119)	1:18:A:ASP:HB3	1:20:A:TYR:HE2	19	0.1
(1,1116)	1:18:A:ASP:HA	1:105:A:TYR:HA	14	0.1
(1,1092)	1:118:A:LEU:H	1:121:A:SER:H	5	0.1
(1,1090)	1:113:A:GLU:HA	1:116:A:ASN:H	1	0.1
(1,1083)	1:76:A:LYS:H	1:80:A:LEU:H	2	0.1
(1,1083)	1:76:A:LYS:H	1:80:A:LEU:H	17	0.1
(1,1062)	1:122:A:LEU:HG	1:43:B:ASN:H	16	0.1
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD11	16	0.1
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD12	16	0.1
(1,1043)	1:116:A:ASN:HD22	1:120:A:ILE:HD13	16	0.1
(1,1042)	1:119:B:MET:HG3	1:124:B:LEU:H	7	0.1
(1,1042)	1:119:B:MET:HG3	1:124:B:LEU:H	14	0.1
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG11	17	0.1
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG12	17	0.1
(1,1039)	1:112:A:LYS:H	1:114:A:VAL:HG13	17	0.1
(1,1034)	1:23:A:ASP:H	1:100:A:LYS:H	16	0.1
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG21	9	0.1
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG22	9	0.1
(1,1020)	1:42:A:GLN:HE22	1:54:A:ILE:HG23	9	0.1
(1,1017)	1:113:A:GLU:HA	1:116:A:ASN:HD22	10	0.1
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	9	0.1
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	9	0.1
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	9	0.1
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD11	13	0.1
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD12	13	0.1
(1,1014)	1:116:A:ASN:HD21	1:120:A:ILE:HD13	13	0.1
(1,1006)	1:123:A:GLY:H	1:125:A:ASN:H	11	0.1
(1,1004)	1:119:A:MET:HE1	1:124:A:LEU:H	19	0.1
(1,1004)	1:119:A:MET:HE2	1:124:A:LEU:H	19	0.1
(1,1004)	1:119:A:MET:HE3	1:124:A:LEU:H	19	0.1
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	17	0.1
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	17	0.1
(1,1001)	1:120:B:ILE:HG21	1:123:B:GLY:H	18	0.1
(1,1001)	1:120:B:ILE:HG22	1:123:B:GLY:H	18	0.1
(1,1001)	1:120:B:ILE:HG23	1:123:B:GLY:H	18	0.1
(1,999)	1:123:A:GLY:H	1:43:B:ASN:HB3	4	0.1
(1,994)	1:69:A:THR:HB	1:121:A:SER:H	6	0.1
(1,984)	1:119:A:MET:H	1:119:A:MET:HE1	10	0.1
(1,984)	1:119:A:MET:H	1:119:A:MET:HE2	10	0.1
(1,984)	1:119:A:MET:H	1:119:A:MET:HE3	10	0.1
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	11	0.1
(1,965)	1:111:A:MET:HG3	1:112:A:LYS:H	19	0.1
(1,961)	1:112:A:LYS:H	1:115:A:ASP:H	20	0.1
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	17	0.1
(1,960)	1:111:A:MET:H	1:111:A:MET:HG2	20	0.1
(1,936)	1:20:A:TYR:H	1:104:A:THR:H	8	0.1
(1,931)	1:99:A:LEU:HA	1:101:A:GLU:H	7	0.1
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD11	13	0.1
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD12	13	0.1
(1,905)	1:93:A:THR:H	1:94:A:LEU:HD13	13	0.1
(1,882)	1:86:A:ILE:HD11	1:87:A:LEU:H	10	0.1
(1,882)	1:86:A:ILE:HD12	1:87:A:LEU:H	10	0.1
(1,882)	1:86:A:ILE:HD13	1:87:A:LEU:H	10	0.1
(1,873)	1:73:A:ILE:HB	1:84:A:SER:H	6	0.1
(1,865)	1:80:A:LEU:HD11	1:82:A:LYS:H	9	0.1
(1,865)	1:80:A:LEU:HD12	1:82:A:LYS:H	9	0.1
(1,865)	1:80:A:LEU:HD13	1:82:A:LYS:H	9	0.1
(1,848)	1:67:A:ILE:HD11	1:70:A:HIS:H	17	0.1
(1,848)	1:67:A:ILE:HD12	1:70:A:HIS:H	17	0.1
(1,848)	1:67:A:ILE:HD13	1:70:A:HIS:H	17	0.1
(1,782)	1:42:A:GLN:H	1:54:A:ILE:H	17	0.1
(1,780)	1:40:A:ILE:H	1:42:A:GLN:H	15	0.1
(1,754)	1:27:A:VAL:HG11	1:33:A:GLY:H	6	0.1
(1,754)	1:27:A:VAL:HG12	1:33:A:GLY:H	6	0.1
(1,754)	1:27:A:VAL:HG13	1:33:A:GLY:H	6	0.1
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	4	0.1
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	13	0.1
(1,745)	1:28:A:GLN:HA	1:31:A:GLU:H	18	0.1
(1,742)	1:31:A:GLU:H	1:95:B:ASP:H	18	0.1
(1,696)	1:92:A:ARG:H	1:92:A:ARG:HG2	5	0.1
(1,676)	1:99:A:LEU:H	1:99:A:LEU:HG	3	0.1
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG21	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG22	10	0.1
(1,638)	1:73:A:ILE:H	1:73:A:ILE:HG23	10	0.1
(1,622)	1:96:B:LYS:HB3	1:97:B:LYS:H	18	0.1
(1,622)	1:96:B:LYS:HB3	1:97:B:LYS:H	20	0.1
(1,587)	1:91:A:ILE:H	1:91:A:ILE:HG13	14	0.1
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	11	0.1
(1,578)	1:100:A:LYS:HB3	1:101:A:GLU:H	18	0.1
(1,564)	1:127:A:VAL:HB	1:128:A:ALA:H	11	0.1
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	1	0.1
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	15	0.1
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	17	0.1
(1,542)	1:27:A:VAL:H	1:28:A:GLN:H	18	0.1
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG21	16	0.1
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG22	16	0.1
(1,538)	1:35:A:VAL:H	1:35:A:VAL:HG23	16	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD21	13	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD22	13	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD23	13	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD21	14	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD22	14	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD23	14	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD21	15	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD22	15	0.1
(1,535)	1:124:B:LEU:H	1:124:B:LEU:HD23	15	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG21	7	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG22	7	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG23	7	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG21	17	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG22	17	0.1
(1,503)	1:54:A:ILE:H	1:54:A:ILE:HG23	17	0.1
(1,491)	1:74:A:GLU:H	1:74:A:GLU:HG3	5	0.1
(1,491)	1:74:A:GLU:H	1:74:A:GLU:HG3	15	0.1
(1,478)	1:111:A:MET:H	1:111:A:MET:HE1	8	0.1
(1,478)	1:111:A:MET:H	1:111:A:MET:HE2	8	0.1
(1,478)	1:111:A:MET:H	1:111:A:MET:HE3	8	0.1
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	4	0.1
(1,470)	1:85:A:VAL:HB	1:86:A:ILE:H	8	0.1
(1,455)	1:105:A:TYR:H	1:106:A:LEU:H	13	0.1
(1,440)	1:100:B:LYS:H	1:100:B:LYS:HB2	19	0.1
(1,418)	1:126:A:ALA:HB1	1:127:A:VAL:H	17	0.1
(1,418)	1:126:A:ALA:HB2	1:127:A:VAL:H	17	0.1
(1,418)	1:126:A:ALA:HB3	1:127:A:VAL:H	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,417)	1:126:A:ALA:HA	1:127:A:VAL:H	3	0.1
(1,373)	1:19:A:VAL:H	1:20:A:TYR:H	10	0.1
(1,371)	1:20:A:TYR:H	1:21:A:LEU:H	7	0.1
