



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2MZD / pdb_00002mzd
BMRB ID : 25484
Title : Characterization of the p300 Taz2-p53 TAD2 Complex and Comparison with the p300 Taz2-p53 TAD1 Complex
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Deposited on : 2015-02-11

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

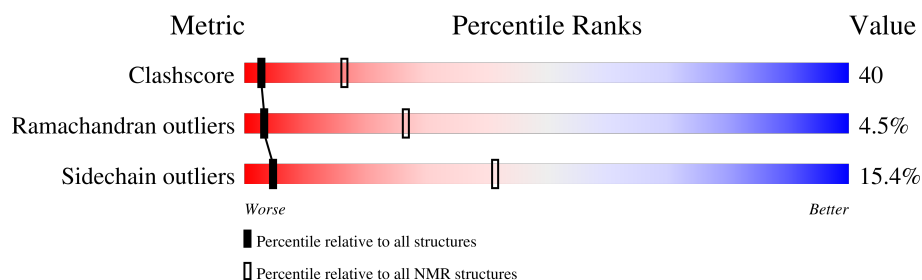
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	90	
2	B	25	

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:7-A:88, B:12-B:22 (93)	0.57	4

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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1791 atoms, of which 903 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1415	420	726	140	119	10	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	CYS	engineered mutation	UNP Q09472
A	24	ALA	CYS	engineered mutation	UNP Q09472
A	67	ALA	CYS	engineered mutation	UNP Q09472
A	68	ALA	CYS	engineered mutation	UNP Q09472

- Molecule 2 is a protein called Cellular tumor antigen p53.

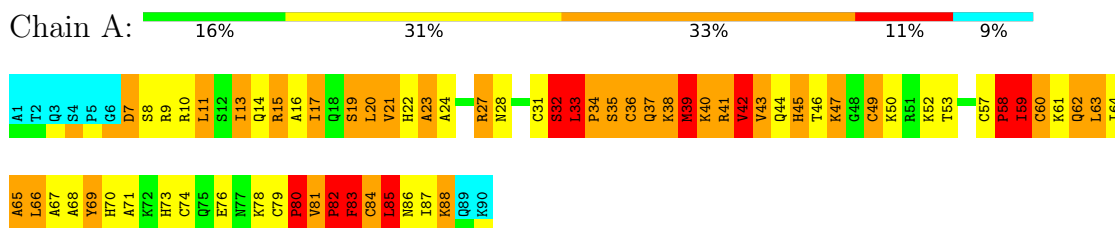
Mol	Chain	Residues	Atoms						Trace
2	B	25	Total	C	H	N	O	S	0
			376	124	177	28	45	2	

4 Residue-property plots

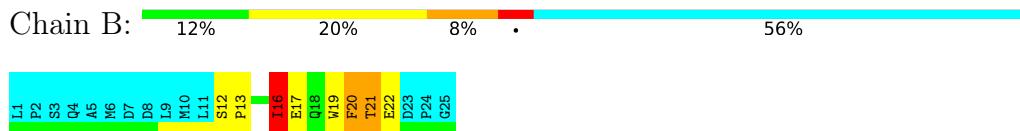
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Histone acetyltransferase p300



- Molecule 2: Cellular tumor antigen p53

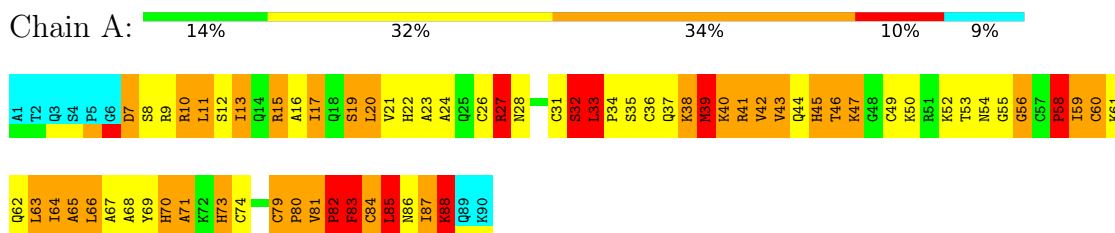


4.2 Scores per residue for each member of the ensemble

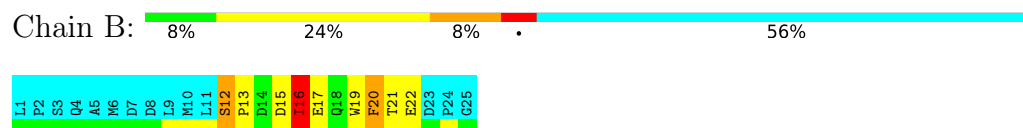
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Histone acetyltransferase p300

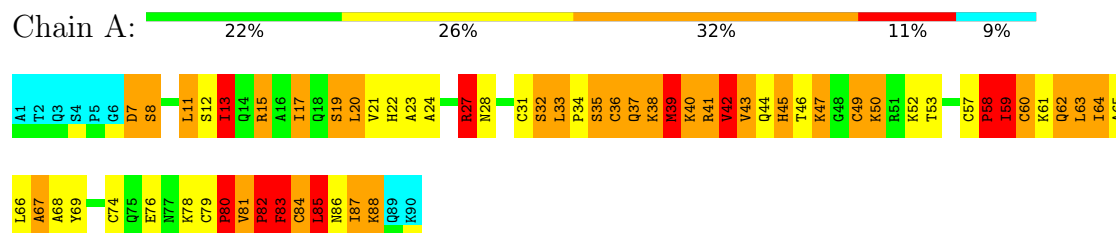


- Molecule 2: Cellular tumor antigen p53

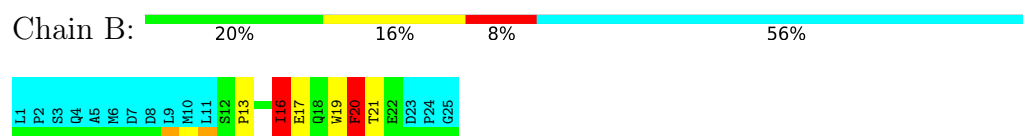


4.2.2 Score per residue for model 2

- Molecule 1: Histone acetyltransferase p300

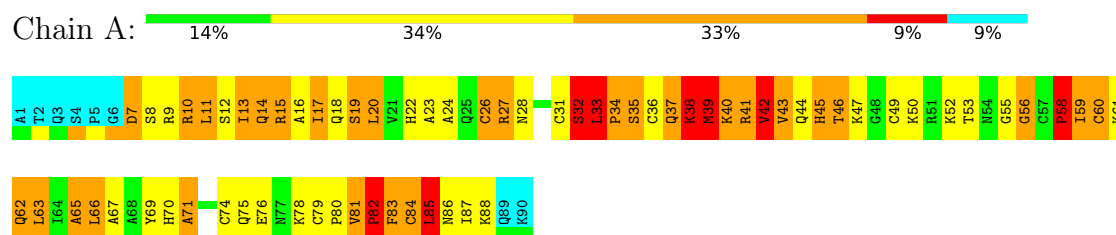


- Molecule 2: Cellular tumor antigen p53

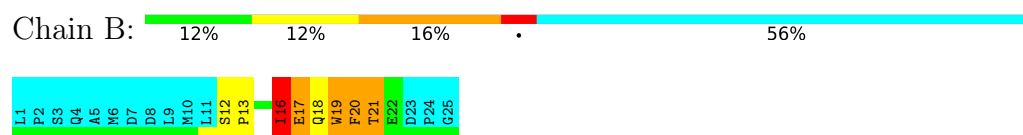


4.2.3 Score per residue for model 3

- Molecule 1: Histone acetyltransferase p300

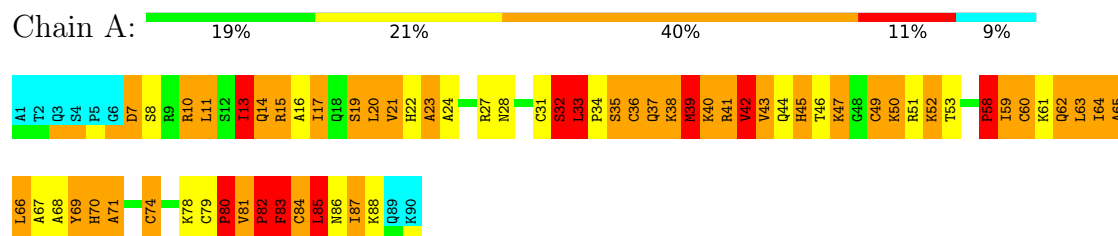


- Molecule 2: Cellular tumor antigen p53

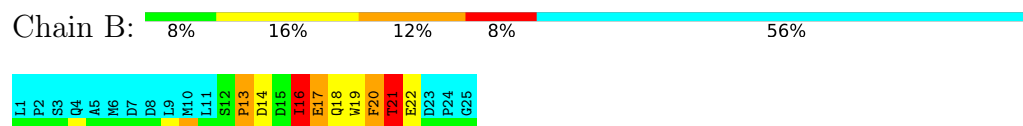


4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Histone acetyltransferase p300

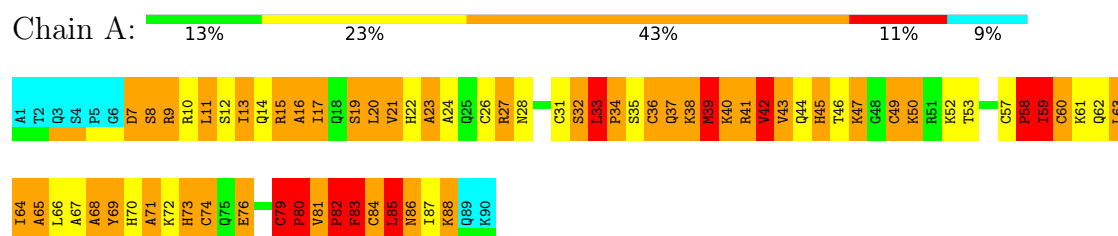


- Molecule 2: Cellular tumor antigen p53

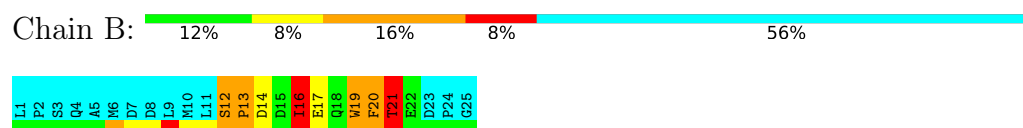


4.2.5 Score per residue for model 5

- Molecule 1: Histone acetyltransferase p300

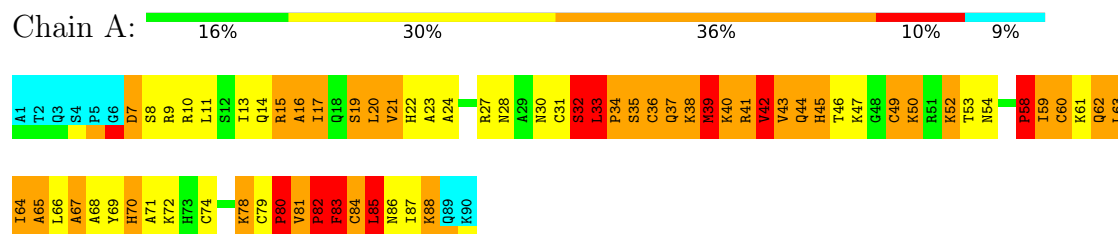


- Molecule 2: Cellular tumor antigen p53



4.2.6 Score per residue for model 6

- Molecule 1: Histone acetyltransferase p300



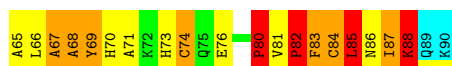
- Molecule 2: Cellular tumor antigen p53





4.2.7 Score per residue for model 7

- Molecule 1: Histone acetyltransferase p300

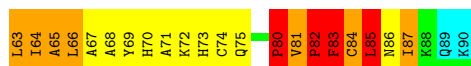
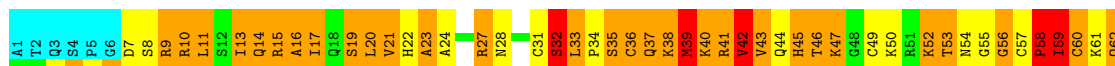


- Molecule 2: Cellular tumor antigen p53

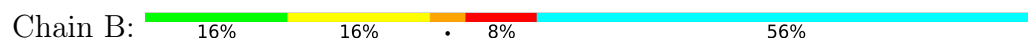


4.2.8 Score per residue for model 8

- Molecule 1: Histone acetyltransferase p300



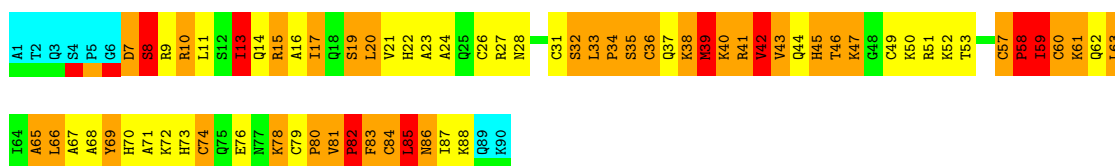
- Molecule 2: Cellular tumor antigen p53



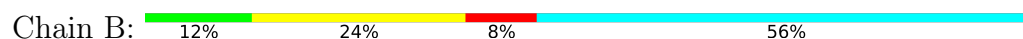
4.2.9 Score per residue for model 9

- Molecule 1: Histone acetyltransferase p300



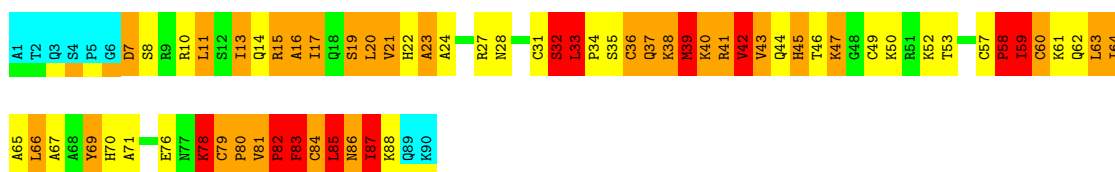


- Molecule 2: Cellular tumor antigen p53

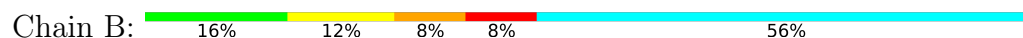


4.2.10 Score per residue for model 10

- Molecule 1: Histone acetyltransferase p300

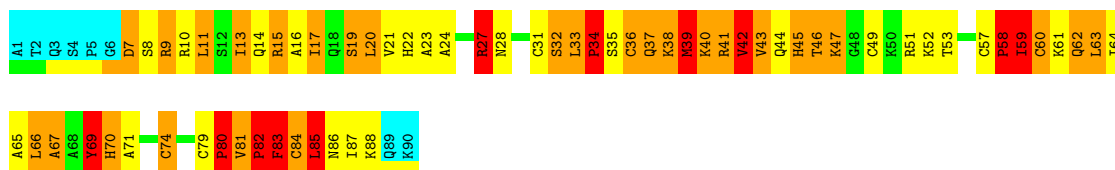


- Molecule 2: Cellular tumor antigen p53

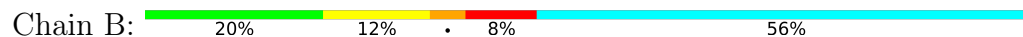


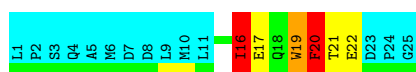
4.2.11 Score per residue for model 11

- Molecule 1: Histone acetyltransferase p300



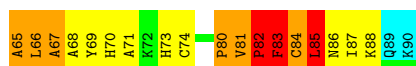
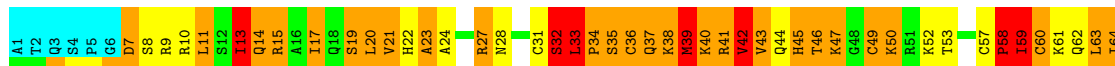
- Molecule 2: Cellular tumor antigen p53



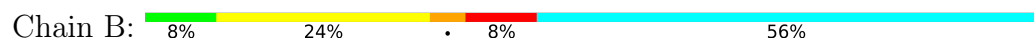


4.2.12 Score per residue for model 12

- Molecule 1: Histone acetyltransferase p300

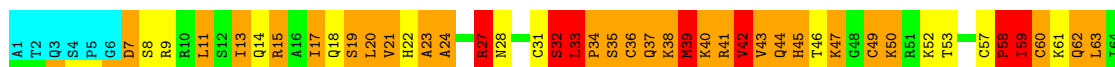


- Molecule 2: Cellular tumor antigen p53



4.2.13 Score per residue for model 13

- Molecule 1: Histone acetyltransferase p300



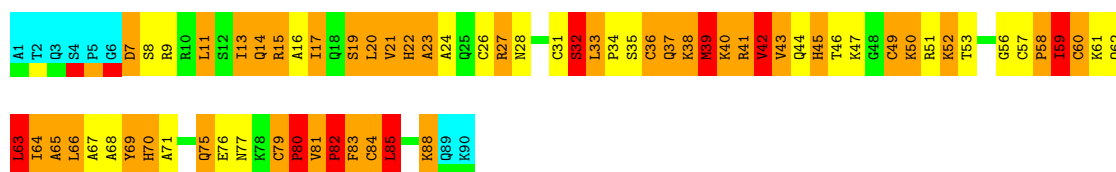
- Molecule 2: Cellular tumor antigen p53



4.2.14 Score per residue for model 14

- Molecule 1: Histone acetyltransferase p300



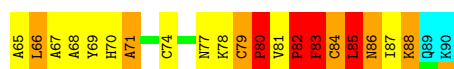
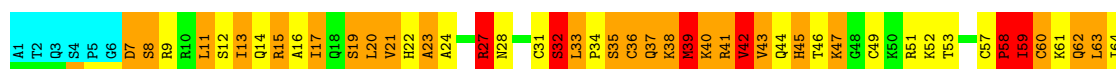


- Molecule 2: Cellular tumor antigen p53



4.2.15 Score per residue for model 15

- Molecule 1: Histone acetyltransferase p300



- Molecule 2: Cellular tumor antigen p53



5 Refinement protocol and experimental data overview

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

Of the 40000 calculated structures, 15 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
TALOS	structure solution	
CNS	structure solution	
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	2
Total number of shifts	1270
Number of shifts mapped to atoms	1270
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality

6.1 Standard geometry

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	3.19±0.08	74±7/642 (11.5± 1.1%)	2.19±0.05	28±2/861 (3.3± 0.2%)
2	B	1.97±0.18	3±1/100 (2.9± 1.3%)	1.68±0.11	2±1/138 (1.1± 0.9%)
All	All	3.05	1147/11130 (10.3%)	2.12	446/14985 (3.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.0±0.7
2	B	0.0±0.0	0.1±0.3
All	All	0	47

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	33	LEU	N-CA	-18.64	1.26	1.46	6	15
1	A	22	HIS	C-O	-12.63	1.09	1.24	14	15
1	A	59	ILE	N-CA	-12.48	1.30	1.46	14	13
1	A	53	THR	N-CA	-12.44	1.30	1.46	11	15
1	A	59	ILE	CA-C	-12.39	1.37	1.52	12	12
1	A	32	SER	N-CA	-12.20	1.29	1.46	14	15
1	A	58	PRO	C-N	-12.13	1.20	1.33	4	13
1	A	59	ILE	C-O	-12.05	1.09	1.24	12	15
1	A	38	LYS	N-CA	-11.80	1.32	1.46	15	15
2	B	21	THR	N-CA	-11.79	1.31	1.47	5	12
1	A	81	VAL	C-O	11.66	1.36	1.24	4	10
2	B	20	PHE	N-CA	-11.42	1.31	1.46	10	4
1	A	58	PRO	C-O	-11.20	1.09	1.24	7	2
1	A	63	LEU	C-O	-10.81	1.11	1.24	11	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	42	VAL	N-CA	-10.70	1.32	1.46	9	15
1	A	81	VAL	C-N	10.68	1.46	1.33	4	7
1	A	37	GLN	CA-C	-10.68	1.38	1.52	15	15
1	A	85	LEU	N-CA	10.43	1.59	1.46	12	7
1	A	45	HIS	CA-C	-10.42	1.39	1.52	9	15
1	A	17	ILE	C-O	-10.28	1.12	1.24	8	15
1	A	37	GLN	C-N	-10.28	1.20	1.33	1	15
1	A	20	LEU	CB-CG	-9.93	1.33	1.53	6	15
1	A	58	PRO	CA-CB	-9.61	1.40	1.53	7	2
1	A	61	LYS	CA-C	-9.36	1.40	1.52	1	14
1	A	74	CYS	CA-CB	9.27	1.64	1.53	7	12
1	A	8	SER	N-CA	-9.25	1.34	1.46	8	14
1	A	38	LYS	CA-CB	-9.23	1.39	1.53	1	15
1	A	31	CYS	CA-C	-9.16	1.40	1.52	4	15
1	A	28	ASN	N-CA	-8.96	1.35	1.46	4	15
1	A	85	LEU	CA-C	8.84	1.64	1.52	15	12
2	B	16	ILE	C-N	-8.79	1.22	1.34	15	15
1	A	60	CYS	C-O	-8.66	1.13	1.24	6	13
1	A	14	GLN	C-O	-8.59	1.14	1.24	11	11
1	A	41	ARG	CA-C	-8.57	1.40	1.52	5	15
1	A	64	ILE	C-O	-8.50	1.14	1.24	2	10
1	A	22	HIS	C-N	-8.46	1.22	1.33	14	15
1	A	20	LEU	N-CA	-8.27	1.36	1.46	9	15
1	A	61	LYS	N-CA	-8.23	1.35	1.46	14	13
1	A	51	ARG	N-CA	-8.19	1.35	1.46	9	5
1	A	61	LYS	CA-CB	-8.17	1.40	1.53	14	13
1	A	82	PRO	C-N	-8.04	1.22	1.33	6	15
1	A	39	MET	C-N	-8.02	1.23	1.33	14	15
1	A	87	ILE	CA-CB	7.87	1.64	1.54	2	13
1	A	60	CYS	C-N	-7.85	1.22	1.33	14	12
1	A	50	LYS	N-CA	7.78	1.56	1.46	13	6
1	A	76	GLU	CA-C	-7.73	1.43	1.52	14	1
1	A	60	CYS	CA-C	-7.73	1.41	1.52	14	11
1	A	40	LYS	C-O	-7.69	1.15	1.24	12	15
1	A	84	CYS	N-CA	-7.68	1.36	1.46	2	10
1	A	88	LYS	N-CA	-7.62	1.37	1.46	7	1
1	A	11	LEU	CA-C	-7.59	1.42	1.52	1	13
1	A	83	PHE	C-O	-7.58	1.14	1.24	12	9
1	A	46	THR	C-O	-7.53	1.15	1.24	8	4
1	A	13	ILE	C-O	-7.49	1.15	1.24	4	8
1	A	10	ARG	C-O	-7.48	1.15	1.24	3	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	27	ARG	C-N	-7.28	1.24	1.33	5	13
1	A	19	SER	CA-C	-7.28	1.43	1.52	9	15
1	A	47	LYS	CA-CB	-7.24	1.42	1.53	3	13
2	B	20	PHE	CA-C	-7.22	1.46	1.52	6	2
1	A	22	HIS	CA-C	-7.21	1.43	1.52	8	15
1	A	81	VAL	N-CA	-7.08	1.37	1.46	2	4
1	A	83	PHE	N-CA	-7.06	1.37	1.46	2	1
1	A	80	PRO	N-CA	-7.04	1.38	1.47	10	10
1	A	82	PRO	CA-C	-6.93	1.44	1.52	3	6
1	A	27	ARG	CA-C	-6.93	1.45	1.53	9	6
1	A	83	PHE	C-N	-6.87	1.24	1.33	12	12
1	A	65	ALA	C-N	-6.86	1.25	1.33	3	8
1	A	73	HIS	CA-C	6.85	1.61	1.52	8	6
1	A	43	VAL	C-N	-6.82	1.24	1.33	2	15
1	A	49	CYS	CA-C	-6.80	1.45	1.53	14	2
1	A	37	GLN	C-O	-6.69	1.16	1.24	9	8
2	B	19	TRP	N-CA	-6.69	1.37	1.46	11	4
1	A	17	ILE	N-CA	-6.69	1.38	1.46	6	6
1	A	44	GLN	N-CA	-6.68	1.37	1.46	13	15
1	A	63	LEU	CA-CB	-6.68	1.42	1.53	7	2
1	A	46	THR	N-CA	-6.60	1.38	1.46	8	6
1	A	43	VAL	N-CA	-6.53	1.39	1.46	6	6
1	A	66	LEU	N-CA	-6.51	1.38	1.46	3	10
1	A	75	GLN	N-CA	-6.49	1.38	1.46	14	1
1	A	15	ARG	C-N	-6.48	1.25	1.33	6	14
1	A	35	SER	N-CA	-6.46	1.37	1.46	4	12
1	A	8	SER	C-N	6.42	1.42	1.33	6	6
1	A	71	ALA	CA-C	-6.41	1.43	1.52	13	5
1	A	59	ILE	CA-CB	-6.40	1.48	1.55	4	2
1	A	10	ARG	CA-C	-6.40	1.45	1.52	3	4
1	A	49	CYS	C-O	-6.37	1.14	1.23	2	6
1	A	53	THR	C-N	6.36	1.42	1.33	11	8
1	A	21	VAL	N-CA	-6.36	1.39	1.46	14	9
1	A	40	LYS	CA-CB	-6.36	1.43	1.53	15	10
1	A	12	SER	N-CA	-6.33	1.38	1.46	1	1
1	A	23	ALA	C-N	-6.32	1.25	1.33	14	9
1	A	59	ILE	C-N	-6.31	1.25	1.33	7	2
1	A	15	ARG	CA-CB	-6.30	1.43	1.53	8	9
1	A	7	ASP	C-O	-6.28	1.16	1.24	15	7
1	A	64	ILE	CA-C	-6.28	1.45	1.52	6	3
1	A	21	VAL	C-O	-6.26	1.17	1.24	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	62	GLN	C-O	-6.25	1.16	1.24	11	7
1	A	34	PRO	C-N	-6.21	1.24	1.33	12	7
2	B	22	GLU	C-N	-6.20	1.25	1.33	13	1
1	A	8	SER	CA-C	6.17	1.61	1.52	13	10
1	A	69	TYR	N-CA	-6.17	1.38	1.46	7	6
1	A	13	ILE	CB-CG1	-6.08	1.41	1.53	13	8
1	A	13	ILE	CA-C	-6.07	1.44	1.52	14	7
2	B	22	GLU	N-CA	-6.06	1.38	1.46	14	3
1	A	80	PRO	C-N	-6.04	1.26	1.33	2	4
1	A	13	ILE	N-CA	6.02	1.53	1.46	3	2
1	A	65	ALA	N-CA	-5.99	1.39	1.46	5	7
1	A	10	ARG	CA-CB	-5.98	1.44	1.53	3	3
1	A	67	ALA	N-CA	-5.93	1.39	1.46	11	8
1	A	55	GLY	C-N	-5.92	1.24	1.33	1	3
1	A	17	ILE	CA-CB	-5.86	1.47	1.54	4	11
1	A	34	PRO	CA-CB	-5.85	1.45	1.53	9	2
1	A	35	SER	C-N	5.85	1.41	1.33	14	10
1	A	84	CYS	CA-C	-5.83	1.45	1.52	11	3
1	A	38	LYS	C-O	-5.82	1.17	1.24	12	2
1	A	11	LEU	C-N	-5.82	1.26	1.33	1	2
1	A	52	LYS	N-CA	-5.81	1.38	1.46	7	1
2	B	21	THR	C-N	-5.81	1.25	1.33	11	2
1	A	50	LYS	C-O	5.78	1.31	1.24	7	2
1	A	49	CYS	CA-CB	5.78	1.62	1.53	8	2
1	A	41	ARG	C-N	-5.76	1.26	1.33	8	5
1	A	65	ALA	C-O	-5.75	1.17	1.24	3	2
1	A	19	SER	C-O	-5.74	1.17	1.24	9	7
1	A	32	SER	CA-C	-5.72	1.46	1.53	14	10
1	A	70	HIS	C-O	-5.72	1.17	1.24	4	4
1	A	20	LEU	CA-CB	-5.72	1.44	1.53	5	5
1	A	68	ALA	CA-C	-5.72	1.45	1.52	5	2
1	A	87	ILE	C-N	-5.71	1.25	1.33	7	1
1	A	76	GLU	C-N	-5.71	1.26	1.33	3	3
1	A	26	CYS	N-CA	-5.70	1.38	1.46	9	3
1	A	50	LYS	CA-CB	-5.68	1.46	1.54	1	1
1	A	18	GLN	CA-C	-5.62	1.45	1.52	13	1
1	A	76	GLU	N-CA	-5.58	1.39	1.46	5	2
1	A	56	GLY	CA-C	-5.56	1.44	1.51	1	4
1	A	41	ARG	C-O	-5.53	1.16	1.24	11	5
1	A	64	ILE	CA-CB	5.52	1.60	1.54	14	1
1	A	88	LYS	C-N	-5.51	1.26	1.33	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	19	SER	CA-CB	-5.48	1.44	1.53	12	1
1	A	62	GLN	N-CA	-5.48	1.39	1.46	3	3
1	A	7	ASP	C-N	-5.47	1.26	1.33	11	2
1	A	16	ALA	CA-C	-5.47	1.46	1.52	5	2
1	A	45	HIS	C-N	-5.47	1.26	1.33	14	2
1	A	7	ASP	N-CA	-5.44	1.39	1.46	6	1
1	A	46	THR	C-N	-5.39	1.26	1.33	3	1
1	A	54	ASN	C-N	-5.39	1.25	1.33	8	2
1	A	58	PRO	N-CA	-5.37	1.40	1.47	14	1
1	A	71	ALA	C-N	-5.37	1.27	1.33	15	3
1	A	57	CYS	CA-CB	5.34	1.63	1.53	7	1
1	A	15	ARG	C-O	-5.32	1.17	1.24	15	1
1	A	38	LYS	CG-CD	-5.26	1.36	1.52	10	1
1	A	77	ASN	N-CA	-5.23	1.39	1.46	14	1
1	A	42	VAL	CA-C	-5.22	1.45	1.52	6	2
1	A	16	ALA	N-CA	-5.21	1.40	1.46	10	1
1	A	21	VAL	C-N	-5.21	1.26	1.33	15	1
1	A	62	GLN	C-N	-5.20	1.26	1.33	15	1
1	A	56	GLY	N-CA	-5.19	1.37	1.45	14	1
1	A	32	SER	C-N	-5.17	1.27	1.33	1	2
1	A	46	THR	CB-OG1	-5.16	1.35	1.43	3	2
1	A	39	MET	CA-C	-5.16	1.46	1.52	6	1
1	A	19	SER	C-N	-5.14	1.27	1.33	5	1
1	A	24	ALA	N-CA	-5.12	1.40	1.46	13	2
1	A	52	LYS	C-N	-5.12	1.26	1.33	7	1
1	A	58	PRO	N-CD	5.11	1.54	1.47	9	1
1	A	12	SER	CA-C	5.11	1.59	1.52	3	1
1	A	88	LYS	CA-C	-5.09	1.47	1.53	1	1
2	B	16	ILE	C-O	-5.08	1.17	1.24	8	1
1	A	16	ALA	C-O	-5.07	1.18	1.24	8	1
1	A	45	HIS	C-O	-5.04	1.18	1.24	4	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	PRO	N-CA-CB	-15.97	91.07	102.73	2	13
1	A	83	PHE	CA-C-N	12.10	144.65	121.54	9	15
1	A	83	PHE	C-N-CA	12.10	144.65	121.54	9	15
1	A	31	CYS	CA-C-N	-11.41	106.32	122.41	2	15
1	A	31	CYS	C-N-CA	-11.41	106.32	122.41	2	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	CYS	CA-C-N	11.08	133.69	119.84	7	11
1	A	57	CYS	C-N-CA	11.08	133.69	119.84	7	11
1	A	7	ASP	N-CA-C	-11.01	97.97	111.40	5	15
1	A	59	ILE	N-CA-C	-9.81	102.33	111.45	15	5
1	A	59	ILE	CA-C-N	9.72	134.28	120.28	1	9
1	A	59	ILE	C-N-CA	9.72	134.28	120.28	1	9
1	A	59	ILE	CB-CA-C	9.65	123.19	111.80	4	13
1	A	58	PRO	CB-CA-C	-9.27	96.57	112.06	3	13
2	B	20	PHE	CA-CB-CG	8.88	122.68	113.80	10	6
1	A	84	CYS	N-CA-C	-8.87	91.90	110.80	9	15
1	A	13	ILE	CB-CA-C	-8.47	101.26	111.94	14	9
2	B	22	GLU	N-CA-C	-8.08	96.73	109.50	10	2
1	A	42	VAL	CB-CA-C	7.70	121.65	111.94	9	7
1	A	58	PRO	CA-N-CD	-7.68	101.25	112.00	7	2
1	A	60	CYS	CB-CA-C	-7.63	97.70	110.68	6	3
1	A	59	ILE	N-CA-CB	-6.99	99.69	111.23	7	2
1	A	81	VAL	N-CA-C	6.82	116.10	108.05	10	4
1	A	32	SER	CA-C-N	6.81	132.65	123.46	5	12
1	A	32	SER	C-N-CA	6.81	132.65	123.46	5	12
1	A	33	LEU	CB-CA-C	6.79	117.72	110.65	1	1
1	A	81	VAL	CA-C-N	6.62	127.53	120.11	9	10
1	A	81	VAL	C-N-CA	6.62	127.53	120.11	9	10
1	A	39	MET	CA-C-N	6.61	129.04	120.44	12	15
1	A	39	MET	C-N-CA	6.61	129.04	120.44	12	15
1	A	86	ASN	N-CA-C	-6.60	105.76	113.88	9	6
1	A	13	ILE	N-CA-CB	6.51	120.34	110.58	1	7
1	A	58	PRO	CA-C-N	6.43	133.55	121.97	7	2
1	A	58	PRO	C-N-CA	6.43	133.55	121.97	7	2
1	A	31	CYS	N-CA-C	-6.43	100.52	110.10	4	13
1	A	58	PRO	N-CA-C	-6.38	99.33	112.47	7	3
1	A	81	VAL	O-C-N	6.28	127.06	121.41	4	4
1	A	36	CYS	N-CA-C	-6.25	104.39	111.14	9	13
2	B	15	ASP	N-CA-C	6.23	119.00	111.40	15	1
2	B	13	PRO	CB-CA-C	-6.20	102.07	111.44	7	3
1	A	80	PRO	CA-C-N	-6.13	117.40	123.04	10	2
1	A	80	PRO	C-N-CA	-6.13	117.40	123.04	10	2
1	A	45	HIS	N-CA-C	-6.06	104.36	110.97	6	6
1	A	7	ASP	CA-CB-CG	6.00	118.60	112.60	3	10
2	B	12	SER	CA-C-N	6.00	126.11	119.87	7	3
2	B	12	SER	C-N-CA	6.00	126.11	119.87	7	3
1	A	83	PHE	N-CA-C	5.98	123.53	110.80	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	49	CYS	CA-C-O	-5.88	115.49	122.13	7	4
1	A	59	ILE	CA-CB-CG1	5.83	120.31	110.40	6	3
1	A	60	CYS	N-CA-C	-5.82	104.85	111.14	9	1
1	A	83	PHE	O-C-N	5.82	130.33	122.59	9	5
2	B	16	ILE	CA-C-N	5.75	128.26	120.38	13	1
2	B	16	ILE	C-N-CA	5.75	128.26	120.38	13	1
1	A	62	GLN	CA-C-N	5.64	128.12	120.44	12	5
1	A	62	GLN	C-N-CA	5.64	128.12	120.44	12	5
1	A	83	PHE	CA-CB-CG	-5.64	108.16	113.80	2	1
1	A	79	CYS	N-CA-C	5.63	122.26	109.81	5	2
1	A	53	THR	CB-CA-C	5.58	120.87	109.55	6	3
1	A	82	PRO	N-CA-C	-5.57	103.37	111.33	3	3
1	A	40	LYS	N-CA-CB	-5.55	101.95	110.01	1	10
1	A	70	HIS	CA-C-N	5.49	127.95	120.54	14	3
1	A	70	HIS	C-N-CA	5.49	127.95	120.54	14	3
1	A	9	ARG	N-CA-CB	5.47	118.00	110.07	8	2
1	A	66	LEU	CA-C-N	5.44	127.51	120.44	3	3
1	A	66	LEU	C-N-CA	5.44	127.51	120.44	3	3
1	A	85	LEU	N-CA-C	5.37	122.24	110.80	6	3
2	B	18	GLN	N-CA-C	-5.37	106.23	112.89	3	3
1	A	59	ILE	CA-CB-CG2	5.36	119.62	110.50	4	2
1	A	13	ILE	N-CA-C	-5.29	105.97	111.58	14	2
1	A	80	PRO	N-CA-CB	-5.21	97.78	103.25	5	1
1	A	71	ALA	CA-C-N	5.14	127.42	120.38	5	1
1	A	71	ALA	C-N-CA	5.14	127.42	120.38	5	1
1	A	50	LYS	N-CA-CB	5.13	118.37	110.46	14	1
1	A	31	CYS	CB-CA-C	-5.11	102.81	110.16	11	1
1	A	69	TYR	CA-CB-CG	5.11	123.09	113.90	11	1
1	A	50	LYS	N-CA-C	-5.05	107.17	113.38	9	1
1	A	62	GLN	CB-CG-CD	5.04	121.17	112.60	7	1
1	A	42	VAL	CA-CB-CG2	-5.03	101.84	110.40	1	1
1	A	17	ILE	CB-CA-C	-5.03	105.43	112.02	13	1
1	A	88	LYS	CA-C-N	-5.02	114.30	122.34	15	1
1	A	88	LYS	C-N-CA	-5.02	114.30	122.34	15	1
1	A	87	ILE	N-CA-C	-5.02	104.82	111.09	10	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	32	SER	Peptide	15
1	A	82	PRO	Peptide	14
1	A	58	PRO	Mainchain,Peptide	13
2	B	21	THR	Peptide	2
1	A	10	ARG	Sidechain	1
1	A	9	ARG	Sidechain	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	632	668	664	56±5
2	B	96	77	77	10±3
All	All	10920	11175	11108	892