(1,347)	1:124:A:LEU:HA	1:125:A:ASN:H	17	0.1
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	8	0.1
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	8	0.1
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	8	0.1
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD21	13	0.1
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD22	13	0.1
(1,334)	1:80:A:LEU:H	1:80:A:LEU:HD23	13	0.1
(1,329)	1:82:A:LYS:H	1:82:A:LYS:HB2	9	0.1
(1,307)	1:89:A:GLU:HB3	1:90:A:GLN:H	6	0.1
(1,257)	1:62:A:ILE:HA	1:62:A:ILE:HD11	9	0.1
(1,257)	1:62:A:ILE:HA	1:62:A:ILE:HD12	9	0.1
(1,257)	1:62:A:ILE:HA	1:62:A:ILE:HD13	9	0.1
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD11	13	0.1
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD12	13	0.1
(1,256)	1:116:A:ASN:HB3	1:120:A:ILE:HD13	13	0.1
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	13	0.1
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	13	0.1
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	13	0.1
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	13	0.1
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	13	0.1
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	13	0.1
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	13	0.1
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	13	0.1
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	13	0.1
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB1	15	0.1
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB2	15	0.1
(1,253)	1:88:A:LEU:HD11	1:117:A:ALA:HB3	15	0.1
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB1	15	0.1
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB2	15	0.1
(1,253)	1:88:A:LEU:HD12	1:117:A:ALA:HB3	15	0.1
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB1	15	0.1
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB2	15	0.1
(1,253)	1:88:A:LEU:HD13	1:117:A:ALA:HB3	15	0.1
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD21	8	0.1
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD22	8	0.1
(1,244)	1:56:A:ALA:HB1	1:88:A:LEU:HD23	8	0.1
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD21	8	0.1
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD22	8	0.1
(1,244)	1:56:A:ALA:HB2	1:88:A:LEU:HD23	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD21	8	0.1
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD22	8	0.1
(1,244)	1:56:A:ALA:HB3	1:88:A:LEU:HD23	8	0.1
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD11	16	0.1
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD12	16	0.1
(1,231)	1:56:B:ALA:HA	1:91:B:ILE:HD13	16	0.1
(1,223)	1:19:A:VAL:HG21	1:105:A:TYR:HA	8	0.1
(1,223)	1:19:A:VAL:HG22	1:105:A:TYR:HA	8	0.1
(1,223)	1:19:A:VAL:HG23	1:105:A:TYR:HA	8	0.1
(1,221)	1:72:A:GLU:HA	1:85:A:VAL:HG21	16	0.1
(1,221)	1:72:A:GLU:HA	1:85:A:VAL:HG22	16	0.1
(1,221)	1:72:A:GLU:HA	1:85:A:VAL:HG23	16	0.1
(1,218)	1:25:A:SER:HA	1:27:A:VAL:HG21	4	0.1
(1,218)	1:25:A:SER:HA	1:27:A:VAL:HG22	4	0.1
(1,218)	1:25:A:SER:HA	1:27:A:VAL:HG23	4	0.1
(1,204)	1:40:A:ILE:HA	1:55:A:VAL:HA	8	0.1
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD11	3	0.1
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD12	3	0.1
(1,184)	1:119:A:MET:HA	1:124:A:LEU:HD13	3	0.1
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD21	6	0.1
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD22	6	0.1
(1,172)	1:106:A:LEU:HA	1:106:A:LEU:HD23	6	0.1
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD21	7	0.1
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD22	7	0.1
(1,127)	1:119:A:MET:HG2	1:124:A:LEU:HD23	7	0.1
(1,120)	1:88:A:LEU:HD11	1:114:A:VAL:HA	6	0.1
(1,120)	1:88:A:LEU:HD12	1:114:A:VAL:HA	6	0.1
(1,120)	1:88:A:LEU:HD13	1:114:A:VAL:HA	6	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	3	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	3	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	3	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	7	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	7	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	7	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD11	16	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD12	16	0.1
(1,119)	1:118:A:LEU:HA	1:118:A:LEU:HD13	16	0.1
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG21	8	0.1
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG22	8	0.1
(1,117)	1:111:A:MET:HE1	1:114:A:VAL:HG23	8	0.1
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG21	8	0.1
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG22	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:111:A:MET:HE2	1:114:A:VAL:HG23	8	0.1
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG21	8	0.1
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG22	8	0.1
(1,117)	1:111:A:MET:HE3	1:114:A:VAL:HG23	8	0.1
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD11	1	0.1
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD12	1	0.1
(1,102)	1:21:A:LEU:HB2	1:21:A:LEU:HD13	1	0.1
(1,101)	1:56:A:ALA:HB1	1:91:A:ILE:HB	12	0.1
(1,101)	1:56:A:ALA:HB2	1:91:A:ILE:HB	12	0.1
(1,101)	1:56:A:ALA:HB3	1:91:A:ILE:HB	12	0.1
(1,95)	1:27:A:VAL:HG21	1:33:A:GLY:HA2	20	0.1
(1,95)	1:27:A:VAL:HG22	1:33:A:GLY:HA2	20	0.1
(1,95)	1:27:A:VAL:HG23	1:33:A:GLY:HA2	20	0.1
(1,92)	1:45:A:THR:HG21	1:49:A:TYR:HA	16	0.1
(1,92)	1:45:A:THR:HG22	1:49:A:TYR:HA	16	0.1
(1,92)	1:45:A:THR:HG23	1:49:A:TYR:HA	16	0.1
(1,78)	1:71:A:VAL:HG21	1:113:A:GLU:HB3	5	0.1
(1,78)	1:71:A:VAL:HG22	1:113:A:GLU:HB3	5	0.1
(1,78)	1:71:A:VAL:HG23	1:113:A:GLU:HB3	5	0.1
(1,43)	1:53:A:VAL:HG11	1:94:A:LEU:HB2	19	0.1
(1,43)	1:53:A:VAL:HG12	1:94:A:LEU:HB2	19	0.1
(1,43)	1:53:A:VAL:HG13	1:94:A:LEU:HB2	19	0.1
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG21	2	0.1
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG22	2	0.1
(1,30)	1:78:A:TYR:HB3	1:104:A:THR:HG23	2	0.1
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG21	15	0.1
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG22	15	0.1
(1,27)	1:103:A:LEU:HB2	1:104:A:THR:HG23	15	0.1

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

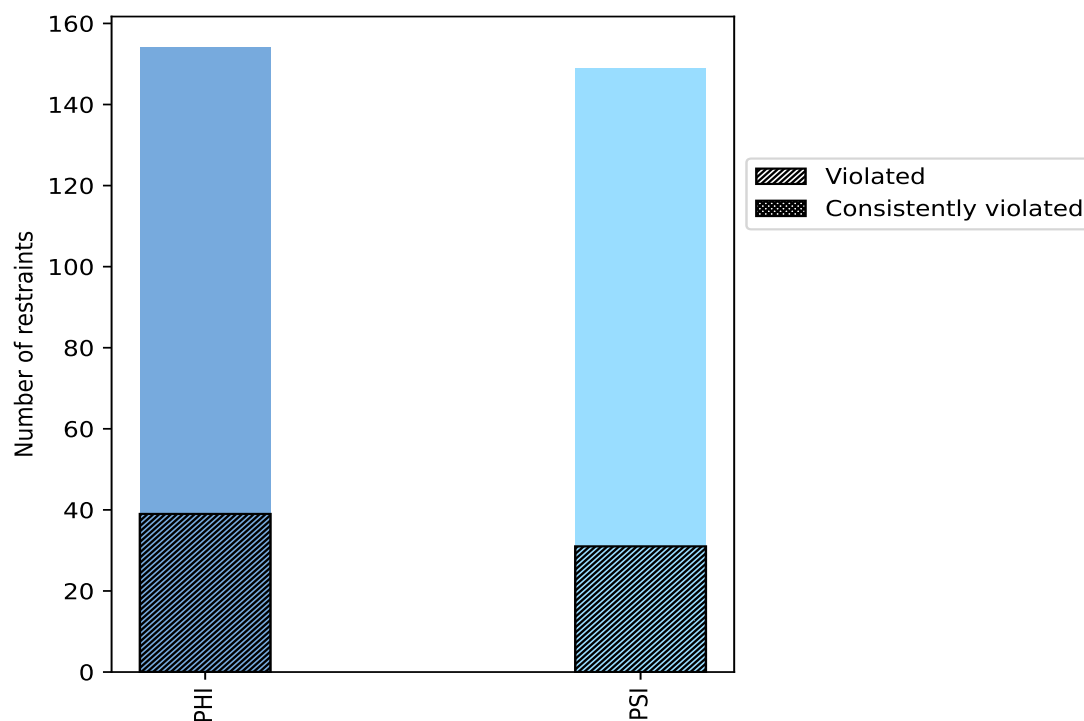
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	154	50.8	39	25.3	12.9	0	0.0	0.0
PSI	149	49.2	31	20.8	10.2	0	0.0	0.0
Total	303	100.0	70	23.1	23.1	0	0.0	0.0

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

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



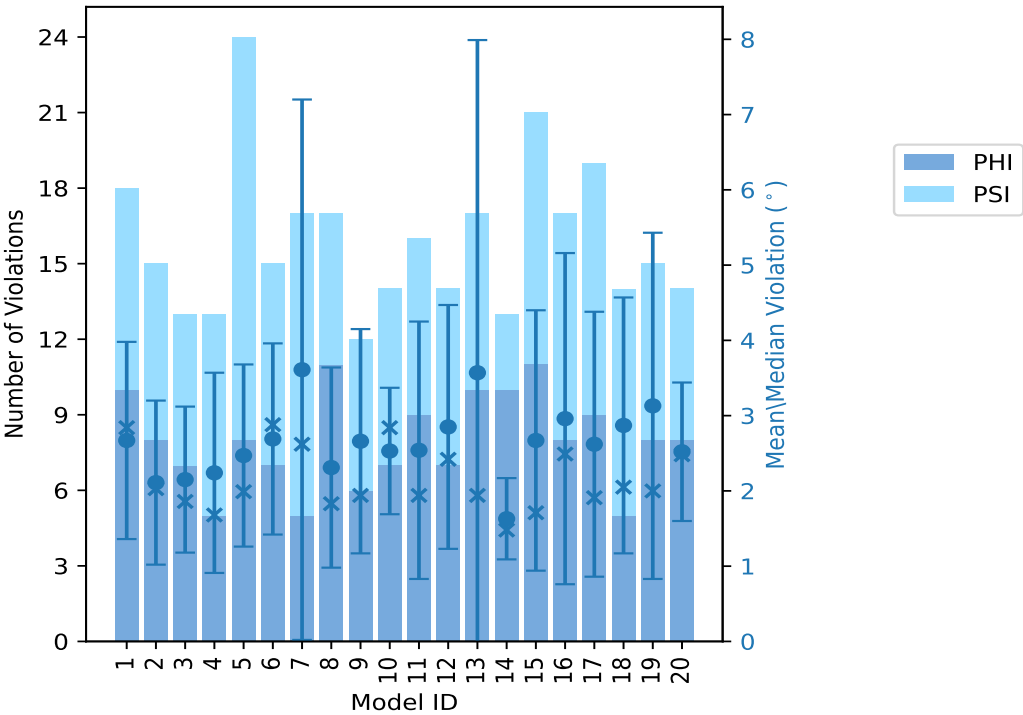
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	10	8	18	2.67	5.04	1.31	2.84
2	8	7	15	2.11	4.41	1.09	2.03
3	7	6	13	2.15	4.21	0.97	1.86
4	5	8	13	2.24	4.89	1.33	1.68
5	8	16	24	2.47	5.3	1.21	1.99
6	7	8	15	2.69	4.76	1.27	2.88
7	5	12	17	3.61	15.38	3.59	2.62
8	11	6	17	2.31	5.27	1.33	1.83
9	6	6	12	2.66	5.32	1.49	1.94
10	7	7	14	2.53	3.73	0.84	2.84
11	9	7	16	2.54	6.8	1.71	1.94
12	7	7	14	2.85	5.7	1.62	2.42
13	10	7	17	3.57	16.27	4.42	1.94
14	10	3	13	1.63	2.64	0.54	1.48
15	11	10	21	2.67	7.11	1.73	1.71
16	8	9	17	2.96	8.47	2.2	2.49
17	9	10	19	2.62	6.99	1.76	1.91
18	5	9	14	2.87	6.02	1.7	2.05
19	8	7	15	3.13	7.26	2.3	2.0
20	8	6	14	2.52	3.91	0.92	2.48