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 40.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD22	2:B:16:ILE:HG13	0.84	1.49	13	7
1:A:42:VAL:HG13	1:A:59:ILE:HD11	0.81	1.53	14	6
1:A:49:CYS:O	1:A:52:LYS:HG3	0.80	1.77	10	11
1:A:79:CYS:HB2	1:A:84:CYS:SG	0.79	2.18	2	1
1:A:66:LEU:HA	1:A:69:TYR:CE1	0.76	2.15	11	1
1:A:52:LYS:HE2	1:A:60:CYS:SG	0.73	2.23	6	4
1:A:46:THR:HG23	1:A:60:CYS:SG	0.72	2.24	5	4
1:A:43:VAL:O	1:A:47:LYS:HG3	0.71	1.86	2	12
1:A:20:LEU:HD11	1:A:63:LEU:HD13	0.70	1.63	4	15
2:B:17:GLU:HA	2:B:20:PHE:CD2	0.69	2.23	5	1
1:A:38:LYS:HG2	2:B:19:TRP:O	0.69	1.86	10	14
1:A:42:VAL:HG21	1:A:59:ILE:HD13	0.68	1.65	9	2
1:A:36:CYS:O	1:A:40:LYS:HB2	0.67	1.89	10	15
1:A:52:LYS:HB3	1:A:60:CYS:CB	0.67	2.20	1	3
1:A:81:VAL:O	1:A:84:CYS:HB3	0.67	1.89	1	8
1:A:71:ALA:HB2	1:A:84:CYS:HA	0.67	1.67	13	11
1:A:59:ILE:O	1:A:63:LEU:HB3	0.66	1.91	7	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:CYS:HA	1:A:85:LEU:HD21	0.65	1.67	14	2
2:B:17:GLU:HA	2:B:20:PHE:CE1	0.65	2.27	10	1
1:A:11:LEU:O	1:A:15:ARG:HG3	0.64	1.91	2	15
1:A:52:LYS:HA	1:A:60:CYS:SG	0.64	2.33	11	8
1:A:66:LEU:HD22	2:B:16:ILE:CG1	0.63	2.23	13	7
1:A:43:VAL:O	1:A:46:THR:HG22	0.63	1.94	11	7
1:A:46:THR:O	1:A:52:LYS:HE3	0.62	1.94	6	8
1:A:43:VAL:HG13	1:A:82:PRO:HG3	0.62	1.72	1	7
2:B:16:ILE:HA	2:B:19:TRP:CE3	0.61	2.30	12	5
1:A:13:ILE:HB	1:A:69:TYR:OH	0.61	1.95	15	3
1:A:7:ASP:O	1:A:11:LEU:HD12	0.61	1.96	3	3
1:A:58:PRO:O	1:A:60:CYS:N	0.61	2.34	7	2
1:A:46:THR:HA	1:A:60:CYS:SG	0.61	2.36	8	7
1:A:23:ALA:HB1	1:A:40:LYS:CA	0.61	2.25	2	15
1:A:63:LEU:HA	1:A:66:LEU:HB3	0.60	1.73	11	15
1:A:17:ILE:HG13	1:A:66:LEU:HD11	0.60	1.73	11	13
1:A:85:LEU:HA	1:A:88:LYS:HB2	0.60	1.74	6	5
1:A:81:VAL:HG12	1:A:82:PRO:O	0.59	1.97	1	15
1:A:67:ALA:HB1	1:A:82:PRO:O	0.59	1.97	2	9
1:A:64:ILE:HG12	1:A:83:PHE:CD1	0.59	2.32	5	8
2:B:13:PRO:O	2:B:16:ILE:HG12	0.59	1.97	6	1
1:A:57:CYS:SG	1:A:58:PRO:HD2	0.59	2.38	7	2
1:A:71:ALA:O	1:A:88:LYS:HE3	0.58	1.99	14	3
2:B:17:GLU:HA	2:B:20:PHE:CE2	0.58	2.33	5	1
1:A:70:HIS:HA	1:A:73:HIS:CE1	0.58	2.34	1	1
1:A:71:ALA:O	1:A:88:LYS:HE2	0.58	1.98	3	2
1:A:17:ILE:HG13	1:A:66:LEU:CD1	0.58	2.29	3	14
1:A:9:ARG:O	1:A:13:ILE:HG13	0.58	1.99	5	4
1:A:49:CYS:O	1:A:52:LYS:HG2	0.57	2.00	6	2
2:B:16:ILE:H	2:B:16:ILE:HD13	0.57	1.59	13	7
1:A:21:VAL:HA	1:A:81:VAL:CG2	0.57	2.30	15	14
1:A:46:THR:O	1:A:52:LYS:HG2	0.57	2.00	1	1
1:A:46:THR:C	1:A:52:LYS:HE3	0.57	2.25	14	7
1:A:70:HIS:CE1	1:A:74:CYS:HB2	0.56	2.35	11	3
2:B:15:ASP:HB3	2:B:19:TRP:CH2	0.56	2.35	12	3
1:A:19:SER:CB	2:B:20:PHE:HB2	0.56	2.30	5	3
1:A:35:SER:HB2	2:B:20:PHE:O	0.56	2.01	8	4
1:A:19:SER:HB3	1:A:39:MET:HG3	0.56	1.77	15	15
1:A:24:ALA:HB1	1:A:80:PRO:O	0.56	2.00	2	10
1:A:23:ALA:O	1:A:40:LYS:HG3	0.55	2.00	5	12
1:A:52:LYS:HB3	1:A:60:CYS:HB3	0.55	1.77	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:PRO:HA	1:A:37:GLN:HB2	0.55	1.79	12	13
1:A:11:LEU:HG	1:A:14:GLN:OE1	0.55	2.01	5	1
1:A:16:ALA:O	1:A:20:LEU:HB2	0.55	2.02	15	11
2:B:15:ASP:O	2:B:18:GLN:HG2	0.55	2.02	13	1
1:A:13:ILE:HG21	1:A:69:TYR:CE1	0.54	2.37	11	1
1:A:60:CYS:SG	1:A:64:ILE:HG13	0.54	2.42	10	3
1:A:20:LEU:CD1	1:A:63:LEU:HD13	0.54	2.32	4	15
1:A:35:SER:HB3	2:B:20:PHE:O	0.54	2.02	12	5
1:A:59:ILE:HA	2:B:19:TRP:CZ3	0.54	2.38	12	5
1:A:65:ALA:O	1:A:69:TYR:HB2	0.54	2.02	3	4
2:B:17:GLU:HA	2:B:20:PHE:CD1	0.54	2.38	6	2
1:A:43:VAL:O	1:A:46:THR:HB	0.54	2.02	8	7
1:A:13:ILE:HG12	2:B:13:PRO:HB3	0.54	1.80	5	4
1:A:23:ALA:HB1	1:A:40:LYS:N	0.54	2.18	6	15
1:A:42:VAL:HG22	1:A:59:ILE:HG13	0.54	1.80	2	8
1:A:13:ILE:HG22	2:B:13:PRO:HB2	0.54	1.80	6	1
1:A:36:CYS:SG	1:A:40:LYS:HE3	0.53	2.43	9	2
1:A:67:ALA:O	1:A:70:HIS:HB3	0.53	2.03	6	7
1:A:52:LYS:HB3	1:A:60:CYS:SG	0.53	2.43	1	3
1:A:38:LYS:HE3	2:B:19:TRP:O	0.53	2.03	13	2
1:A:41:ARG:O	1:A:45:HIS:HB2	0.53	2.04	11	14
1:A:68:ALA:O	1:A:71:ALA:HB3	0.53	2.04	13	9
1:A:42:VAL:CG1	1:A:59:ILE:HD11	0.53	2.30	14	1
1:A:78:LYS:O	1:A:85:LEU:HG	0.52	2.04	13	3
1:A:42:VAL:HG22	1:A:59:ILE:HD11	0.52	1.80	6	1
1:A:17:ILE:HG21	1:A:70:HIS:CG	0.52	2.38	13	2
1:A:26:CYS:O	1:A:40:LYS:HE2	0.52	2.04	3	2
1:A:46:THR:OG1	1:A:63:LEU:HD23	0.52	2.04	8	5
1:A:40:LYS:O	1:A:43:VAL:HB	0.52	2.05	7	12
1:A:68:ALA:HA	1:A:83:PHE:O	0.52	2.05	1	4
1:A:84:CYS:O	1:A:86:ASN:N	0.52	2.43	10	12
1:A:24:ALA:HB1	1:A:80:PRO:C	0.52	2.30	7	11
1:A:59:ILE:HA	2:B:19:TRP:CH2	0.52	2.40	12	1
1:A:13:ILE:O	1:A:17:ILE:HG13	0.52	2.05	6	1
1:A:39:MET:HG2	2:B:19:TRP:O	0.51	2.05	10	3
1:A:50:LYS:C	1:A:52:LYS:H	0.51	2.12	7	9
1:A:79:CYS:SG	1:A:80:PRO:HD3	0.51	2.46	5	2
1:A:79:CYS:HG	1:A:80:PRO:HD3	0.51	1.64	1	1
1:A:76:GLU:HG2	1:A:78:LYS:H	0.51	1.65	9	2
1:A:24:ALA:CB	1:A:81:VAL:HG22	0.51	2.36	9	13
1:A:17:ILE:N	1:A:66:LEU:HD11	0.50	2.21	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ARG:O	1:A:27:ARG:HD3	0.50	2.07	2	5
1:A:59:ILE:HB	2:B:19:TRP:CH2	0.50	2.42	2	3
1:A:68:ALA:O	1:A:72:LYS:HB2	0.50	2.07	5	1
1:A:57:CYS:O	1:A:61:LYS:HB2	0.50	2.07	7	2
1:A:42:VAL:HG13	1:A:59:ILE:CD1	0.50	2.34	15	1
2:B:14:ASP:HA	2:B:17:GLU:OE1	0.49	2.07	5	1
1:A:9:ARG:NE	1:A:9:ARG:HA	0.49	2.23	7	2
1:A:62:GLN:O	1:A:65:ALA:HB3	0.49	2.08	15	12
1:A:79:CYS:HA	1:A:85:LEU:CD1	0.49	2.38	6	3
1:A:79:CYS:HA	1:A:85:LEU:HD11	0.49	1.84	13	4
2:B:17:GLU:O	2:B:20:PHE:HD2	0.49	1.90	7	4
1:A:42:VAL:CG2	1:A:59:ILE:HD11	0.49	2.38	3	3
1:A:39:MET:CG	2:B:20:PHE:HA	0.49	2.37	11	3
1:A:81:VAL:O	1:A:84:CYS:HB2	0.49	2.08	12	1
1:A:85:LEU:HA	1:A:88:LYS:CD	0.49	2.38	14	1
2:B:20:PHE:CE2	2:B:21:THR:HB	0.48	2.43	8	2
1:A:59:ILE:O	1:A:63:LEU:N	0.48	2.45	14	7
1:A:8:SER:O	1:A:12:SER:HB2	0.48	2.08	5	3
2:B:20:PHE:CE1	2:B:21:THR:HG22	0.48	2.43	2	1
1:A:83:PHE:CD1	1:A:86:ASN:HB3	0.48	2.44	2	1
1:A:79:CYS:H	1:A:85:LEU:HG	0.48	1.68	15	1
1:A:32:SER:C	1:A:34:PRO:HD3	0.48	2.33	6	11
1:A:70:HIS:CD2	1:A:74:CYS:HB2	0.48	2.43	13	1
2:B:16:ILE:HD13	2:B:16:ILE:N	0.48	2.23	8	11
1:A:39:MET:HE3	2:B:19:TRP:HB2	0.48	1.86	11	3
1:A:43:VAL:HG13	1:A:82:PRO:HD3	0.47	1.86	13	1
1:A:59:ILE:HD11	2:B:19:TRP:CE2	0.47	2.44	1	1
1:A:17:ILE:CG1	1:A:66:LEU:HD11	0.47	2.38	11	1
1:A:76:GLU:OE2	1:A:85:LEU:HD12	0.47	2.10	5	1
1:A:20:LEU:HD11	1:A:63:LEU:CD1	0.47	2.38	6	3
1:A:66:LEU:HD13	2:B:16:ILE:HG13	0.46	1.87	7	1
1:A:83:PHE:HB3	1:A:87:ILE:HD13	0.46	1.87	10	1
1:A:70:HIS:NE2	1:A:74:CYS:HB2	0.46	2.25	9	1
1:A:17:ILE:HG21	1:A:70:HIS:ND1	0.46	2.25	11	1
2:B:20:PHE:CE2	2:B:21:THR:HG22	0.46	2.45	15	1
2:B:16:ILE:H	2:B:16:ILE:CD1	0.46	2.21	1	4
1:A:10:ARG:HA	1:A:13:ILE:CD1	0.46	2.41	5	1
1:A:77:ASN:HA	1:A:85:LEU:CB	0.46	2.41	15	1
1:A:21:VAL:HA	1:A:81:VAL:HG22	0.46	1.87	1	1
1:A:85:LEU:C	1:A:85:LEU:HD22	0.46	2.36	15	2
1:A:46:THR:HG23	1:A:52:LYS:HE2	0.46	1.87	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LYS:C	1:A:52:LYS:N	0.46	2.73	7	7
2:B:16:ILE:HD13	2:B:16:ILE:H	0.46	1.71	2	4
1:A:60:CYS:HA	1:A:63:LEU:HB3	0.46	1.88	1	2
1:A:74:CYS:O	1:A:88:LYS:HE3	0.46	2.11	4	2
1:A:20:LEU:HD13	1:A:66:LEU:CD2	0.46	2.41	11	5
1:A:68:ALA:O	1:A:72:LYS:HD2	0.46	2.11	6	1
1:A:83:PHE:CD1	1:A:83:PHE:N	0.45	2.80	4	2
1:A:13:ILE:O	1:A:16:ALA:HB3	0.45	2.11	6	1
1:A:39:MET:CG	2:B:20:PHE:HB3	0.45	2.40	10	1
1:A:7:ASP:CG	1:A:11:LEU:HD13	0.45	2.37	10	5
1:A:59:ILE:HA	1:A:62:GLN:HB2	0.45	1.88	9	1
1:A:66:LEU:HD22	2:B:16:ILE:CB	0.45	2.41	2	5
1:A:33:LEU:HG	1:A:36:CYS:H	0.45	1.72	12	11
1:A:33:LEU:HD11	1:A:35:SER:HB2	0.45	1.89	6	1
1:A:52:LYS:HB2	1:A:60:CYS:SG	0.45	2.52	6	1
1:A:63:LEU:HD12	1:A:63:LEU:O	0.45	2.12	1	8
1:A:42:VAL:HG22	1:A:59:ILE:CD1	0.45	2.41	14	2
1:A:64:ILE:HG12	1:A:83:PHE:CE1	0.45	2.47	12	1
1:A:46:THR:OG1	1:A:52:LYS:HG2	0.45	2.11	3	1
1:A:47:LYS:HA	1:A:52:LYS:HE3	0.45	1.89	2	4
1:A:21:VAL:O	1:A:24:ALA:HB3	0.45	2.12	7	11
1:A:17:ILE:HG21	1:A:70:HIS:CD2	0.45	2.47	3	2
1:A:42:VAL:HG22	1:A:59:ILE:CG1	0.45	2.42	5	2
1:A:17:ILE:HG12	1:A:66:LEU:CD1	0.45	2.42	6	1
1:A:17:ILE:HD11	1:A:69:TYR:CE2	0.45	2.46	10	1
1:A:46:THR:OG1	1:A:60:CYS:HB3	0.44	2.12	2	3
1:A:59:ILE:O	1:A:63:LEU:CB	0.44	2.65	9	1
1:A:34:PRO:HG3	1:A:37:GLN:HE21	0.44	1.72	5	1
1:A:10:ARG:O	1:A:14:GLN:HG3	0.44	2.13	8	1
1:A:39:MET:HE1	2:B:16:ILE:HG22	0.43	1.89	6	1
1:A:50:LYS:O	1:A:54:ASN:HB3	0.43	2.13	6	1
1:A:20:LEU:HD13	1:A:66:LEU:HD23	0.43	1.90	11	3
1:A:38:LYS:CE	2:B:19:TRP:HA	0.43	2.43	15	1
2:B:18:GLN:O	2:B:22:GLU:HG3	0.43	2.13	8	1
1:A:33:LEU:HG	1:A:36:CYS:N	0.43	2.28	12	5
2:B:17:GLU:O	2:B:20:PHE:HD1	0.43	1.97	2	3
1:A:38:LYS:HG3	2:B:19:TRP:CE3	0.43	2.48	9	1
1:A:46:THR:OG1	1:A:60:CYS:HA	0.43	2.13	15	1
1:A:46:THR:HG23	1:A:60:CYS:CB	0.43	2.43	6	1
1:A:33:LEU:HD11	1:A:35:SER:HB3	0.43	1.89	10	1
1:A:23:ALA:HB1	1:A:40:LYS:HA	0.43	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LYS:O	1:A:44:GLN:HG2	0.43	2.13	6	1
1:A:33:LEU:HD11	1:A:35:SER:OG	0.43	2.13	8	1
1:A:46:THR:HG23	1:A:60:CYS:HB3	0.43	1.91	1	1
1:A:71:ALA:CB	1:A:84:CYS:HA	0.42	2.44	7	1
1:A:38:LYS:NZ	2:B:22:GLU:HG2	0.42	2.28	10	1
1:A:81:VAL:HB	1:A:84:CYS:CB	0.42	2.43	1	1
1:A:76:GLU:OE2	1:A:78:LYS:HE3	0.42	2.13	10	1
1:A:7:ASP:CA	1:A:11:LEU:HD13	0.42	2.45	2	1
1:A:79:CYS:O	1:A:85:LEU:HD13	0.42	2.14	2	1
2:B:14:ASP:O	2:B:18:GLN:HG2	0.42	2.14	4	1
1:A:60:CYS:O	1:A:64:ILE:HG13	0.42	2.14	2	1
1:A:39:MET:HG2	2:B:20:PHE:HA	0.42	1.92	6	1
1:A:46:THR:OG1	1:A:59:ILE:HD13	0.42	2.14	10	1
1:A:47:LYS:HA	1:A:52:LYS:CE	0.42	2.44	12	2
1:A:84:CYS:SG	1:A:85:LEU:N	0.42	2.92	3	2
2:B:17:GLU:O	2:B:20:PHE:CD2	0.42	2.72	4	2
1:A:13:ILE:HG23	2:B:13:PRO:HA	0.42	1.91	9	1
1:A:16:ALA:HB1	2:B:16:ILE:CG1	0.42	2.45	9	1
1:A:13:ILE:HA	2:B:13:PRO:HB3	0.42	1.90	14	1
1:A:13:ILE:CG2	1:A:69:TYR:CE1	0.42	3.02	11	1
1:A:17:ILE:HD13	1:A:70:HIS:ND1	0.42	2.29	12	1
1:A:80:PRO:HB2	1:A:81:VAL:HG23	0.42	1.91	1	1
1:A:10:ARG:HA	1:A:13:ILE:HD12	0.42	1.91	5	1
1:A:21:VAL:HG22	1:A:81:VAL:HG21	0.41	1.91	1	1
1:A:60:CYS:CA	1:A:63:LEU:HB3	0.41	2.45	3	1
1:A:34:PRO:HA	1:A:37:GLN:CG	0.41	2.46	6	1
1:A:33:LEU:C	1:A:35:SER:N	0.41	2.77	11	2
1:A:46:THR:C	1:A:52:LYS:HE2	0.41	2.40	9	2
1:A:85:LEU:HD22	1:A:85:LEU:C	0.41	2.40	6	2
1:A:17:ILE:HG13	1:A:66:LEU:HD12	0.41	1.92	5	1
1:A:17:ILE:CG1	1:A:66:LEU:CD1	0.41	2.98	13	1
1:A:88:LYS:O	1:A:88:LYS:HG3	0.41	2.15	15	1
1:A:13:ILE:HG23	2:B:13:PRO:HB3	0.41	1.92	12	1
2:B:17:GLU:HA	2:B:20:PHE:HB3	0.41	1.92	12	1
1:A:79:CYS:HA	1:A:85:LEU:CD2	0.41	2.44	15	1
1:A:84:CYS:C	1:A:86:ASN:H	0.41	2.22	15	1
1:A:66:LEU:HD22	2:B:16:ILE:HB	0.41	1.92	2	1
1:A:88:LYS:O	1:A:88:LYS:HD3	0.41	2.15	7	1
1:A:7:ASP:O	1:A:11:LEU:HD13	0.41	2.15	15	2
1:A:13:ILE:HA	1:A:16:ALA:HB3	0.41	1.92	15	1
1:A:27:ARG:O	1:A:27:ARG:HD2	0.41	2.16	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:CD1	1:A:35:SER:HB2	0.41	2.46	6	1
1:A:38:LYS:CD	2:B:19:TRP:HA	0.41	2.46	12	1
2:B:13:PRO:O	2:B:17:GLU:HG3	0.40	2.16	1	1
1:A:9:ARG:O	2:B:13:PRO:HG3	0.40	2.16	3	1
1:A:33:LEU:O	1:A:36:CYS:HB2	0.40	2.16	3	1
1:A:7:ASP:C	1:A:11:LEU:HD13	0.40	2.42	2	1
1:A:14:GLN:O	1:A:18:GLN:HG3	0.40	2.15	3	1
1:A:53:THR:HG21	1:A:64:ILE:HD12	0.40	1.93	8	1
1:A:17:ILE:HD11	1:A:69:TYR:CZ	0.40	2.52	2	1
1:A:34:PRO:HG3	1:A:37:GLN:OE1	0.40	2.16	2	1
1:A:39:MET:HG2	2:B:19:TRP:C	0.40	2.41	11	1
1:A:34:PRO:HA	1:A:37:GLN:CB	0.40	2.46	12	1
1:A:22:HIS:O	1:A:26:CYS:CB	0.40	2.70	14	1
1:A:34:PRO:HG3	1:A:37:GLN:NE2	0.40	2.31	5	1
1:A:13:ILE:HA	1:A:16:ALA:CB	0.40	2.47	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	82/90 (91%)	71±2 (87±2%)	7±1 (8±2%)	4±1 (5±1%)	3	23
2	B	11/25 (44%)	10±1 (89±8%)	1±1 (11±8%)	0±0 (0±0%)	100	100
All	All	1395/1725 (81%)	1211 (87%)	121 (9%)	63 (5%)	3	27