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	
PHI	PSI	Total	Count ¹	%
17	9	26	1	5.0
6	5	11	2	10.0
5	4	9	3	15.0
1	1	2	4	20.0
0	2	2	5	25.0
2	2	4	6	30.0
0	0	0	7	35.0
0	0	0	8	40.0
0	0	0	9	45.0
1	1	2	10	50.0
1	2	3	11	55.0

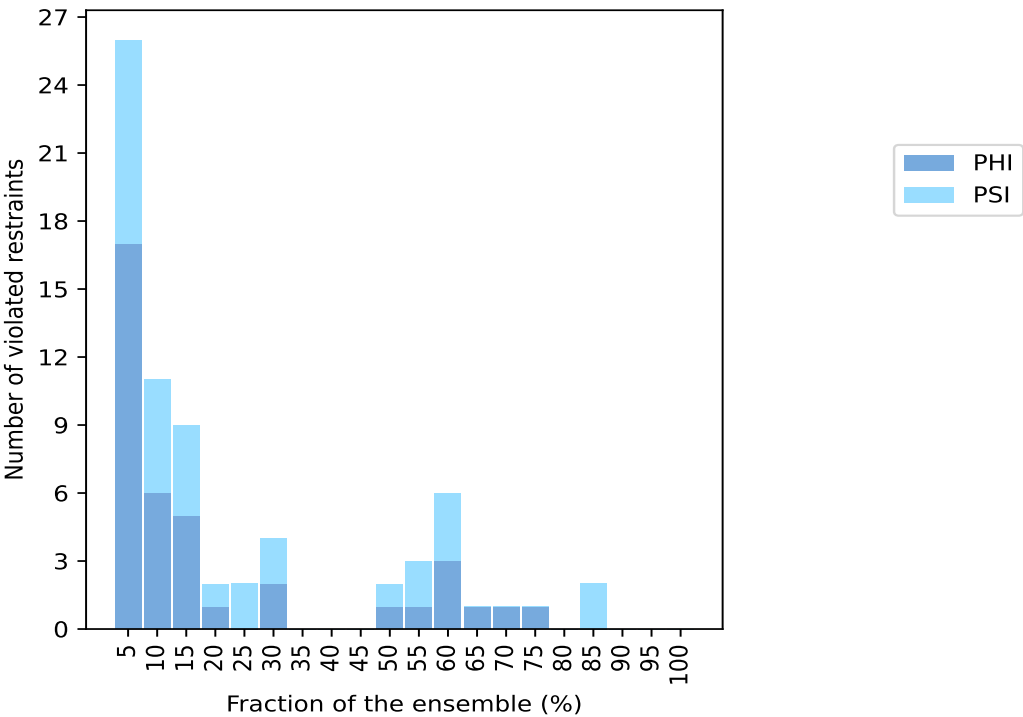
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
3	3	6	12	60.0
1	0	1	13	65.0
1	0	1	14	70.0
1	0	1	15	75.0
0	0	0	16	80.0
0	2	2	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	0	0	20	100.0