All 10 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	83	PHE	15
1	A	85	LEU	15
1	A	80	PRO	11
1	A	79	CYS	7
1	A	78	LYS	4
1	A	56	GLY	3

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Mol	Chain	Res	Type	Models (Total)
1	A	82	PRO	2
1	A	52	LYS	2
1	A	58	PRO	2
1	A	59	ILE	2

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	71/77 (92%)	62±1 (87±2%)	9±1 (13±2%)	6	47
2	B	11/23 (48%)	8±1 (69±9%)	3±1 (31±9%)	1	15
All	All	1230/1500 (82%)	1041 (85%)	189 (15%)	5	41

All 34 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	39	MET	15
1	A	42	VAL	15
2	B	16	ILE	15
1	A	58	PRO	14
1	A	85	LEU	14
2	B	20	PHE	12
1	A	27	ARG	11
1	A	59	ILE	11
1	A	33	LEU	10
1	A	13	ILE	9
2	B	17	GLU	8
1	A	88	LYS	7
2	B	21	THR	7
1	A	87	ILE	6
2	B	12	SER	5
1	A	75	GLN	4
2	B	15	ASP	2
1	A	50	LYS	2
1	A	52	LYS	2
1	A	78	LYS	2

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Mol	Chain	Res	Type	Models (Total)
2	B	22	GLU	2
1	A	72	LYS	2
1	A	34	PRO	2
1	A	69	TYR	2
1	A	38	LYS	1
1	A	83	PHE	1
1	A	73	HIS	1
1	A	30	ASN	1
1	A	8	SER	1
1	A	9	ARG	1
1	A	32	SER	1
1	A	44	GLN	1
1	A	86	ASN	1
1	A	63	LEU	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 82% 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 [i](#)

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

Total number of shifts	990
Number of shifts mapped to atoms	990
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	87	-0.51 ± 0.14	Should be checked
$^{13}\text{C}_\beta$	83	0.25 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	-0.85 ± 0.11	Should be applied
^{15}N	74	-0.76 ± 0.37	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 72%, i.e. 920 atoms were assigned a chemical shift out of a possible 1274. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	372/458 (81%)	153/184 (83%)	149/186 (80%)	70/88 (80%)
Sidechain	548/743 (74%)	375/479 (78%)	173/224 (77%)	0/40 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/73 (0%)	0/36 (0%)	0/28 (0%)	0/9 (0%)
Overall	920/1274 (72%)	528/699 (76%)	322/438 (74%)	70/137 (51%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 990 atoms were assigned a chemical shift out of a possible 1541. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	400/564 (71%)	165/227 (73%)	161/230 (70%)	74/107 (69%)
Sidechain	590/904 (65%)	403/584 (69%)	187/276 (68%)	0/44 (0%)
Aromatic	0/73 (0%)	0/36 (0%)	0/28 (0%)	0/9 (0%)
Overall	990/1541 (64%)	568/847 (67%)	348/534 (65%)	74/160 (46%)

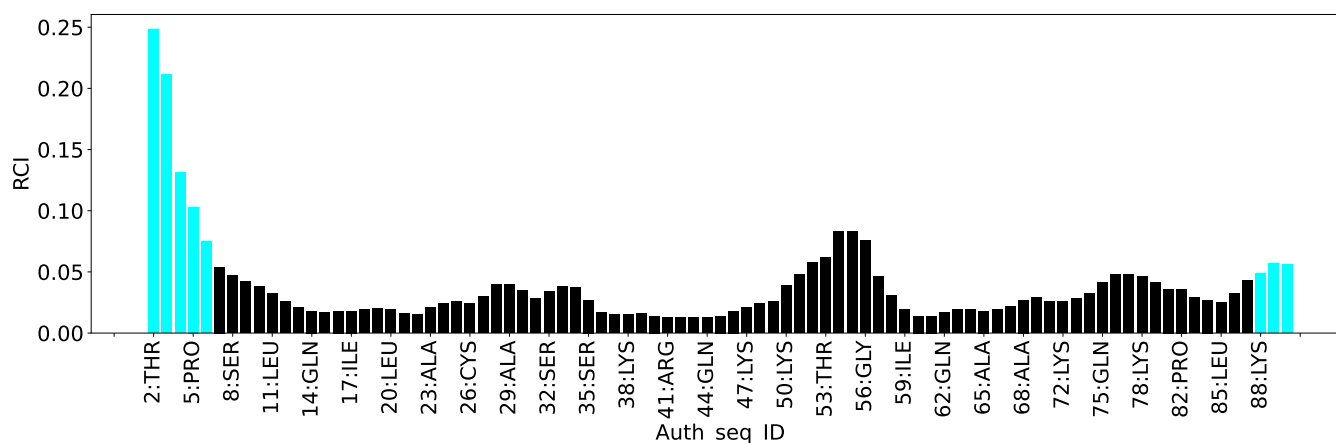
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping

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	280
Number of shifts mapped to atoms	280
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	25	-0.01 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	24	—	None (insufficient data)
$^{13}\text{C}'$	21	—	None (insufficient data)
^{15}N	22	—	None (insufficient data)

7.2.3 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 10%, i.e. 123 atoms were assigned a chemical shift out of a possible 1274. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	52/458 (11%)	21/184 (11%)	21/186 (11%)	10/88 (11%)
Sidechain	64/743 (9%)	43/479 (9%)	20/224 (9%)	1/40 (2%)
Aromatic	7/73 (10%)	6/36 (17%)	0/28 (0%)	1/9 (11%)
Overall	123/1274 (10%)	70/699 (10%)	41/438 (9%)	12/137 (9%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 18%, i.e. 279 atoms were assigned a chemical shift out of a possible 1541. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	115/564 (20%)	47/227 (21%)	46/230 (20%)	22/107 (21%)
Sidechain	157/904 (17%)	107/584 (18%)	48/276 (17%)	2/44 (5%)
Aromatic	7/73 (10%)	6/36 (17%)	0/28 (0%)	1/9 (11%)
Overall	279/1541 (18%)	160/847 (19%)	94/534 (18%)	25/160 (16%)

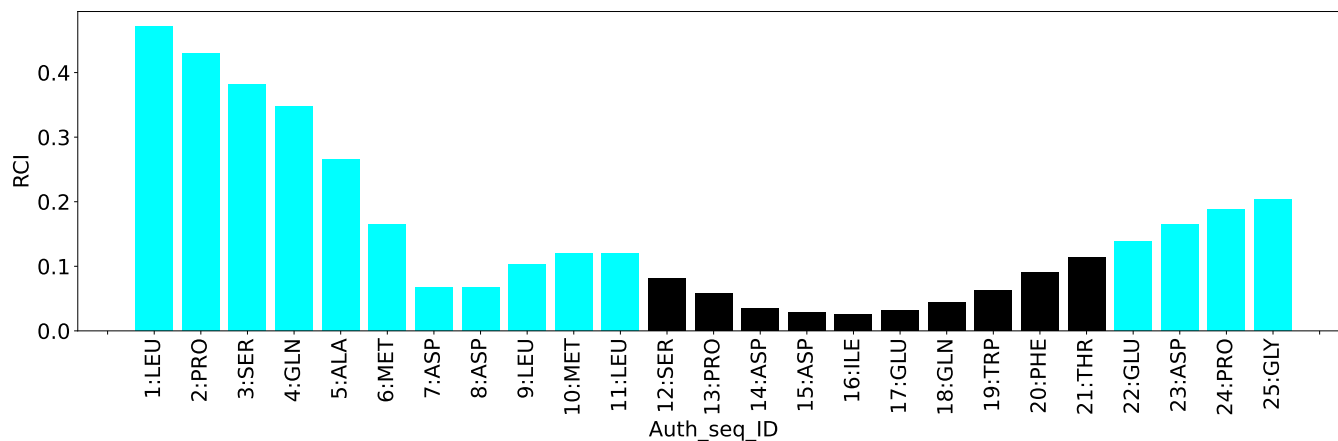
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2081
Intra-residue ($ i-j =0$)	535
Sequential ($ i-j =1$)	546
Medium range ($ i-j >1$ and $ i-j <5$)	595
Long range ($ i-j \geq 5$)	277
Inter-chain	40
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	180
Number of unmapped restraints	0
Number of restraints per residue	19.7
Number of long range restraints per residue ¹	2.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	120.5	0.2
0.2-0.5 (Medium)	142.4	0.5
>0.5 (Large)	32.1	4.51

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)	28.4	10.0
10.0-20.0 (Medium)	3.8	19.74
>20.0 (Large)	3.5	136.54

9 Distance violation analysis ⓘ

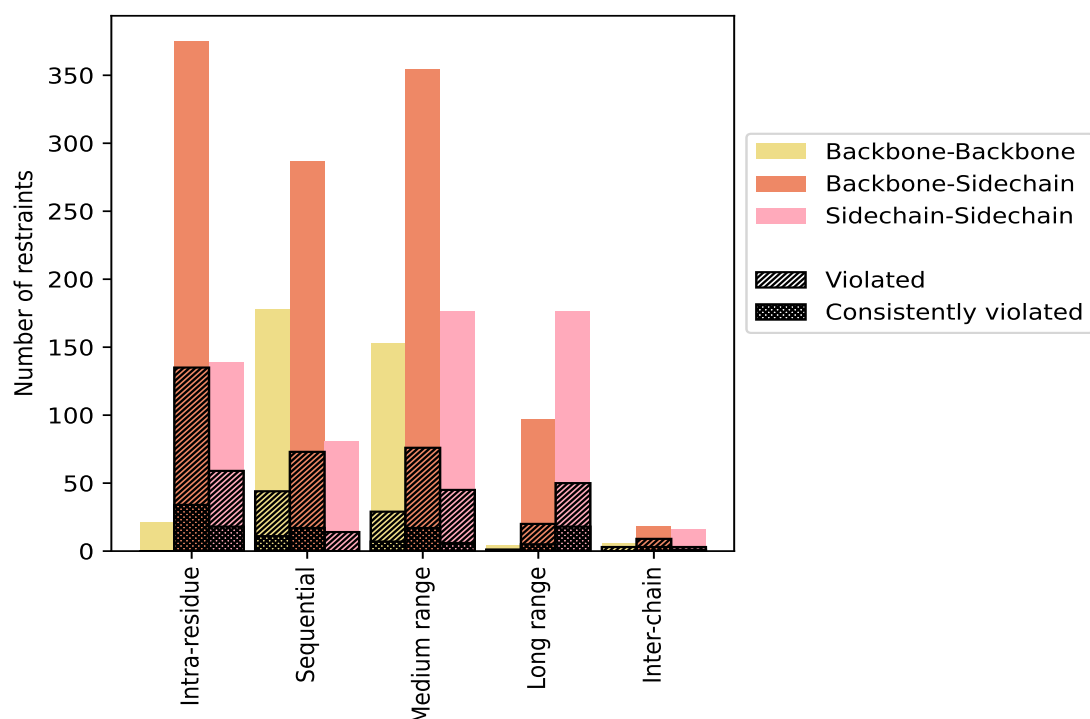
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	535	25.7	194	36.3	9.3	52	9.7	2.5
Backbone-Backbone	21	1.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	375	18.0	135	36.0	6.5	34	9.1	1.6
Sidechain-Sidechain	139	6.7	59	42.4	2.8	18	12.9	0.9
Sequential ($i-j =1$)	546	26.2	131	24.0	6.3	28	5.1	1.3
Backbone-Backbone	178	8.6	44	24.7	2.1	11	6.2	0.5
Backbone-Sidechain	287	13.8	73	25.4	3.5	17	5.9	0.8
Sidechain-Sidechain	81	3.9	14	17.3	0.7	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	595	28.6	136	22.9	6.5	26	4.4	1.2
Backbone-Backbone	153	7.4	29	19.0	1.4	7	4.6	0.3
Backbone-Sidechain	266	12.8	62	23.3	3.0	13	4.9	0.6
Sidechain-Sidechain	176	8.5	45	25.6	2.2	6	3.4	0.3
Long range ($i-j \geq 5$)	277	13.3	71	25.6	3.4	24	8.7	1.2
Backbone-Backbone	4	0.2	1	25.0	0.0	1	25.0	0.0
Backbone-Sidechain	97	4.7	20	20.6	1.0	5	5.2	0.2
Sidechain-Sidechain	176	8.5	50	28.4	2.4	18	10.2	0.9
Inter-chain	40	1.9	15	37.5	0.7	4	10.0	0.2
Backbone-Backbone	6	0.3	3	50.0	0.1	0	0.0	0.0
Backbone-Sidechain	18	0.9	9	50.0	0.4	3	16.7	0.1
Sidechain-Sidechain	16	0.8	3	18.8	0.1	1	6.2	0.0
Hydrogen bond	88	4.2	14	15.9	0.7	4	4.5	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2081	100.0	561	27.0	27.0	138	6.6	6.6
Backbone-Backbone	362	17.4	77	21.3	3.7	19	5.2	0.9
Backbone-Sidechain	1131	54.3	313	27.7	15.0	76	6.7	3.7
Sidechain-Sidechain	588	28.3	171	29.1	8.2	43	7.3	2.1

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 disulfied bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	118	65	78	39	8	308	0.31	3.49	0.35	0.22
2	99	69	76	42	8	294	0.33	4.25	0.4	0.24
3	106	66	75	44	7	298	0.32	2.94	0.32	0.24
4	104	66	79	43	8	300	0.33	4.51	0.43	0.24
5	105	71	80	37	9	302	0.32	3.35	0.36	0.23
6	108	72	78	36	7	301	0.3	3.46	0.35	0.23
7	110	70	83	47	8	318	0.31	2.91	0.33	0.23
8	108	70	76	40	9	303	0.32	3.82	0.39	0.23
9	108	66	77	40	7	298	0.35	4.35	0.46	0.24
10	106	71	76	37	7	297	0.32	3.24	0.37	0.23

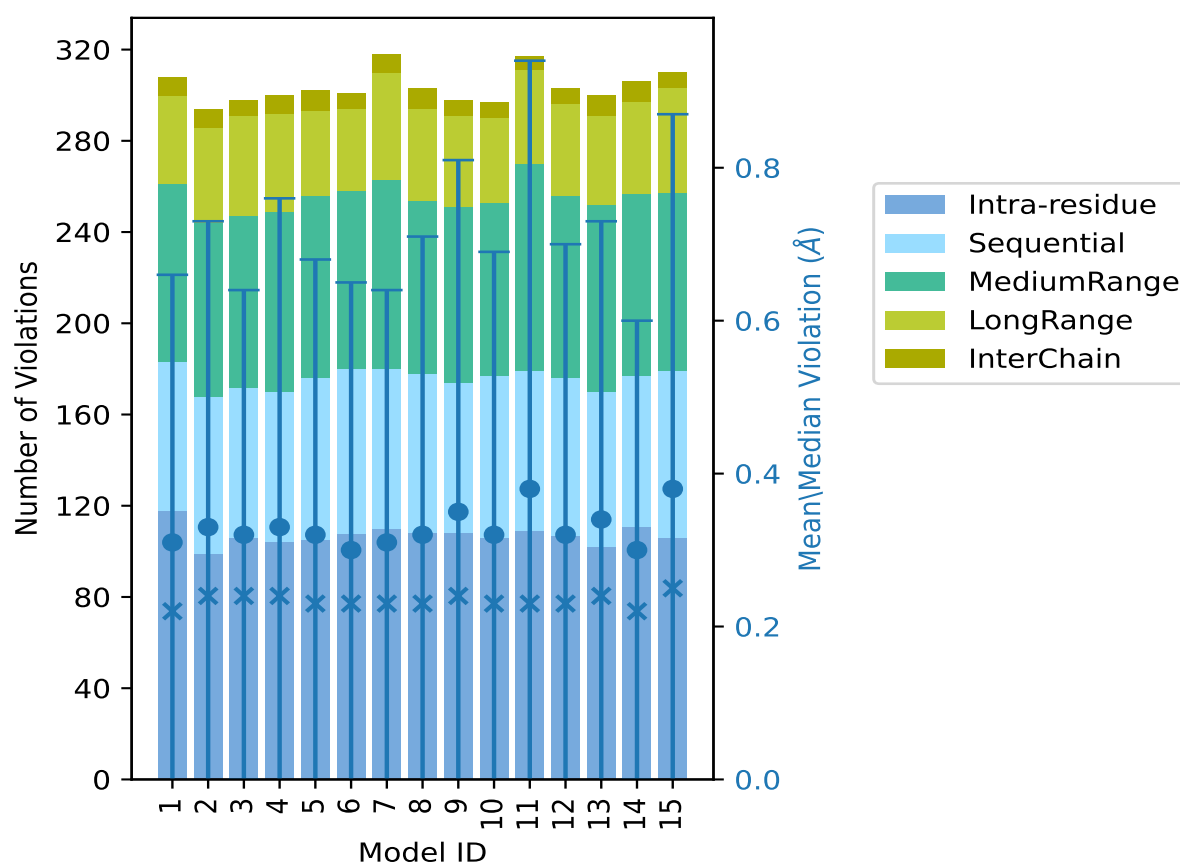
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	109	70	91	41	6	317	0.38	4.27	0.56	0.23
12	107	69	80	40	7	303	0.32	4.28	0.38	0.23
13	102	68	82	39	9	300	0.34	3.37	0.39	0.24
14	111	66	80	40	9	306	0.3	2.53	0.3	0.22
15	106	73	78	46	7	310	0.38	4.06	0.49	0.25

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

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



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

9.3 Distance violation statistics for the ensemble

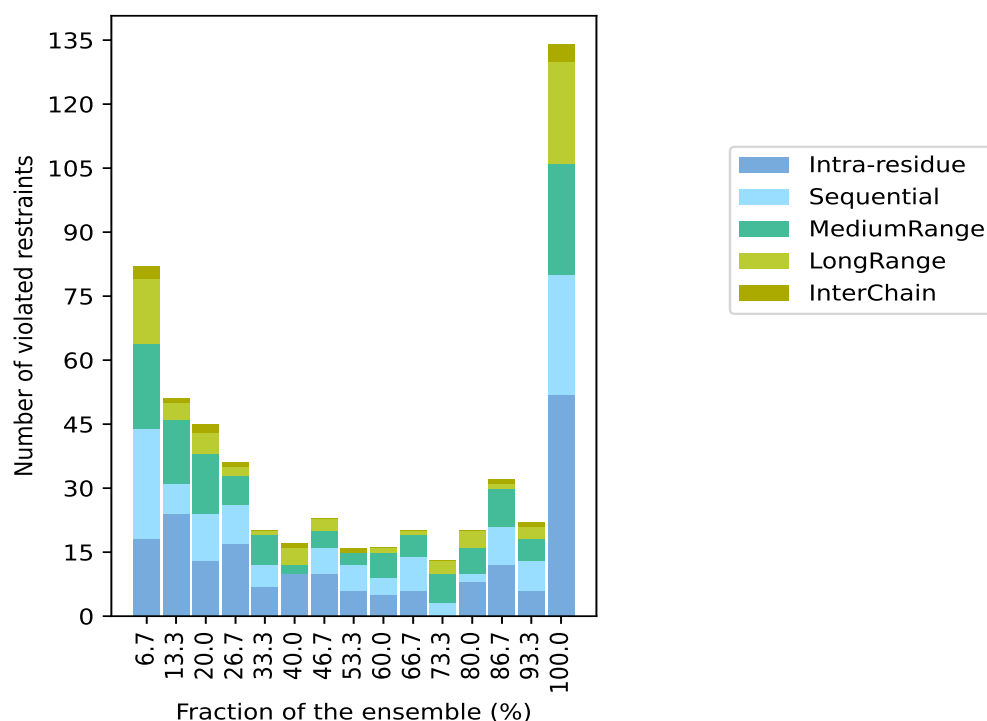
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1446(IR:341, SQ:415, MR:459, LR:206, IC:25) restraints are 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	%
18	26	20	15	3	82	1	6.7
24	7	15	4	1	51	2	13.3
13	11	14	5	2	45	3	20.0
17	9	7	2	1	36	4	26.7
7	5	7	1	0	20	5	33.3
10	0	2	4	1	17	6	40.0
10	6	4	3	0	23	7	46.7
6	6	3	0	1	16	8	53.3
5	4	6	1	0	16	9	60.0
6	8	5	1	0	20	10	66.7
0	3	7	3	0	13	11	73.3
8	2	6	4	0	20	12	80.0
12	9	9	1	1	32	13	86.7
6	7	5	3	1	22	14	93.3
52	28	26	24	4	134	15	100.0

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

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

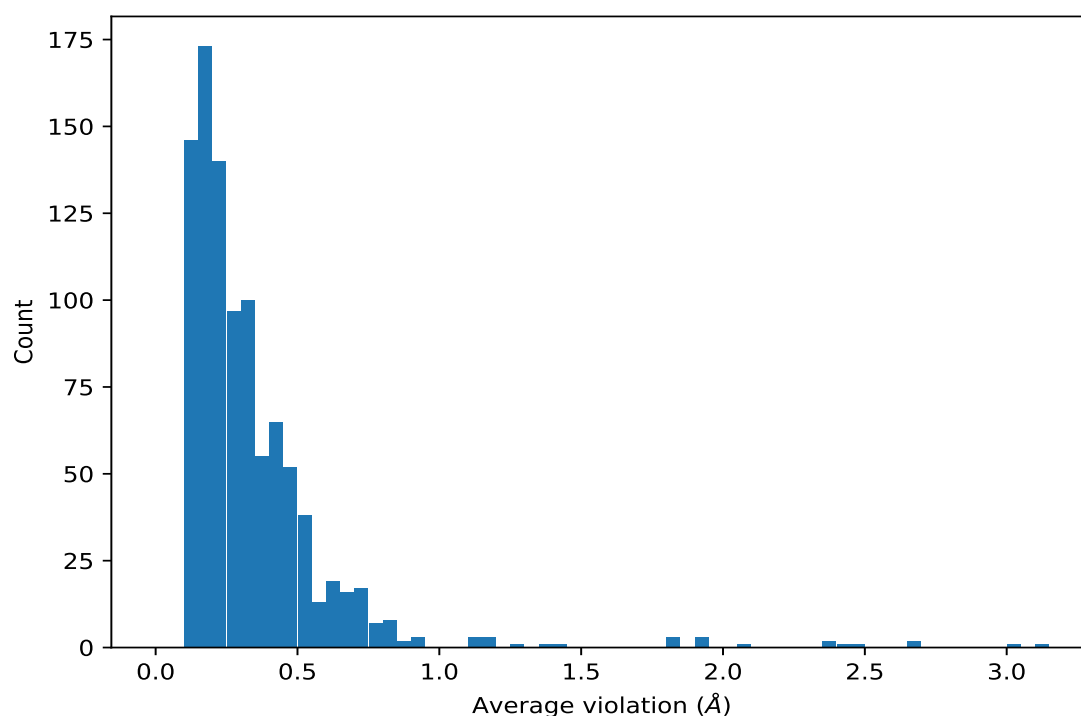
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	15	3.1	1.22	3.24
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	15	3.03	0.32	2.97
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	15	2.45	1.34	2.84
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	15	1.81	0.18	1.79
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	15	1.81	0.18	1.79
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	15	1.81	0.18	1.79
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	15	1.38	0.16	1.41
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	15	1.19	0.25	1.2
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	15	1.19	0.25	1.2
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	15	1.19	0.25	1.2
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	15	0.89	0.79	0.4
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	15	0.8	0.02	0.8
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	15	0.8	0.02	0.8
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	15	0.8	0.02	0.8
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	15	0.79	0.39	1.03
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	15	0.77	0.15	0.78

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	15	0.77	0.15	0.78
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	15	0.77	0.15	0.78
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	15	0.74	0.45	0.68
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	15	0.72	0.05	0.7
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	15	0.72	0.05	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	15	0.72	0.05	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	15	0.72	0.05	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	15	0.72	0.05	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	15	0.72	0.05	0.7
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	15	0.71	0.03	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	15	0.71	0.03	0.71
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	15	0.68	0.02	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	15	0.68	0.02	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	15	0.68	0.02	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	15	0.68	0.02	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	15	0.68	0.02	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	15	0.68	0.02	0.67
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	15	0.67	0.13	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	15	0.67	0.13	0.74
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	15	0.65	0.38	0.69
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	15	0.63	0.03	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	15	0.63	0.03	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	15	0.63	0.03	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	15	0.63	0.03	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	15	0.63	0.03	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	15	0.63	0.03	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	15	0.63	0.03	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	15	0.63	0.03	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	15	0.63	0.03	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	15	0.61	0.02	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	15	0.61	0.02	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	15	0.61	0.02	0.61
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	15	0.53	0.12	0.55
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	15	0.53	0.12	0.55
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	15	0.53	0.12	0.55
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	15	0.51	0.09	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	15	0.51	0.09	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	15	0.51	0.09	0.53
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	15	0.51	0.07	0.53
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	15	0.51	0.07	0.53
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	15	0.51	0.01	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	15	0.51	0.01	0.51
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	15	0.48	0.03	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	15	0.48	0.03	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	15	0.48	0.03	0.49
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	15	0.48	0.03	0.49
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	15	0.48	0.03	0.49
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	15	0.48	0.03	0.49
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	15	0.48	0.03	0.49
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	15	0.48	0.03	0.49
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	15	0.48	0.03	0.49
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	15	0.47	0.13	0.57
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	15	0.46	0.1	0.5
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	15	0.46	0.1	0.5
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	15	0.46	0.1	0.5
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	15	0.46	0.1	0.5
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	15	0.45	0.01	0.45
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	15	0.45	0.01	0.45
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	15	0.45	0.01	0.45
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	15	0.45	0.01	0.45
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	15	0.45	0.01	0.45
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	15	0.45	0.01	0.45
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	15	0.45	0.06	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	15	0.45	0.06	0.47
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	15	0.45	0.06	0.47
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	15	0.45	0.01	0.45
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	15	0.45	0.01	0.45
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	15	0.45	0.01	0.45
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	15	0.45	0.01	0.45
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	15	0.45	0.01	0.45
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	15	0.45	0.01	0.45
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	15	0.45	0.03	0.44
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	15	0.45	0.03	0.44
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	15	0.45	0.03	0.44
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	15	0.45	0.12	0.46
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	15	0.45	0.12	0.46
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	15	0.44	0.03	0.43
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	15	0.44	0.03	0.43
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	15	0.44	0.02	0.43
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	15	0.44	0.02	0.43
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	15	0.44	0.02	0.43
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	15	0.43	0.04	0.44
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	15	0.43	0.04	0.44
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	15	0.43	0.04	0.44
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	15	0.43	0.03	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	15	0.43	0.03	0.42
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	15	0.41	0.03	0.42
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	15	0.41	0.03	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	15	0.41	0.01	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	15	0.41	0.01	0.41
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	15	0.4	0.07	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	15	0.4	0.07	0.4
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	15	0.4	0.07	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	15	0.4	0.07	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	15	0.4	0.07	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	15	0.4	0.07	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	15	0.4	0.07	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	15	0.4	0.07	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	15	0.4	0.07	0.4
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	15	0.4	0.02	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	15	0.4	0.02	0.39
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	15	0.39	0.02	0.39
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	15	0.39	0.02	0.39
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	15	0.37	0.08	0.37
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	15	0.37	0.08	0.37
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	15	0.37	0.08	0.37
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	15	0.37	0.05	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	15	0.37	0.05	0.36
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	15	0.37	0.02	0.36
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	15	0.37	0.02	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	15	0.37	0.02	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	15	0.37	0.01	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	15	0.37	0.01	0.37
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	15	0.37	0.1	0.4
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	15	0.37	0.1	0.4
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	15	0.37	0.1	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	15	0.36	0.07	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	15	0.36	0.07	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	15	0.36	0.07	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	15	0.36	0.03	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	15	0.36	0.03	0.36
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	15	0.35	0.05	0.37
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	15	0.35	0.05	0.37
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	15	0.35	0.05	0.37
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	15	0.34	0.07	0.33
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	15	0.34	0.07	0.33
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	15	0.34	0.07	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	15	0.33	0.02	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	15	0.33	0.02	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	15	0.32	0.02	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	15	0.32	0.02	0.33
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	15	0.32	0.06	0.32
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	15	0.32	0.06	0.32
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	15	0.32	0.06	0.32
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	15	0.32	0.02	0.32
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	15	0.32	0.02	0.32
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	15	0.32	0.05	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	15	0.32	0.05	0.31
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	15	0.32	0.04	0.31
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	15	0.32	0.04	0.31
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	15	0.31	0.06	0.32
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	15	0.31	0.06	0.32
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	15	0.31	0.03	0.32
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	15	0.31	0.03	0.32
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	15	0.31	0.03	0.32
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	15	0.31	0.04	0.3
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	15	0.31	0.02	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	15	0.3	0.18	0.25
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	15	0.3	0.03	0.29
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	15	0.3	0.03	0.29
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	15	0.3	0.01	0.3
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	15	0.3	0.01	0.3
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	15	0.3	0.01	0.3
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	15	0.3	0.02	0.3
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	15	0.3	0.04	0.31
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	15	0.3	0.04	0.31
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	15	0.3	0.04	0.31
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	15	0.29	0.05	0.29
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	15	0.29	0.03	0.3
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	15	0.29	0.03	0.3
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	15	0.29	0.04	0.3
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	15	0.29	0.04	0.3
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	15	0.29	0.05	0.28
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	15	0.29	0.05	0.28
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	15	0.29	0.05	0.28
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	15	0.29	0.01	0.29
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	15	0.29	0.01	0.29
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	15	0.28	0.08	0.33
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	15	0.28	0.08	0.33
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	15	0.28	0.08	0.28
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	15	0.28	0.02	0.28
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	15	0.28	0.02	0.28
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	15	0.28	0.03	0.27
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	15	0.28	0.03	0.29
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	15	0.28	0.03	0.29
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	15	0.27	0.05	0.27
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	15	0.27	0.05	0.27
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	15	0.27	0.03	0.27
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	15	0.27	0.05	0.28
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	15	0.27	0.05	0.28
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	15	0.26	0.04	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	15	0.26	0.04	0.28
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	15	0.26	0.02	0.26
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	15	0.26	0.02	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	15	0.26	0.04	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	15	0.26	0.04	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	15	0.26	0.04	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	15	0.26	0.03	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	15	0.26	0.03	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	15	0.26	0.03	0.26
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	15	0.26	0.03	0.26
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	15	0.26	0.03	0.26
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	15	0.25	0.02	0.25
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	15	0.24	0.06	0.27
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	15	0.24	0.06	0.27
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	15	0.24	0.04	0.24
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	15	0.24	0.04	0.24
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	15	0.23	0.06	0.23
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	15	0.23	0.04	0.23
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	15	0.23	0.04	0.24
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	15	0.23	0.03	0.24
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	15	0.23	0.09	0.2
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	15	0.23	0.01	0.23
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	15	0.23	0.1	0.18
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	15	0.23	0.02	0.23
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	15	0.23	0.04	0.22
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	15	0.23	0.04	0.22
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	15	0.23	0.04	0.22
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	15	0.23	0.03	0.23
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	15	0.22	0.05	0.2
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	15	0.22	0.05	0.2
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	15	0.22	0.05	0.2
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	15	0.22	0.03	0.21
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	15	0.22	0.02	0.22
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	15	0.21	0.02	0.21
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	15	0.21	0.04	0.21
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	15	0.21	0.03	0.2
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	15	0.21	0.02	0.21
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	15	0.2	0.03	0.2
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	15	0.2	0.03	0.2
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	15	0.2	0.03	0.2
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	15	0.2	0.06	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	15	0.2	0.02	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	15	0.2	0.02	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	15	0.2	0.02	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	15	0.2	0.02	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	15	0.2	0.02	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	15	0.2	0.02	0.2
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	15	0.2	0.04	0.2
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	15	0.2	0.03	0.19
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	15	0.2	0.01	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	15	0.2	0.02	0.2
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	15	0.2	0.01	0.19
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	15	0.19	0.04	0.2
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	15	0.19	0.04	0.2
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	15	0.19	0.03	0.19
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	15	0.19	0.02	0.19
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	15	0.19	0.02	0.19
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	15	0.19	0.02	0.19
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	15	0.19	0.04	0.17
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	15	0.19	0.04	0.17
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	15	0.18	0.04	0.18
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	15	0.18	0.02	0.18
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	15	0.18	0.04	0.18
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	15	0.18	0.02	0.18
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	15	0.18	0.03	0.18
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	15	0.18	0.04	0.17
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	15	0.17	0.03	0.17
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	15	0.17	0.02	0.17
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	15	0.16	0.04	0.16
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	15	0.16	0.03	0.17
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	15	0.16	0.03	0.16
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	15	0.16	0.02	0.15
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	15	0.16	0.02	0.15
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	15	0.15	0.03	0.15
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	15	0.15	0.02	0.14
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	15	0.13	0.01	0.13
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	15	0.13	0.02	0.13
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	15	0.13	0.02	0.13
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	15	0.12	0.02	0.12
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	14	0.75	0.06	0.76
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	14	0.75	0.06	0.76
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	14	0.75	0.06	0.76
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	14	0.53	0.08	0.52
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	14	0.53	0.08	0.52
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	14	0.53	0.14	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	14	0.53	0.14	0.54
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	14	0.53	0.14	0.54
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	14	0.47	0.07	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	14	0.47	0.07	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	14	0.47	0.07	0.48
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	14	0.42	0.07	0.44
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	14	0.42	0.07	0.44
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	14	0.42	0.07	0.44
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	14	0.38	0.13	0.44
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	14	0.38	0.13	0.44
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	14	0.35	0.04	0.34
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	14	0.35	0.04	0.34
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	14	0.35	0.04	0.34
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	14	0.35	0.02	0.34
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	14	0.35	0.02	0.34
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	14	0.33	0.07	0.36
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	14	0.32	0.1	0.34
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	14	0.32	0.1	0.34
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	14	0.32	0.05	0.32
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	14	0.27	0.05	0.28
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	14	0.26	0.07	0.26
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	14	0.26	0.07	0.26
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	14	0.26	0.07	0.26
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	14	0.24	0.07	0.26
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	14	0.21	0.04	0.23
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	14	0.2	0.02	0.2
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	14	0.2	0.02	0.2
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	14	0.2	0.02	0.2
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	14	0.17	0.09	0.14
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	14	0.17	0.03	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	14	0.17	0.03	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	14	0.17	0.03	0.16
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	14	0.17	0.02	0.16
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	14	0.16	0.03	0.16
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	14	0.13	0.02	0.13
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	14	0.12	0.01	0.12
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	13	1.26	1.3	0.33
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	13	0.61	0.21	0.58
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	13	0.61	0.21	0.58
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	13	0.56	0.56	0.37
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	13	0.53	0.18	0.63
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	13	0.51	0.02	0.52