¹ Number of models with violations

10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ

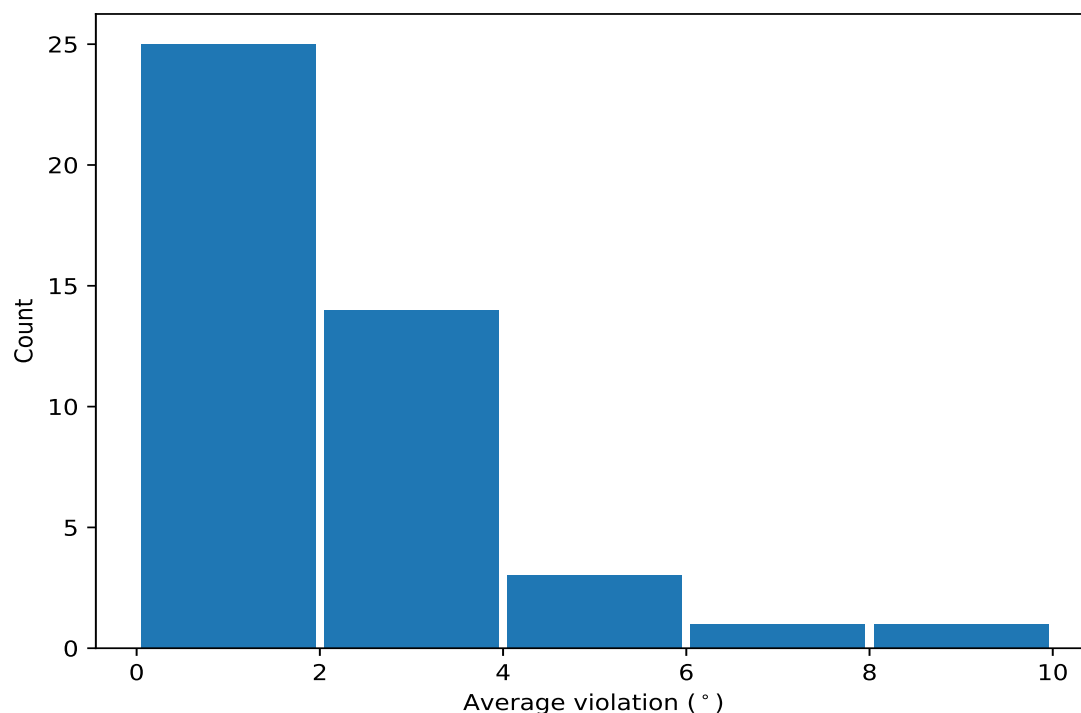


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	17	3.27	0.76	3.09
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	17	3.22	0.81	3.15
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	15	3.69	1.96	3.27
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	14	4.07	1.73	3.66
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	13	1.65	0.45	1.64
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	12	5.47	3.3	4.4
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	12	4.99	2.11	4.76
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	12	3.67	1.05	3.9
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	12	3.57	0.95	3.61
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	12	2.21	0.68	2.12
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	12	1.71	0.35	1.69
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	11	2.38	0.63	2.05
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	11	1.66	0.72	1.3
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	11	1.44	0.31	1.43
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	10	1.65	0.74	1.42
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	10	1.42	0.24	1.36
(1,194)	1:44:B:ASP:C	1:45:B:THR:N	1:45:B:THR:CA	1:45:B:THR:C	6	2.31	0.38	2.26
(1,43)	1:44:A:ASP:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	6	1.86	0.45	1.88
(1,48)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	6	1.75	0.58	1.47
(1,267)	1:103:B:LEU:N	1:103:B:LEU:CA	1:103:B:LEU:C	1:104:B:THR:N	6	1.62	0.47	1.55

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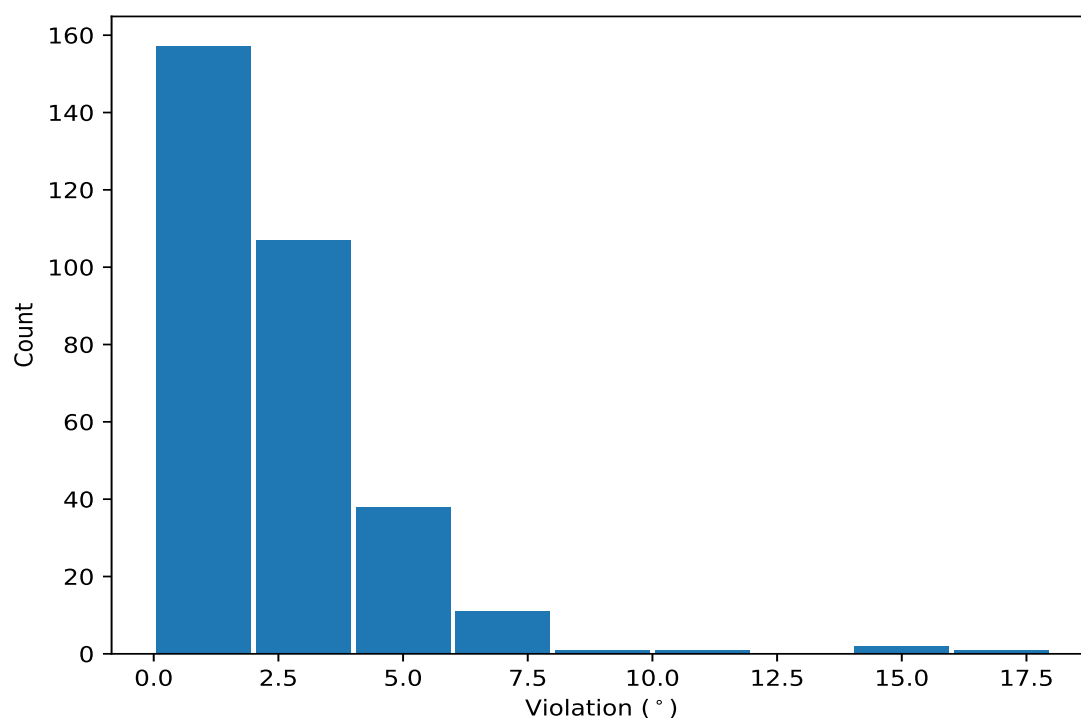
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,199)	1:47:B:ASN:N	1:47:B:ASN:CA	1:47:B:ASN:C	1:48:B:LYS:N	5	1.91	0.27	1.95
(1,116)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	5	1.42	0.47	1.27
(1,137)	1:116:A:ASN:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	4	6.58	6.2	4.49
(1,28)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:VAL:N	4	1.32	0.15	1.32
(1,136)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ALA:N	3	9.21	4.03	8.47
(1,251)	1:91:B:ILE:C	1:92:B:ARG:N	1:92:B:ARG:CA	1:92:B:ARG:C	3	3.1	1.53	2.05
(1,100)	1:91:A:ILE:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	3	3.06	1.56	2.06
(1,287)	1:116:B:ASN:N	1:116:B:ASN:CA	1:116:B:ASN:C	1:117:B:ALA:N	3	2.34	0.29	2.49
(1,8)	1:17:A:GLY:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	3	2.0	1.23	1.27
(1,78)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:LYS:N	3	1.93	0.49	1.68
(1,160)	1:17:B:GLY:C	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	3	1.84	1.11	1.09
(1,259)	1:97:B:LYS:N	1:97:B:LYS:CA	1:97:B:LYS:C	1:98:B:ARG:N	3	1.32	0.05	1.35
(1,177)	1:29:B:GLY:C	1:30:B:SER:N	1:30:B:SER:CA	1:30:B:SER:C	3	1.26	0.1	1.31
(1,229)	1:74:B:GLU:N	1:74:B:GLU:CA	1:74:B:GLU:C	1:75:B:LYS:N	2	2.21	0.84	2.21
(1,222)	1:68:B:PRO:C	1:69:B:THR:N	1:69:B:THR:CA	1:69:B:THR:C	2	2.18	0.71	2.18
(1,82)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:LYS:N	2	1.82	0.05	1.82
(1,233)	1:76:B:LYS:N	1:76:B:LYS:CA	1:76:B:LYS:C	1:77:B:LYS:N	2	1.67	0.28	1.67
(1,83)	1:76:A:LYS:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	2	1.45	0.09	1.45
(1,179)	1:34:B:GLY:N	1:34:B:GLY:CA	1:34:B:GLY:C	1:35:B:VAL:N	2	1.3	0.18	1.3
(1,50)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:TYR:N	2	1.23	0.01	1.23
(1,234)	1:76:B:LYS:C	1:77:B:LYS:N	1:77:B:LYS:CA	1:77:B:LYS:C	2	1.16	0.06	1.16
(1,19)	1:24:A:LEU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	2	1.14	0.04	1.14
(1,4)	1:14:A:ILE:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	2	1.13	0.06	1.13
(1,25)	1:29:A:GLY:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	2	1.07	0.01	1.07

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

10.5 All violated dihedral-angle restraints

10.5.1 Histogram : Distribution of violations

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	1:116:A:ASN:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	13	16.27
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	7	15.38
(1,136)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ALA:N	13	14.48
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	7	10.52
(1,136)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ALA:N	16	8.47
(1,137)	1:116:A:ASN:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	16	7.71
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	19	7.26
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	15	7.11
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	19	7.09
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	17	6.99
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	11	6.8
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	17	6.79
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	19	6.76
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	15	6.61
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	19	6.5
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	18	6.02
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	11	5.99
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	12	5.7
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	18	5.36
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	9	5.32
(1,124)	1:109:A:ASP:N	1:109:A:ASP:CA	1:109:A:ASP:C	1:110:A:LYS:N	5	5.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,251)	1:91:B:ILE:C	1:92:B:ARG:N	1:92:B:ARG:CA	1:92:B:ARG:C	8	5.27
(1,100)	1:91:A:ILE:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	8	5.26
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	12	5.21
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	9	5.17
(1,275)	1:109:B:ASP:N	1:109:B:ASP:CA	1:109:B:ASP:C	1:110:B:LYS:N	5	5.09
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	1	5.04
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	1	5.04
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	12	5.03
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	12	4.95
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	4	4.89
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	16	4.77
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	6	4.76
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	18	4.75
(1,136)	1:116:A:ASN:N	1:116:A:ASN:CA	1:116:A:ASN:C	1:117:A:ALA:N	15	4.69
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	6	4.67
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	16	4.62
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	17	4.52
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	7	4.48
(1,125)	1:109:A:ASP:C	1:110:A:LYS:N	1:110:A:LYS:CA	1:110:A:LYS:C	5	4.43
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	4	4.42
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	2	4.41
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	17	4.38
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	13	4.34
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	13	4.33
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	15	4.3
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	18	4.28
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	3	4.21
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	3	4.18
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	9	4.15
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	6	4.11
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	18	4.11
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	2	4.1
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	9	4.03
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	15	3.96
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	20	3.91
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	6	3.9
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	8	3.89
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	1	3.88
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	5	3.75
(1,276)	1:109:B:ASP:C	1:110:B:LYS:N	1:110:B:LYS:CA	1:110:B:LYS:C	5	3.73
(1,8)	1:17:A:GLY:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	10	3.73
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	1	3.71
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	18	3.7
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	4	3.66
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	4	3.62
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	20	3.62
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	6	3.58
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	11	3.55
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	1	3.53
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	20	3.51
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	20	3.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	16	3.47
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	1	3.44
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	1	3.43
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	1	3.42
(1,160)	1:17:B:GLY:C	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	10	3.41
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	16	3.38
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	11	3.36
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	8	3.34
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	5	3.32
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	10	3.3
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	6	3.27
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	11	3.26
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	15	3.23
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	10	3.18
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	11	3.18
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	20	3.15
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	15	3.1
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	10	3.1
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	20	3.09
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	2	3.07
(1,229)	1:74:B:GLU:N	1:74:B:GLU:CA	1:74:B:GLU:C	1:75:B:LYS:N	7	3.05
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	2	3.03
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	17	3.03
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	12	2.94
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	7	2.94
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	10	2.92
(1,48)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	20	2.92
(1,222)	1:68:B:PRO:C	1:69:B:THR:N	1:69:B:THR:CA	1:69:B:THR:C	6	2.89
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	1	2.88
(1,71)	1:68:A:PRO:C	1:69:A:THR:N	1:69:A:THR:CA	1:69:A:THR:C	6	2.88
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	10	2.85
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	5	2.84
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	10	2.83
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	1	2.81
(1,194)	1:44:B:ASP:C	1:45:B:THR:N	1:45:B:THR:CA	1:45:B:THR:C	5	2.79
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	5	2.79
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	12	2.77
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	7	2.76
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	7	2.74
(1,194)	1:44:B:ASP:C	1:45:B:THR:N	1:45:B:THR:CA	1:45:B:THR:C	15	2.73
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	17	2.71
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	3	2.69
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	7	2.69
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	17	2.69
(1,43)	1:44:A:ASP:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	15	2.68
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	12	2.65
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	14	2.64
(1,78)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:LYS:N	7	2.62
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	16	2.61
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	8	2.61
(1,287)	1:116:B:ASN:N	1:116:B:ASN:CA	1:116:B:ASN:C	1:117:B:ALA:N	15	2.59

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	2	2.51
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	7	2.5
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	16	2.5
(1,287)	1:116:B:ASN:N	1:116:B:ASN:CA	1:116:B:ASN:C	1:117:B:ALA:N	16	2.49
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	5	2.44
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	8	2.42
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	14	2.41
(1,267)	1:103:B:LEU:N	1:103:B:LEU:CA	1:103:B:LEU:C	1:104:B:THR:N	11	2.39
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	17	2.38
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	2	2.38
(1,172)	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1:26:B:PRO:N	10	2.38
(1,20)	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1:26:A:PRO:N	10	2.38
(1,209)	1:53:B:VAL:N	1:53:B:VAL:CA	1:53:B:VAL:C	1:54:B:ILE:N	13	2.37
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	3	2.37
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	19	2.36
(1,116)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	8	2.3
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	19	2.3
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	13	2.28
(1,194)	1:44:B:ASP:C	1:45:B:THR:N	1:45:B:THR:CA	1:45:B:THR:C	11	2.28
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	5	2.27
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	9	2.26
(1,199)	1:47:B:ASN:N	1:47:B:ASN:CA	1:47:B:ASN:C	1:48:B:LYS:N	7	2.23
(1,194)	1:44:B:ASP:C	1:45:B:THR:N	1:45:B:THR:CA	1:45:B:THR:C	3	2.23
(1,173)	1:26:B:PRO:C	1:27:B:VAL:N	1:27:B:VAL:CA	1:27:B:VAL:C	14	2.2
(1,194)	1:44:B:ASP:C	1:45:B:THR:N	1:45:B:THR:CA	1:45:B:THR:C	19	2.19
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	12	2.19
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	17	2.18
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	12	2.11
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	2	2.1
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	13	2.09
(1,100)	1:91:A:ILE:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	18	2.06
(1,251)	1:91:B:ILE:C	1:92:B:ARG:N	1:92:B:ARG:CA	1:92:B:ARG:C	18	2.05
(1,199)	1:47:B:ASN:N	1:47:B:ASN:CA	1:47:B:ASN:C	1:48:B:LYS:N	20	2.05
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	6	2.05
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	2	2.03
(1,48)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	7	2.03
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	5	2.0
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	19	2.0
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	9	1.99
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	5	1.98
(1,251)	1:91:B:ILE:C	1:92:B:ARG:N	1:92:B:ARG:CA	1:92:B:ARG:C	20	1.98
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	6	1.97
(1,43)	1:44:A:ASP:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	3	1.97
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	14	1.95
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	13	1.95
(1,233)	1:76:B:LYS:N	1:76:B:LYS:CA	1:76:B:LYS:C	1:77:B:LYS:N	5	1.95
(1,199)	1:47:B:ASN:N	1:47:B:ASN:CA	1:47:B:ASN:C	1:48:B:LYS:N	5	1.95
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	14	1.95
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	18	1.95
(1,287)	1:116:B:ASN:N	1:116:B:ASN:CA	1:116:B:ASN:C	1:117:B:ALA:N	13	1.94
(1,267)	1:103:B:LEU:N	1:103:B:LEU:CA	1:103:B:LEU:C	1:104:B:THR:N	8	1.93