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	13	0.51	0.02	0.52
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	13	0.51	0.02	0.52
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	13	0.49	0.17	0.47
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	13	0.49	0.17	0.47
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	13	0.49	0.17	0.47
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	13	0.44	0.37	0.28
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	13	0.41	0.14	0.38
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	13	0.32	0.09	0.35
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	13	0.32	0.09	0.35
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	13	0.32	0.03	0.32
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	13	0.31	0.13	0.29
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	13	0.31	0.13	0.29
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	13	0.31	0.13	0.29
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	13	0.31	0.13	0.29
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	13	0.31	0.13	0.29
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	13	0.31	0.13	0.29
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	13	0.31	0.04	0.32
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	13	0.27	0.05	0.28
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	13	0.27	0.05	0.28
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	13	0.26	0.03	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	13	0.26	0.03	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	13	0.26	0.03	0.27
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	13	0.25	0.05	0.25
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	13	0.24	0.19	0.17
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	13	0.23	0.01	0.23
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	13	0.22	0.05	0.23
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	13	0.22	0.05	0.23
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	13	0.21	0.03	0.22
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	13	0.21	0.05	0.22
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	13	0.21	0.02	0.2
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	13	0.21	0.02	0.2
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	13	0.21	0.02	0.2
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	13	0.19	0.06	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	13	0.19	0.06	0.16
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	13	0.18	0.02	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	13	0.18	0.07	0.15
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	13	0.18	0.07	0.15
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	13	0.18	0.07	0.15
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	13	0.18	0.03	0.18
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	13	0.17	0.01	0.17
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	13	0.17	0.04	0.18
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	13	0.16	0.03	0.16
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	13	0.16	0.04	0.16
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	13	0.15	0.03	0.15
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	13	0.15	0.03	0.15
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	13	0.15	0.03	0.15
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	13	0.15	0.04	0.14
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	13	0.14	0.02	0.14
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	13	0.14	0.02	0.15
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	13	0.13	0.01	0.13
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	13	0.12	0.01	0.12
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	12	0.64	0.61	0.22
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	12	0.44	0.05	0.44
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	12	0.44	0.05	0.44
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	12	0.44	0.38	0.24
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	12	0.42	0.05	0.43
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	12	0.42	0.05	0.43
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	12	0.42	0.05	0.43
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	12	0.41	0.05	0.42
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	12	0.41	0.05	0.42
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	12	0.41	0.05	0.42
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	12	0.31	0.11	0.36
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	12	0.31	0.11	0.36
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	12	0.3	0.16	0.26
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	12	0.3	0.16	0.26
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	12	0.3	0.16	0.26
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	12	0.3	0.16	0.26
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	12	0.26	0.03	0.26
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	12	0.26	0.03	0.26
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	12	0.23	0.08	0.2
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	12	0.23	0.08	0.2
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	12	0.22	0.06	0.22
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	12	0.22	0.06	0.22
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	12	0.22	0.06	0.22
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	12	0.22	0.06	0.22
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	12	0.22	0.06	0.22
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	12	0.22	0.06	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	12	0.22	0.06	0.22
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	12	0.22	0.06	0.22
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	12	0.22	0.06	0.22
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	12	0.2	0.05	0.2
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	12	0.2	0.06	0.23
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	12	0.19	0.06	0.18
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	12	0.18	0.07	0.16
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	12	0.16	0.04	0.16
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	12	0.15	0.03	0.16
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	12	0.15	0.04	0.14
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	12	0.15	0.04	0.14
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	12	0.14	0.03	0.14
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	12	0.14	0.01	0.14
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	12	0.14	0.02	0.13
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	12	0.12	0.01	0.12
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	12	0.12	0.01	0.11
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	11	0.55	0.14	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	11	0.55	0.14	0.56
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	11	0.32	0.09	0.3
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	11	0.28	0.12	0.28
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	11	0.28	0.12	0.28
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	11	0.25	0.07	0.28
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	11	0.25	0.07	0.28
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	11	0.25	0.03	0.25
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	11	0.24	0.01	0.24
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	11	0.19	0.02	0.19
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	11	0.17	0.05	0.17
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	11	0.16	0.06	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	11	0.15	0.03	0.14
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	11	0.13	0.01	0.13
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	11	0.13	0.02	0.13
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	11	0.12	0.0	0.12
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	10	1.92	0.57	2.14
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	10	1.92	0.57	2.14
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	10	1.92	0.57	2.14
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	10	0.41	0.25	0.39
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	10	0.32	0.05	0.33
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	10	0.32	0.05	0.33
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	10	0.28	0.09	0.32
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	10	0.24	0.07	0.26
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	10	0.24	0.07	0.26
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	10	0.24	0.06	0.25
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	10	0.22	0.1	0.18
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	10	0.19	0.04	0.2
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	10	0.18	0.04	0.17
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	10	0.17	0.05	0.15
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	10	0.17	0.05	0.15
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	10	0.17	0.05	0.15
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	10	0.17	0.05	0.15
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	10	0.17	0.05	0.15
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	10	0.17	0.05	0.15
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	10	0.16	0.04	0.16
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	10	0.16	0.04	0.16
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	10	0.16	0.04	0.16
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	10	0.15	0.03	0.16
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	10	0.15	0.03	0.16
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	10	0.15	0.03	0.16
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	10	0.15	0.03	0.14
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	10	0.15	0.02	0.15
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	10	0.14	0.02	0.15
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	10	0.14	0.02	0.15
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	10	0.14	0.02	0.15
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	10	0.14	0.03	0.13
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	10	0.12	0.01	0.12
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	10	0.11	0.01	0.11
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	9	0.58	0.09	0.62
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	9	0.58	0.09	0.62
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	9	0.58	0.09	0.62
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	9	0.34	0.09	0.35
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	9	0.34	0.09	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	9	0.34	0.09	0.35
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	9	0.31	0.1	0.33
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	9	0.29	0.08	0.33
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	9	0.29	0.08	0.33
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	9	0.23	0.07	0.21
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	9	0.23	0.07	0.21
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	9	0.23	0.07	0.21
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	9	0.23	0.06	0.24
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	9	0.23	0.06	0.24
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	9	0.21	0.04	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	9	0.2	0.04	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	9	0.2	0.04	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	9	0.2	0.04	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	9	0.2	0.04	0.21
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	9	0.17	0.04	0.17
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	9	0.16	0.03	0.16
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	9	0.16	0.03	0.16
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	9	0.15	0.02	0.14
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	9	0.15	0.03	0.15
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	9	0.14	0.02	0.14
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	9	0.13	0.02	0.13
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	9	0.12	0.01	0.12
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	9	0.12	0.01	0.12
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	8	0.33	0.07	0.34
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	8	0.33	0.07	0.34
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	8	0.33	0.07	0.34
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	8	0.32	0.07	0.34
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	8	0.29	0.08	0.3
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	8	0.29	0.08	0.3
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	8	0.25	0.09	0.23
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	8	0.25	0.09	0.23
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	8	0.23	0.05	0.23
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	8	0.23	0.05	0.23
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	8	0.22	0.12	0.14
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	8	0.22	0.12	0.14
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	8	0.22	0.03	0.22
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	8	0.16	0.03	0.16
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	8	0.16	0.03	0.16
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	8	0.14	0.04	0.13
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	8	0.14	0.03	0.14
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	8	0.14	0.02	0.14
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	8	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	8	0.13	0.03	0.12
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	8	0.12	0.02	0.11
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	8	0.11	0.01	0.11
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	8	0.11	0.01	0.11
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	7	0.88	0.8	0.25
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	7	0.6	0.34	0.4
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	7	0.6	0.34	0.4
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	7	0.6	0.34	0.4
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	7	0.38	0.04	0.38
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	7	0.38	0.04	0.38
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	7	0.28	0.06	0.3
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	7	0.28	0.06	0.3
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	7	0.27	0.06	0.3
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	7	0.27	0.06	0.3
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	7	0.25	0.09	0.27
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	7	0.25	0.09	0.27
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	7	0.23	0.07	0.24
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	7	0.23	0.07	0.24
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	7	0.22	0.11	0.17
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	7	0.22	0.11	0.17
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	7	0.2	0.05	0.19
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	7	0.2	0.05	0.19
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	7	0.2	0.05	0.19
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	7	0.2	0.03	0.19
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	7	0.16	0.02	0.17
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	7	0.15	0.05	0.12
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	7	0.15	0.05	0.12
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	7	0.15	0.05	0.12
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	7	0.14	0.03	0.13
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	7	0.14	0.02	0.14
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	7	0.14	0.02	0.15
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	7	0.14	0.03	0.14
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	7	0.14	0.03	0.14
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	7	0.14	0.03	0.14
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	7	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	7	0.13	0.03	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	7	0.13	0.03	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	7	0.13	0.03	0.12
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	7	0.13	0.02	0.12
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	7	0.13	0.02	0.12
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	7	0.12	0.01	0.12
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	7	0.12	0.02	0.12
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	7	0.12	0.01	0.11
(1,18)	2:5:B:ALA:H	1:17:A:ILE:H	6	0.84	1.53	0.16
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE2	6	0.81	0.69	0.5
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE3	6	0.81	0.69	0.5
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE2	6	0.81	0.69	0.5
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE3	6	0.81	0.69	0.5
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD11	6	0.3	0.03	0.3
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD12	6	0.3	0.03	0.3
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD13	6	0.3	0.03	0.3
(1,700)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	6	0.3	0.02	0.29
(1,1967)	1:90:A:LYS:HE2	1:90:A:LYS:HA	6	0.28	0.02	0.29
(1,1967)	1:90:A:LYS:HE3	1:90:A:LYS:HA	6	0.28	0.02	0.29
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE2	6	0.27	0.03	0.29
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE3	6	0.27	0.03	0.29
(1,1630)	1:50:A:LYS:HA	1:50:A:LYS:HG2	6	0.19	0.11	0.16
(1,1413)	1:38:A:LYS:HE2	1:38:A:LYS:HB2	6	0.17	0.03	0.16
(1,1413)	1:38:A:LYS:HE3	1:38:A:LYS:HB2	6	0.17	0.03	0.16
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE2	6	0.16	0.03	0.16
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE3	6	0.16	0.03	0.16
(1,1623)	1:49:A:CYS:HB2	1:57:A:CYS:HB3	6	0.16	0.04	0.15
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD21	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD22	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD23	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD21	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD22	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD23	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD21	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD22	6	0.16	0.03	0.16
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD23	6	0.16	0.03	0.16
(1,972)	1:3:A:GLN:HB3	1:8:A:SER:HA	6	0.14	0.02	0.14
(1,741)	1:73:A:HIS:HB3	1:73:A:HIS:H	6	0.13	0.02	0.12
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB1	6	0.13	0.02	0.14
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB2	6	0.13	0.02	0.14
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB3	6	0.13	0.02	0.14
(1,227)	1:22:A:HIS:HB3	1:22:A:HIS:H	6	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,286)	1:26:A:CYS:HB3	1:26:A:CYS:H	6	0.12	0.01	0.12
(1,429)	1:37:A:GLN:HG3	1:37:A:GLN:H	6	0.12	0.01	0.12
(1,847)	2:11:B:LEU:HD21	2:11:B:LEU:H	5	0.43	0.07	0.43
(1,847)	2:11:B:LEU:HD22	2:11:B:LEU:H	5	0.43	0.07	0.43
(1,847)	2:11:B:LEU:HD23	2:11:B:LEU:H	5	0.43	0.07	0.43
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD11	5	0.3	0.08	0.31
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD12	5	0.3	0.08	0.31
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD13	5	0.3	0.08	0.31
(1,1938)	1:81:A:VAL:HG11	1:84:A:CYS:HB3	5	0.3	0.09	0.31
(1,1938)	1:81:A:VAL:HG12	1:84:A:CYS:HB3	5	0.3	0.09	0.31
(1,1938)	1:81:A:VAL:HG13	1:84:A:CYS:HB3	5	0.3	0.09	0.31
(1,1969)	1:90:A:LYS:HE2	1:90:A:LYS:HB2	5	0.23	0.01	0.22
(1,1969)	1:90:A:LYS:HE3	1:90:A:LYS:HB2	5	0.23	0.01	0.22
(1,1953)	1:85:A:LEU:HD11	1:85:A:LEU:HB3	5	0.21	0.08	0.21
(1,1953)	1:85:A:LEU:HD12	1:85:A:LEU:HB3	5	0.21	0.08	0.21
(1,1953)	1:85:A:LEU:HD13	1:85:A:LEU:HB3	5	0.21	0.08	0.21
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE2	5	0.21	0.03	0.23
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE3	5	0.21	0.03	0.23
(1,628)	1:55:A:GLY:H	1:57:A:CYS:H	5	0.2	0.05	0.18
(1,122)	1:13:A:ILE:HG12	1:14:A:GLN:H	5	0.19	0.02	0.2
(1,701)	1:62:A:GLN:HG2	1:62:A:GLN:HE21	5	0.19	0.04	0.19
(1,701)	1:62:A:GLN:HG3	1:62:A:GLN:HE21	5	0.19	0.04	0.19
(1,1855)	1:69:A:TYR:HB3	1:72:A:LYS:HB2	5	0.17	0.06	0.18
(1,578)	1:51:A:ARG:HB2	1:55:A:GLY:H	5	0.16	0.08	0.13
(1,578)	1:51:A:ARG:HB3	1:55:A:GLY:H	5	0.16	0.08	0.13
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	5	0.14	0.04	0.14
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	5	0.14	0.04	0.14
(1,125)	1:13:A:ILE:HB	1:14:A:GLN:H	5	0.14	0.01	0.14
(1,761)	1:77:A:ASN:HB3	1:77:A:ASN:H	5	0.13	0.01	0.13
(1,242)	1:23:A:ALA:HB1	1:24:A:ALA:H	5	0.13	0.02	0.14
(1,242)	1:23:A:ALA:HB2	1:24:A:ALA:H	5	0.13	0.02	0.14
(1,242)	1:23:A:ALA:HB3	1:24:A:ALA:H	5	0.13	0.02	0.14
(2,54)	1:44:A:GLN:O	1:48:A:GLY:N	5	0.13	0.02	0.14
(1,1150)	1:19:A:SER:HA	1:22:A:HIS:HB3	5	0.12	0.01	0.13
(1,1173)	1:20:A:LEU:HA	1:39:A:MET:HB3	5	0.12	0.01	0.12
(1,1312)	1:30:A:ASN:HA	1:31:A:CYS:HB3	5	0.12	0.01	0.12
(2,36)	1:35:A:SER:O	1:39:A:MET:N	5	0.12	0.01	0.11
(1,704)	1:62:A:GLN:H	1:63:A:LEU:H	5	0.11	0.01	0.11
(1,483)	1:41:A:ARG:HB2	1:41:A:ARG:H	5	0.11	0.0	0.11
(1,557)	1:49:A:CYS:H	1:50:A:LYS:HE2	4	2.08	1.13	2.6
(1,637)	1:57:A:CYS:H	1:60:A:CYS:HB2	4	1.4	0.63	1.76
(1,658)	1:59:A:ILE:H	1:60:A:CYS:HA	4	0.64	0.52	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB2	4	0.45	0.22	0.42
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB3	4	0.45	0.22	0.42
(1,1072)	1:13:A:ILE:HG21	1:17:A:ILE:HG13	4	0.42	0.1	0.47
(1,1072)	1:13:A:ILE:HG22	1:17:A:ILE:HG13	4	0.42	0.1	0.47
(1,1072)	1:13:A:ILE:HG23	1:17:A:ILE:HG13	4	0.42	0.1	0.47
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD11	4	0.34	0.18	0.32
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD12	4	0.34	0.18	0.32
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD13	4	0.34	0.18	0.32
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD11	4	0.34	0.18	0.32
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD12	4	0.34	0.18	0.32
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD13	4	0.34	0.18	0.32
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE2	4	0.33	0.07	0.36
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE3	4	0.33	0.07	0.36
(1,65)	1:6:A:GLY:H	1:7:A:ASP:H	4	0.31	0.03	0.32
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE1	4	0.28	0.15	0.22
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE2	4	0.28	0.15	0.22
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE1	4	0.28	0.15	0.22
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE2	4	0.28	0.15	0.22
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE1	4	0.28	0.15	0.22
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE2	4	0.28	0.15	0.22
(1,1464)	1:40:A:LYS:HG2	1:40:A:LYS:HE3	4	0.27	0.01	0.28
(1,1464)	1:40:A:LYS:HG3	1:40:A:LYS:HE3	4	0.27	0.01	0.28
(1,64)	1:5:A:PRO:HA	1:9:A:ARG:H	4	0.26	0.14	0.22
(1,787)	1:87:A:ILE:HG12	1:87:A:ILE:H	4	0.23	0.03	0.23
(1,787)	1:87:A:ILE:HG13	1:87:A:ILE:H	4	0.23	0.03	0.23
(1,89)	1:10:A:ARG:HG2	1:10:A:ARG:H	4	0.23	0.03	0.23
(1,89)	1:10:A:ARG:HG3	1:10:A:ARG:H	4	0.23	0.03	0.23
(1,699)	1:62:A:GLN:HB2	1:62:A:GLN:HE21	4	0.22	0.02	0.22
(1,851)	2:11:B:LEU:HD11	2:12:B:SER:H	4	0.22	0.05	0.22
(1,851)	2:11:B:LEU:HD12	2:12:B:SER:H	4	0.22	0.05	0.22
(1,851)	2:11:B:LEU:HD13	2:12:B:SER:H	4	0.22	0.05	0.22
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD11	4	0.18	0.05	0.18
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD12	4	0.18	0.05	0.18
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD13	4	0.18	0.05	0.18
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD11	4	0.18	0.05	0.18
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD12	4	0.18	0.05	0.18
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD13	4	0.18	0.05	0.18
(1,571)	1:51:A:ARG:HG2	1:51:A:ARG:H	4	0.18	0.07	0.16
(1,571)	1:51:A:ARG:HG3	1:51:A:ARG:H	4	0.18	0.07	0.16
(1,570)	1:51:A:ARG:HB2	1:51:A:ARG:H	4	0.18	0.03	0.18
(1,570)	1:51:A:ARG:HB3	1:51:A:ARG:H	4	0.18	0.03	0.18
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG21	4	0.17	0.05	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG22	4	0.17	0.05	0.16
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG23	4	0.17	0.05	0.16
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD2	4	0.17	0.06	0.16
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD3	4	0.17	0.06	0.16
(1,12)	1:62:A:GLN:HE22	2:11:B:LEU:HG	4	0.17	0.06	0.16
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD11	4	0.16	0.03	0.16
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD12	4	0.16	0.03	0.16
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD13	4	0.16	0.03	0.16
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD11	4	0.16	0.03	0.16
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD12	4	0.16	0.03	0.16
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD13	4	0.16	0.03	0.16
(1,1681)	1:52:A:LYS:HD3	1:60:A:CYS:HB2	4	0.15	0.05	0.15
(1,767)	1:78:A:LYS:HB3	1:78:A:LYS:H	4	0.14	0.03	0.12
(1,1968)	1:90:A:LYS:HE2	1:90:A:LYS:HB3	4	0.13	0.05	0.11
(1,1968)	1:90:A:LYS:HE3	1:90:A:LYS:HB3	4	0.13	0.05	0.11
(1,1988)	2:17:B:GLU:HA	2:18:B:GLN:HA	4	0.13	0.01	0.13
(1,1632)	1:50:A:LYS:HA	1:50:A:LYS:HG3	4	0.13	0.01	0.12
(1,744)	1:74:A:CYS:HB3	1:74:A:CYS:H	4	0.12	0.03	0.12
(1,845)	2:11:B:LEU:HG	2:11:B:LEU:H	4	0.12	0.02	0.12
(1,441)	1:38:A:LYS:HB3	1:38:A:LYS:H	4	0.12	0.01	0.12
(1,1298)	1:27:A:ARG:HA	1:28:A:ASN:HB3	4	0.11	0.01	0.11
(1,821)	2:8:B:ASP:HA	2:9:B:LEU:H	4	0.11	0.01	0.11
(1,1091)	1:15:A:ARG:HA	1:16:A:ALA:HA	4	0.11	0.0	0.11
(1,146)	1:15:A:ARG:HB2	1:15:A:ARG:H	4	0.1	0.0	0.1
(1,1426)	1:38:A:LYS:HA	1:41:A:ARG:HB2	4	0.1	0.0	0.1
(1,228)	1:22:A:HIS:HB2	1:22:A:HIS:H	4	0.1	0.0	0.1
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD2	3	2.65	0.57	2.91
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD3	3	2.65	0.57	2.91
(1,556)	1:49:A:CYS:H	1:50:A:LYS:HE3	3	2.41	0.39	2.2
(1,1645)	1:50:A:LYS:HD2	1:52:A:LYS:HG3	3	2.37	1.02	3.07
(1,1645)	1:50:A:LYS:HD3	1:52:A:LYS:HG3	3	2.37	1.02	3.07
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG21	3	1.13	0.23	1.23
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG22	3	1.13	0.23	1.23
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG23	3	1.13	0.23	1.23
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG21	3	0.92	0.16	0.92
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG22	3	0.92	0.16	0.92
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG23	3	0.92	0.16	0.92
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD11	3	0.37	0.11	0.44
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD12	3	0.37	0.11	0.44
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD13	3	0.37	0.11	0.44
(1,776)	1:85:A:LEU:HD21	1:85:A:LEU:H	3	0.37	0.06	0.35
(1,776)	1:85:A:LEU:HD22	1:85:A:LEU:H	3	0.37	0.06	0.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,776)	1:85:A:LEU:HD23	1:85:A:LEU:H	3	0.37	0.06	0.35
(1,1584)	1:46:A:THR:HG21	1:60:A:CYS:HB3	3	0.36	0.04	0.36
(1,1584)	1:46:A:THR:HG22	1:60:A:CYS:HB3	3	0.36	0.04	0.36
(1,1584)	1:46:A:THR:HG23	1:60:A:CYS:HB3	3	0.36	0.04	0.36
(1,1607)	1:47:A:LYS:HD2	1:82:A:PRO:HB3	3	0.33	0.02	0.32
(1,1607)	1:47:A:LYS:HD3	1:82:A:PRO:HB3	3	0.33	0.02	0.32
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE1	3	0.31	0.02	0.31
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE2	3	0.31	0.02	0.31
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG2	3	0.3	0.11	0.33
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG3	3	0.3	0.11	0.33
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD11	3	0.25	0.15	0.19
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD12	3	0.25	0.15	0.19
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD13	3	0.25	0.15	0.19
(1,1041)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	3	0.23	0.02	0.23
(1,1041)	1:11:A:LEU:HD12	1:11:A:LEU:HB2	3	0.23	0.02	0.23
(1,1041)	1:11:A:LEU:HD13	1:11:A:LEU:HB2	3	0.23	0.02	0.23
(1,133)	1:14:A:GLN:HG2	1:14:A:GLN:H	3	0.23	0.09	0.29
(1,133)	1:14:A:GLN:HG3	1:14:A:GLN:H	3	0.23	0.09	0.29
(1,567)	1:50:A:LYS:H	1:51:A:ARG:H	3	0.22	0.0	0.22
(1,629)	1:56:A:GLY:H	1:57:A:CYS:H	3	0.21	0.02	0.22
(1,554)	1:49:A:CYS:HA	1:50:A:LYS:H	3	0.2	0.03	0.18
(1,673)	1:60:A:CYS:HB2	1:61:A:LYS:H	3	0.2	0.09	0.14
(1,79)	1:8:A:SER:HB2	1:8:A:SER:H	3	0.19	0.06	0.17
(1,79)	1:8:A:SER:HB3	1:8:A:SER:H	3	0.19	0.06	0.17
(1,679)	1:61:A:LYS:HB2	1:61:A:LYS:H	3	0.18	0.1	0.11
(1,577)	1:51:A:ARG:HA	1:54:A:ASN:HD21	3	0.17	0.05	0.18
(1,622)	1:54:A:ASN:HA	1:56:A:GLY:H	3	0.16	0.02	0.17
(1,664)	1:59:A:ILE:HA	1:62:A:GLN:HE22	3	0.16	0.03	0.15
(1,1048)	1:11:A:LEU:HA	1:14:A:GLN:HB2	3	0.16	0.02	0.16
(1,562)	1:50:A:LYS:HB2	1:50:A:LYS:H	3	0.16	0.03	0.15
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD2	3	0.15	0.02	0.16
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD3	3	0.15	0.02	0.16
(1,1679)	1:52:A:LYS:HA	1:60:A:CYS:HB2	3	0.15	0.03	0.17
(1,602)	1:53:A:THR:H	1:54:A:ASN:H	3	0.15	0.01	0.15
(1,224)	1:21:A:VAL:HG11	1:25:A:GLN:HE21	3	0.14	0.02	0.16
(1,224)	1:21:A:VAL:HG12	1:25:A:GLN:HE21	3	0.14	0.02	0.16
(1,224)	1:21:A:VAL:HG13	1:25:A:GLN:HE21	3	0.14	0.02	0.16
(1,1780)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	3	0.14	0.02	0.14
(1,1780)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	3	0.14	0.02	0.14
(1,1780)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	3	0.14	0.02	0.14
(1,838)	2:10:B:MET:HG2	2:10:B:MET:H	3	0.14	0.03	0.13
(1,1062)	1:13:A:ILE:HA	1:13:A:ILE:HG13	3	0.13	0.03	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1321)	1:31:A:CYS:HB3	1:37:A:GLN:HG3	3	0.13	0.0	0.13
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD1	3	0.13	0.01	0.13
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD2	3	0.13	0.01	0.13
(1,285)	1:25:A:GLN:H	1:27:A:ARG:H	3	0.12	0.01	0.12
(1,364)	1:32:A:SER:HB3	1:32:A:SER:H	3	0.12	0.0	0.12
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD1	3	0.12	0.02	0.11
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD2	3	0.12	0.02	0.11
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD1	3	0.12	0.02	0.11
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD2	3	0.12	0.02	0.11
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD1	3	0.12	0.02	0.11
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD2	3	0.12	0.02	0.11
(1,51)	1:3:A:GLN:HA	1:7:A:ASP:H	3	0.12	0.01	0.11
(1,962)	1:2:A:THR:HB	1:3:A:GLN:HA	3	0.12	0.02	0.1
(1,1684)	1:52:A:LYS:HG2	1:60:A:CYS:HB3	3	0.12	0.01	0.11
(1,1430)	1:38:A:LYS:HB3	1:41:A:ARG:HB2	3	0.11	0.01	0.11
(1,1471)	1:40:A:LYS:HA	1:42:A:VAL:HB	3	0.11	0.01	0.11
(1,546)	1:48:A:GLY:H	1:49:A:CYS:H	3	0.11	0.0	0.11
(2,52)	1:43:A:VAL:O	1:47:A:LYS:N	3	0.11	0.01	0.12
(1,239)	1:23:A:ALA:HB1	1:23:A:ALA:H	3	0.11	0.0	0.11
(1,239)	1:23:A:ALA:HB2	1:23:A:ALA:H	3	0.11	0.0	0.11
(1,239)	1:23:A:ALA:HB3	1:23:A:ALA:H	3	0.11	0.0	0.11
(1,590)	1:52:A:LYS:HA	1:53:A:THR:H	3	0.11	0.0	0.11
(1,566)	1:50:A:LYS:HG3	1:50:A:LYS:H	2	0.73	0.02	0.73
(1,57)	1:4:A:SER:H	1:7:A:ASP:HB2	2	0.52	0.1	0.52
(1,57)	1:4:A:SER:H	1:7:A:ASP:HB3	2	0.52	0.1	0.52
(1,1353)	1:33:A:LEU:HD11	1:36:A:CYS:HB2	2	0.52	0.02	0.52
(1,1353)	1:33:A:LEU:HD12	1:36:A:CYS:HB2	2	0.52	0.02	0.52
(1,1353)	1:33:A:LEU:HD13	1:36:A:CYS:HB2	2	0.52	0.02	0.52
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG21	2	0.49	0.26	0.49
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG22	2	0.49	0.26	0.49
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG23	2	0.49	0.26	0.49
(1,750)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	2	0.4	0.07	0.4
(1,750)	1:75:A:GLN:HB3	1:75:A:GLN:HE21	2	0.4	0.07	0.4
(1,1332)	1:33:A:LEU:HD11	1:33:A:LEU:HB2	2	0.4	0.01	0.4
(1,1332)	1:33:A:LEU:HD12	1:33:A:LEU:HB2	2	0.4	0.01	0.4
(1,1332)	1:33:A:LEU:HD13	1:33:A:LEU:HB2	2	0.4	0.01	0.4
(1,647)	1:59:A:ILE:HB	1:59:A:ILE:H	2	0.3	0.03	0.3
(1,1335)	1:33:A:LEU:HD21	1:33:A:LEU:HB3	2	0.3	0.01	0.3
(1,1335)	1:33:A:LEU:HD22	1:33:A:LEU:HB3	2	0.3	0.01	0.3
(1,1335)	1:33:A:LEU:HD23	1:33:A:LEU:HB3	2	0.3	0.01	0.3
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD11	2	0.28	0.15	0.28
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD12	2	0.28	0.15	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD13	2	0.28	0.15	0.28
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD11	2	0.27	0.07	0.27
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD12	2	0.27	0.07	0.27
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD13	2	0.27	0.07	0.27
(1,1915)	1:78:A:LYS:HE2	1:78:A:LYS:HB3	2	0.26	0.03	0.26
(1,1915)	1:78:A:LYS:HE3	1:78:A:LYS:HB3	2	0.26	0.03	0.26
(1,1350)	1:33:A:LEU:HB2	1:36:A:CYS:HB2	2	0.24	0.0	0.24
(1,1352)	1:33:A:LEU:HD11	1:36:A:CYS:HB3	2	0.22	0.01	0.22
(1,1352)	1:33:A:LEU:HD12	1:36:A:CYS:HB3	2	0.22	0.01	0.22
(1,1352)	1:33:A:LEU:HD13	1:36:A:CYS:HB3	2	0.22	0.01	0.22
(1,381)	1:33:A:LEU:HD11	1:33:A:LEU:H	2	0.22	0.02	0.22
(1,381)	1:33:A:LEU:HD12	1:33:A:LEU:H	2	0.22	0.02	0.22
(1,381)	1:33:A:LEU:HD13	1:33:A:LEU:H	2	0.22	0.02	0.22
(1,736)	1:72:A:LYS:HG2	1:72:A:LYS:H	2	0.22	0.08	0.22
(1,736)	1:72:A:LYS:HG3	1:72:A:LYS:H	2	0.22	0.08	0.22
(1,119)	1:13:A:ILE:HG12	1:13:A:ILE:H	2	0.2	0.03	0.2
(1,942)	2:22:B:GLU:HA	2:23:B:ASP:H	2	0.2	0.09	0.2
(1,1629)	1:50:A:LYS:HA	1:50:A:LYS:HE2	2	0.2	0.04	0.2
(1,1629)	1:50:A:LYS:HA	1:50:A:LYS:HE3	2	0.2	0.04	0.2
(1,665)	1:59:A:ILE:HA	1:63:A:LEU:H	2	0.19	0.02	0.19
(1,1550)	1:44:A:GLN:HA	1:47:A:LYS:HG2	2	0.18	0.01	0.18
(1,1550)	1:44:A:GLN:HA	1:47:A:LYS:HG3	2	0.18	0.01	0.18
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD11	2	0.18	0.01	0.18
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD12	2	0.18	0.01	0.18
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD13	2	0.18	0.01	0.18
(1,340)	1:29:A:ALA:HB1	1:30:A:ASN:HD21	2	0.18	0.06	0.18
(1,340)	1:29:A:ALA:HB2	1:30:A:ASN:HD21	2	0.18	0.06	0.18
(1,340)	1:29:A:ALA:HB3	1:30:A:ASN:HD21	2	0.18	0.06	0.18
(1,812)	2:6:B:MET:HG2	2:6:B:MET:H	2	0.18	0.0	0.18
(1,812)	2:6:B:MET:HG3	2:6:B:MET:H	2	0.18	0.0	0.18
(1,711)	1:63:A:LEU:H	1:64:A:ILE:H	2	0.17	0.0	0.17
(1,388)	1:33:A:LEU:HB3	1:35:A:SER:H	2	0.16	0.01	0.16
(1,414)	1:36:A:CYS:HB2	1:36:A:CYS:H	2	0.16	0.0	0.16
(1,681)	1:61:A:LYS:H	1:62:A:GLN:H	2	0.16	0.01	0.16
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB1	2	0.16	0.05	0.16
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB2	2	0.16	0.05	0.16
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB3	2	0.16	0.05	0.16
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB1	2	0.16	0.05	0.16
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB2	2	0.16	0.05	0.16
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB3	2	0.16	0.05	0.16
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB1	2	0.16	0.05	0.16
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB2	2	0.16	0.05	0.16