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	7	1.93
(1,199)	1:47:B:ASN:N	1:47:B:ASN:CA	1:47:B:ASN:C	1:48:B:LYS:N	17	1.91
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	9	1.9
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	13	1.88
(1,58)	1:53:A:VAL:N	1:53:A:VAL:CA	1:53:A:VAL:C	1:54:A:ILE:N	14	1.88
(1,43)	1:44:A:ASP:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	5	1.88
(1,100)	1:91:A:ILE:C	1:92:A:ARG:N	1:92:A:ARG:CA	1:92:A:ARG:C	20	1.87
(1,43)	1:44:A:ASP:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	19	1.87
(1,267)	1:103:B:LEU:N	1:103:B:LEU:CA	1:103:B:LEU:C	1:104:B:THR:N	3	1.86
(1,82)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:LYS:N	1	1.86
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	8	1.83
(1,81)	1:75:A:LYS:C	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	4	1.81
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	17	1.79
(1,82)	1:76:A:LYS:N	1:76:A:LYS:CA	1:76:A:LYS:C	1:77:A:LYS:N	5	1.77
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	17	1.75
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	20	1.72
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	15	1.71
(1,232)	1:75:B:LYS:C	1:76:B:LYS:N	1:76:B:LYS:CA	1:76:B:LYS:C	4	1.7
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	10	1.7
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	9	1.7
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	19	1.69
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	19	1.69
(1,78)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:LYS:N	4	1.68
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	8	1.67
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	17	1.66
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	19	1.65
(1,194)	1:44:B:ASP:C	1:45:B:THR:N	1:45:B:THR:CA	1:45:B:THR:C	8	1.65
(1,106)	1:95:A:ASP:N	1:95:A:ASP:CA	1:95:A:ASP:C	1:96:A:LYS:N	13	1.65
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	9	1.64
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	3	1.63
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	15	1.62
(1,48)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	5	1.62
(1,43)	1:44:A:ASP:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	11	1.6
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	5	1.59
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	15	1.54
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	7	1.54
(1,83)	1:76:A:LYS:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	1	1.54
(1,28)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:VAL:N	13	1.53
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	16	1.52
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	7	1.5
(1,78)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:LYS:N	12	1.5
(1,179)	1:34:B:GLY:N	1:34:B:GLY:CA	1:34:B:GLY:C	1:35:B:VAL:N	3	1.48
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	5	1.48
(1,21)	1:26:A:PRO:C	1:27:A:VAL:N	1:27:A:VAL:CA	1:27:A:VAL:C	14	1.48
(1,222)	1:68:B:PRO:C	1:69:B:THR:N	1:69:B:THR:CA	1:69:B:THR:C	16	1.47
(1,116)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	4	1.47
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	12	1.46
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	15	1.45
(1,129)	1:112:A:LYS:C	1:113:A:GLU:N	1:113:A:GLU:CA	1:113:A:GLU:C	15	1.44
(1,115)	1:102:A:LYS:C	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	16	1.43
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	16	1.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	10	1.42
(1,199)	1:47:B:ASN:N	1:47:B:ASN:CA	1:47:B:ASN:C	1:48:B:LYS:N	3	1.42
(1,233)	1:76:B:LYS:N	1:76:B:LYS:CA	1:76:B:LYS:C	1:77:B:LYS:N	1	1.4
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	15	1.39
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	18	1.39
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	20	1.39
(1,80)	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	1:76:A:LYS:N	18	1.39
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	8	1.37
(1,229)	1:74:B:GLU:N	1:74:B:GLU:CA	1:74:B:GLU:C	1:75:B:LYS:N	20	1.37
(1,83)	1:76:A:LYS:C	1:77:A:LYS:N	1:77:A:LYS:CA	1:77:A:LYS:C	6	1.36
(1,259)	1:97:B:LYS:N	1:97:B:LYS:CA	1:97:B:LYS:C	1:98:B:ARG:N	4	1.35
(1,259)	1:97:B:LYS:N	1:97:B:LYS:CA	1:97:B:LYS:C	1:98:B:ARG:N	11	1.35
(1,177)	1:29:B:GLY:C	1:30:B:SER:N	1:30:B:SER:CA	1:30:B:SER:C	12	1.35
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	9	1.35
(1,28)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:VAL:N	6	1.34
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	15	1.33
(1,171)	1:24:B:LEU:C	1:25:B:SER:N	1:25:B:SER:CA	1:25:B:SER:C	1	1.32
(1,48)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	17	1.32
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	13	1.31
(1,177)	1:29:B:GLY:C	1:30:B:SER:N	1:30:B:SER:CA	1:30:B:SER:C	9	1.31
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	19	1.31
(1,48)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	3	1.31
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	7	1.3
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	8	1.3
(1,48)	1:47:A:ASN:N	1:47:A:ASN:CA	1:47:A:ASN:C	1:48:A:LYS:N	16	1.3
(1,28)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:VAL:N	3	1.3
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	6	1.29
(1,116)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	11	1.27
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	1	1.27
(1,8)	1:17:A:GLY:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	11	1.27
(1,157)	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	1:16:B:ARG:N	17	1.26
(1,137)	1:116:A:ASN:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	15	1.26
(1,92)	1:83:A:ASP:C	1:84:A:SER:N	1:84:A:SER:CA	1:84:A:SER:C	11	1.26
(1,259)	1:97:B:LYS:N	1:97:B:LYS:CA	1:97:B:LYS:C	1:98:B:ARG:N	3	1.25
(1,267)	1:103:B:LEU:N	1:103:B:LEU:CA	1:103:B:LEU:C	1:104:B:THR:N	5	1.24
(1,280)	1:112:B:LYS:C	1:113:B:GLU:N	1:113:B:GLU:CA	1:113:B:GLU:C	15	1.23
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	14	1.23
(1,50)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:TYR:N	2	1.23
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	19	1.22
(1,234)	1:76:B:LYS:C	1:77:B:LYS:N	1:77:B:LYS:CA	1:77:B:LYS:C	1	1.22
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	20	1.22
(1,50)	1:48:A:LYS:N	1:48:A:LYS:CA	1:48:A:LYS:C	1:49:A:TYR:N	7	1.22
(1,267)	1:103:B:LEU:N	1:103:B:LEU:CA	1:103:B:LEU:C	1:104:B:THR:N	2	1.2
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	2	1.2
(1,257)	1:95:B:ASP:N	1:95:B:ASP:CA	1:95:B:ASP:C	1:96:B:LYS:N	2	1.19
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	6	1.19
(1,118)	1:104:A:THR:C	1:105:A:TYR:N	1:105:A:TYR:CA	1:105:A:TYR:C	4	1.19
(1,43)	1:44:A:ASP:C	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	8	1.19
(1,4)	1:14:A:ILE:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	17	1.19
(1,288)	1:116:B:ASN:C	1:117:B:ALA:N	1:117:B:ALA:CA	1:117:B:ALA:C	13	1.18
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	14	1.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:24:A:LEU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	1	1.18
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	14	1.14
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	10	1.14
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	14	1.12
(1,181)	1:35:B:VAL:N	1:35:B:VAL:CA	1:35:B:VAL:C	1:36:B:ARG:N	18	1.12
(1,156)	1:14:B:ILE:C	1:15:B:ARG:N	1:15:B:ARG:CA	1:15:B:ARG:C	17	1.12
(1,28)	1:34:A:GLY:N	1:34:A:GLY:CA	1:34:A:GLY:C	1:35:A:VAL:N	19	1.12
(1,1)	1:11:A:GLN:C	1:12:A:ASP:N	1:12:A:ASP:CA	1:12:A:ASP:C	11	1.12
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	4	1.11
(1,179)	1:34:B:GLY:N	1:34:B:GLY:CA	1:34:B:GLY:C	1:35:B:VAL:N	6	1.11
(1,177)	1:29:B:GLY:C	1:30:B:SER:N	1:30:B:SER:CA	1:30:B:SER:C	16	1.11
(1,5)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:ARG:N	17	1.11
(1,44)	1:45:A:THR:N	1:45:A:THR:CA	1:45:A:THR:C	1:46:A:GLY:N	5	1.1
(1,267)	1:103:B:LEU:N	1:103:B:LEU:CA	1:103:B:LEU:C	1:104:B:THR:N	4	1.09
(1,234)	1:76:B:LYS:C	1:77:B:LYS:N	1:77:B:LYS:CA	1:77:B:LYS:C	4	1.09
(1,160)	1:17:B:GLY:C	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	16	1.09
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	2	1.09
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	2	1.09
(1,26)	1:31:A:GLU:C	1:32:A:GLN:N	1:32:A:GLN:CA	1:32:A:GLN:C	15	1.09
(1,19)	1:24:A:LEU:C	1:25:A:SER:N	1:25:A:SER:CA	1:25:A:SER:C	9	1.09
(1,74)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:VAL:N	8	1.08
(1,25)	1:29:A:GLY:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	13	1.08
(1,137)	1:116:A:ASN:C	1:117:A:ALA:N	1:117:A:ALA:CA	1:117:A:ALA:C	14	1.07
(1,4)	1:14:A:ILE:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	10	1.07
(1,225)	1:70:B:HIS:N	1:70:B:HIS:CA	1:70:B:HIS:C	1:71:B:VAL:N	8	1.06
(1,147)	1:121:A:SER:C	1:122:A:LEU:N	1:122:A:LEU:CA	1:122:A:LEU:C	8	1.06
(1,25)	1:29:A:GLY:C	1:30:A:SER:N	1:30:A:SER:CA	1:30:A:SER:C	15	1.06
(1,107)	1:95:A:ASP:C	1:96:A:LYS:N	1:96:A:LYS:CA	1:96:A:LYS:C	17	1.04
(1,160)	1:17:B:GLY:C	1:18:B:ASP:N	1:18:B:ASP:CA	1:18:B:ASP:C	11	1.03
(1,116)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	2	1.03
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	13	1.03
(1,269)	1:104:B:THR:C	1:105:B:TYR:N	1:105:B:TYR:CA	1:105:B:TYR:C	16	1.02
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	1	1.02
(1,116)	1:103:A:LEU:N	1:103:A:LEU:CA	1:103:A:LEU:C	1:104:A:THR:N	5	1.02
(1,103)	1:93:A:THR:C	1:94:A:LEU:N	1:94:A:LEU:CA	1:94:A:LEU:C	18	1.02
(1,254)	1:93:B:THR:C	1:94:B:LEU:N	1:94:B:LEU:CA	1:94:B:LEU:C	13	1.01
(1,243)	1:83:B:ASP:C	1:84:B:SER:N	1:84:B:SER:CA	1:84:B:SER:C	11	1.01
(1,214)	1:55:B:VAL:C	1:56:B:ALA:N	1:56:B:ALA:CA	1:56:B:ALA:C	12	1.01
(1,191)	1:42:B:GLN:N	1:42:B:GLN:CA	1:42:B:GLN:C	1:43:B:ASN:N	5	1.01
(1,8)	1:17:A:GLY:C	1:18:A:ASP:N	1:18:A:ASP:CA	1:18:A:ASP:C	12	1.01
(1,203)	1:49:B:TYR:N	1:49:B:TYR:CA	1:49:B:TYR:C	1:50:B:SER:N	18	1.0
(1,108)	1:96:A:LYS:C	1:97:A:LYS:N	1:97:A:LYS:CA	1:97:A:LYS:C	14	1.0