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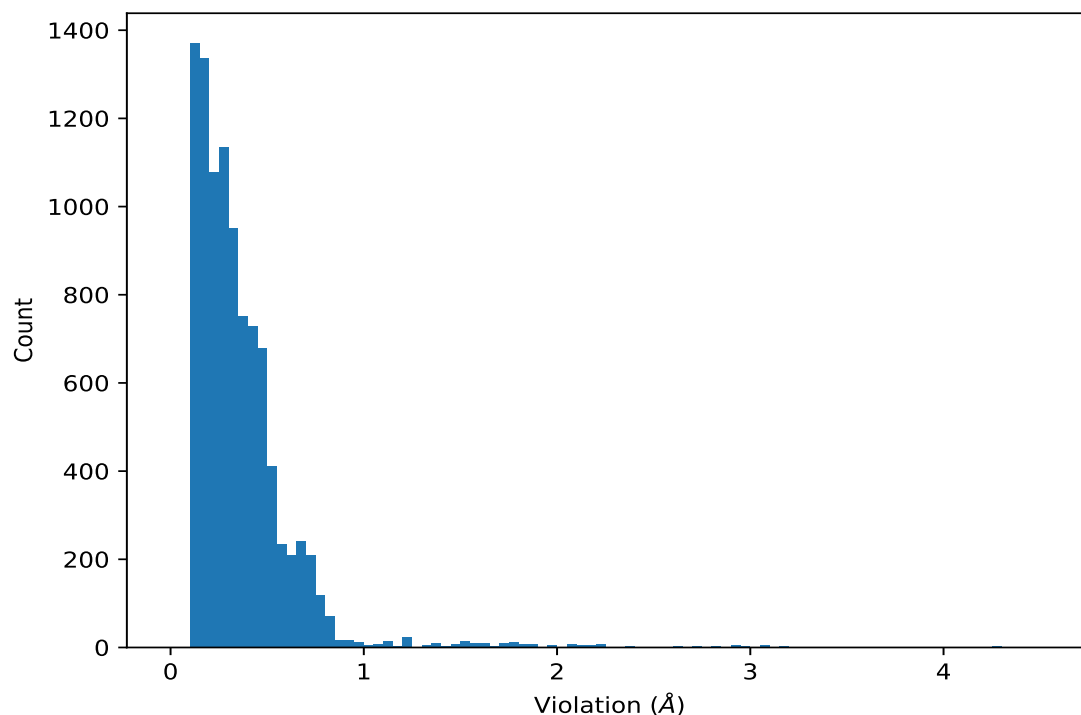
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB3	2	0.16	0.05	0.16
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD11	2	0.15	0.05	0.15
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD12	2	0.15	0.05	0.15
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD13	2	0.15	0.05	0.15
(1,16)	1:69:A:TYR:HA	2:10:B:MET:HB2	2	0.15	0.03	0.15
(1,1378)	1:34:A:PRO:HA	1:38:A:LYS:HG2	2	0.15	0.02	0.15
(1,742)	1:73:A:HIS:HB2	1:73:A:HIS:H	2	0.14	0.01	0.14
(1,1852)	1:69:A:TYR:HA	1:72:A:LYS:HA	2	0.14	0.03	0.14
(1,375)	1:32:A:SER:H	1:36:A:CYS:HB3	2	0.14	0.02	0.14
(1,565)	1:50:A:LYS:HG2	1:50:A:LYS:H	2	0.14	0.02	0.14
(1,1295)	1:27:A:ARG:HB2	1:27:A:ARG:HD2	2	0.14	0.02	0.14
(1,1295)	1:27:A:ARG:HB2	1:27:A:ARG:HD3	2	0.14	0.02	0.14
(1,726)	1:68:A:ALA:HB1	1:68:A:ALA:H	2	0.13	0.03	0.13
(1,726)	1:68:A:ALA:HB2	1:68:A:ALA:H	2	0.13	0.03	0.13
(1,726)	1:68:A:ALA:HB3	1:68:A:ALA:H	2	0.13	0.03	0.13
(1,1658)	1:51:A:ARG:HD2	1:55:A:GLY:HA2	2	0.13	0.02	0.13
(1,1658)	1:51:A:ARG:HD2	1:55:A:GLY:HA3	2	0.13	0.02	0.13
(1,1658)	1:51:A:ARG:HD3	1:55:A:GLY:HA2	2	0.13	0.02	0.13
(1,1658)	1:51:A:ARG:HD3	1:55:A:GLY:HA3	2	0.13	0.02	0.13
(1,1913)	1:78:A:LYS:HA	1:78:A:LYS:HG2	2	0.13	0.02	0.13
(1,117)	1:13:A:ILE:HB	1:13:A:ILE:H	2	0.12	0.02	0.12
(1,377)	1:33:A:LEU:HB2	1:33:A:LEU:H	2	0.12	0.01	0.12
(1,393)	1:33:A:LEU:HB2	1:36:A:CYS:H	2	0.12	0.02	0.12
(1,1249)	1:23:A:ALA:HA	1:40:A:LYS:HE3	2	0.12	0.01	0.12
(1,1369)	1:34:A:PRO:HA	1:37:A:GLN:HG2	2	0.12	0.02	0.12
(1,759)	1:76:A:GLU:HB3	1:76:A:GLU:H	2	0.12	0.0	0.12
(1,1916)	1:78:A:LYS:HB2	1:78:A:LYS:HD2	2	0.12	0.0	0.12
(1,1916)	1:78:A:LYS:HB2	1:78:A:LYS:HD3	2	0.12	0.0	0.12
(1,945)	2:22:B:GLU:HB2	2:23:B:ASP:H	2	0.11	0.01	0.11
(1,1110)	1:17:A:ILE:HB	1:18:A:GLN:HB2	2	0.11	0.01	0.11
(1,1377)	1:34:A:PRO:HA	1:38:A:LYS:HG3	2	0.11	0.01	0.11
(1,165)	1:17:A:ILE:HG12	1:17:A:ILE:H	2	0.11	0.0	0.11
(1,257)	1:24:A:ALA:H	1:25:A:GLN:HG2	2	0.11	0.0	0.11
(2,10)	1:9:A:ARG:O	1:13:A:ILE:N	2	0.11	0.0	0.11
(2,61)	1:59:A:ILE:O	1:63:A:LEU:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	4	4.51
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	9	4.35
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	12	4.28
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	11	4.27
(1,18)	2:5:B:ALA:H	1:17:A:ILE:H	2	4.25
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	11	4.13
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	4	4.09
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	15	4.06
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	8	3.82
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	11	3.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	11	3.59
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	1	3.49
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	6	3.46
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	13	3.37
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	5	3.35
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	12	3.34
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	5	3.32
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	10	3.24
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD2	11	3.18
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD3	11	3.18
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	9	3.17
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	4	3.16
(1,1645)	1:50:A:LYS:HD2	1:52:A:LYS:HG3	11	3.12
(1,1645)	1:50:A:LYS:HD3	1:52:A:LYS:HG3	11	3.12
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	13	3.09
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	8	3.09
(1,1645)	1:50:A:LYS:HD2	1:52:A:LYS:HG3	15	3.07
(1,1645)	1:50:A:LYS:HD3	1:52:A:LYS:HG3	15	3.07
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	6	3.06
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	8	3.01
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	15	2.97
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	1	2.96
(1,557)	1:49:A:CYS:H	1:50:A:LYS:HE2	11	2.96
(1,556)	1:49:A:CYS:H	1:50:A:LYS:HE3	9	2.96
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	3	2.94
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	2	2.93
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	7	2.91
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD2	15	2.91
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD3	15	2.91
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	7	2.9
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	2	2.89
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	8	2.85
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	12	2.84
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	2	2.82
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	9	2.8
(1,557)	1:49:A:CYS:H	1:50:A:LYS:HE2	15	2.8
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	1	2.78
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	3	2.77
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	5	2.73
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	10	2.71
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	10	2.7
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	10	2.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	6	2.64
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	6	2.64
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	6	2.64
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	15	2.58
(1,992)	1:5:A:PRO:HA	1:8:A:SER:HA	14	2.53
(1,557)	1:49:A:CYS:H	1:50:A:LYS:HE2	9	2.41
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	4	2.35
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	4	2.35
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	4	2.35
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	13	2.35
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	9	2.26
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	13	2.23
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	13	2.23
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	13	2.23
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	14	2.21
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	14	2.21
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	14	2.21
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	13	2.2
(1,556)	1:49:A:CYS:H	1:50:A:LYS:HE3	11	2.2
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	14	2.19
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	15	2.19
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	6	2.19
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	6	2.19
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	6	2.19
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	7	2.15
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	3	2.14
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	3	2.14
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	3	2.14
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	11	2.14
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	11	2.14
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	11	2.14
(1,556)	1:49:A:CYS:H	1:50:A:LYS:HE3	15	2.08
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	15	2.05
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	15	2.05
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	15	2.05
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	1	2.05
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	1	2.05
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	1	2.05
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	10	1.99
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	10	1.99
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	10	1.99
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	3	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	3	1.95
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	3	1.95
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	4	1.88
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	4	1.88
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	4	1.88
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	5	1.86
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	5	1.86
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	5	1.86
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD2	9	1.85
(1,1597)	1:47:A:LYS:HA	1:50:A:LYS:HD3	9	1.85
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	7	1.83
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	7	1.83
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	7	1.83
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE2	11	1.82
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE3	11	1.82
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE2	11	1.82
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE3	11	1.82
(1,637)	1:57:A:CYS:H	1:60:A:CYS:HB2	10	1.79
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	9	1.79
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	9	1.79
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	9	1.79
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	13	1.79
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	13	1.79
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	13	1.79
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	7	1.78
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	7	1.78
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	7	1.78
(1,637)	1:57:A:CYS:H	1:60:A:CYS:HB2	14	1.76
(1,637)	1:57:A:CYS:H	1:60:A:CYS:HB2	5	1.75
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	8	1.71
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	8	1.71
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	8	1.71
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE2	15	1.7
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE3	15	1.7
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE2	15	1.7
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE3	15	1.7
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	15	1.7
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	15	1.7
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	15	1.7
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	3	1.69
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	15	1.67
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	11	1.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	14	1.64
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	2	1.64
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	2	1.64
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	2	1.64
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	14	1.61
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	14	1.61
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	14	1.61
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	11	1.6
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	11	1.6
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	11	1.6
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	5	1.59
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	5	1.59
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	5	1.59
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	7	1.57
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	10	1.55
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	13	1.55
(1,3)	1:39:A:MET:HE1	2:19:B:TRP:HZ2	12	1.55
(1,3)	1:39:A:MET:HE2	2:19:B:TRP:HZ2	12	1.55
(1,3)	1:39:A:MET:HE3	2:19:B:TRP:HZ2	12	1.55
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	13	1.54
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	14	1.54
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	11	1.54
(1,973)	1:3:A:GLN:HG2	1:11:A:LEU:HD11	6	1.53
(1,973)	1:3:A:GLN:HG2	1:11:A:LEU:HD12	6	1.53
(1,973)	1:3:A:GLN:HG2	1:11:A:LEU:HD13	6	1.53
(1,973)	1:3:A:GLN:HG3	1:11:A:LEU:HD11	6	1.53
(1,973)	1:3:A:GLN:HG3	1:11:A:LEU:HD12	6	1.53
(1,973)	1:3:A:GLN:HG3	1:11:A:LEU:HD13	6	1.53
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	14	1.52
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	14	1.52
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	14	1.52
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	15	1.51
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	7	1.5
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	13	1.5
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	12	1.47
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	5	1.47
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	7	1.46
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	7	1.46
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	7	1.46
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	8	1.46
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	9	1.46
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	13	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	11	1.41
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	4	1.41
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	1	1.38
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	1	1.38
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	1	1.38
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	15	1.37
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG21	1	1.36
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG22	1	1.36
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG23	1	1.36
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	9	1.36
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	2	1.35
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	1	1.34
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	13	1.33
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	8	1.3
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	8	1.3
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	8	1.3
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	3	1.28
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	6	1.24
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	6	1.24
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	6	1.24
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	2	1.24
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	2	1.24
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	2	1.24
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	12	1.24
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG21	15	1.23
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG22	15	1.23
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG23	15	1.23
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	6	1.23
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	13	1.21
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	13	1.21
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	13	1.21
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	3	1.2
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	3	1.2
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	3	1.2
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	4	1.2
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	4	1.2
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	4	1.2
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	12	1.2
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	12	1.2
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	12	1.2
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	11	1.2
(1,658)	1:59:A:ILE:H	1:60:A:CYS:HA	9	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	15	1.17
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	7	1.16
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	12	1.16
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	13	1.14
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	6	1.14
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	6	1.14
(1,658)	1:59:A:ILE:H	1:60:A:CYS:HA	7	1.13
(1,42)	2:21:B:THR:H	1:39:A:MET:HB3	11	1.13
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	11	1.12
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	13	1.12
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	9	1.12
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	9	1.12
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	9	1.12
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	11	1.11
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG21	1	1.11
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG22	1	1.11
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG23	1	1.11
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	7	1.09
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	13	1.09
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	9	1.08
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	8	1.07
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	12	1.06
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	10	1.06
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	3	1.05
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	12	1.05
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	15	1.04
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	12	1.03
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	5	1.03
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	3	1.01
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	4	1.0
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	2	0.99
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	9	0.98
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	9	0.98
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	9	0.98
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	12	0.98
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	12	0.98
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	12	0.98
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	8	0.97
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	1	0.97
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	1	0.97
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	3	0.96
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	3	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	3	0.96
(1,1645)	1:50:A:LYS:HD2	1:52:A:LYS:HG3	9	0.93
(1,1645)	1:50:A:LYS:HD3	1:52:A:LYS:HG3	9	0.93
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	7	0.93
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	7	0.93
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	7	0.93
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	10	0.93
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	10	0.93
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	10	0.93
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG21	15	0.92
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG22	15	0.92
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG23	15	0.92
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	10	0.91
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	10	0.91
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	10	0.91
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	11	0.9
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	11	0.9
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	11	0.9
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	2	0.89
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	2	0.89
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	2	0.89
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	5	0.89
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	2	0.88
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	2	0.88
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	2	0.88
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	5	0.86
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	5	0.86
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	5	0.86
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	15	0.86
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	15	0.86
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	15	0.86
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD21	8	0.85
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD22	8	0.85
(1,1942)	1:82:A:PRO:HD3	1:85:A:LEU:HD23	8	0.85
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	11	0.84
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	8	0.84
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	8	0.84
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	8	0.84
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	15	0.84
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	15	0.84
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	15	0.84
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	10	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	10	0.83
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	10	0.83
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	11	0.82
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	11	0.82
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	11	0.82
(1,809)	2:5:B:ALA:H	2:7:B:ASP:HB2	5	0.82
(1,809)	2:5:B:ALA:H	2:7:B:ASP:HB3	5	0.82
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	7	0.82
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	7	0.82
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	7	0.82
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG21	14	0.81
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG22	14	0.81
(1,1715)	1:58:A:PRO:HD2	1:59:A:ILE:HG23	14	0.81
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	14	0.81
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	14	0.81
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	14	0.81
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	14	0.81
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	14	0.81
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	14	0.81
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	14	0.81
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	14	0.81
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	14	0.81
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	1	0.81
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	1	0.81
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	1	0.81
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	14	0.81
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	14	0.81
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	14	0.81
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	15	0.81
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	15	0.81
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	15	0.81
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	5	0.8
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	5	0.8
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	5	0.8
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	5	0.8
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	5	0.8
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	5	0.8
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	6	0.8
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	6	0.8
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	6	0.8
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	6	0.8
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	6	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	6	0.8
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	10	0.8
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	10	0.8
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	10	0.8
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	10	0.8
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	10	0.8
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	10	0.8
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	5	0.8
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	5	0.8
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	5	0.8
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	7	0.8
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	7	0.8
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	7	0.8
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	8	0.8
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	8	0.8
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	8	0.8
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	9	0.8
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	9	0.8
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	9	0.8
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	10	0.8
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	10	0.8
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	10	0.8
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	14	0.79
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	14	0.79
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	14	0.79
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	14	0.79
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	14	0.79
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	14	0.79
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	9	0.79
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	9	0.79
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	9	0.79
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	9	0.79
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	9	0.79
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	9	0.79
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	9	0.79
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	9	0.79
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	9	0.79
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	2	0.79
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	2	0.79
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	2	0.79
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	3	0.79
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	3	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	3	0.79
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	4	0.79
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	4	0.79
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	4	0.79
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	12	0.79
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	12	0.79
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	12	0.79
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	7	0.79
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	14	0.79
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	14	0.79
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	14	0.79
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	7	0.78
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	7	0.78
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	7	0.78
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	7	0.78
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	7	0.78
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	7	0.78
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	7	0.78
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	7	0.78
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	7	0.78
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	9	0.78
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	9	0.78
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	9	0.78
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	9	0.78
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	9	0.78
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	9	0.78
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	9	0.78
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	9	0.78
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	9	0.78
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	13	0.78
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	13	0.78
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	13	0.78
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	8	0.78
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	8	0.78
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	8	0.78
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	9	0.77
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	9	0.77
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	9	0.77
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	13	0.77
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	13	0.77
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	13	0.77
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	4	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	4	0.77
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	4	0.77
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	3	0.76
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	3	0.76
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	3	0.76
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	3	0.76
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	3	0.76
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	3	0.76
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	3	0.76
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	3	0.76
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	3	0.76
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	8	0.76
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	8	0.76
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	8	0.76
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	8	0.76
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	8	0.76
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	8	0.76
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	8	0.76
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	8	0.76
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	8	0.76
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	15	0.76
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	15	0.76
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	15	0.76
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	15	0.76
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	15	0.76
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	15	0.76
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	15	0.76
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	15	0.76
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	15	0.76
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	3	0.76
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	3	0.76
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	3	0.76
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	3	0.76
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	3	0.76
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	3	0.76
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	3	0.76
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	3	0.76
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	3	0.76
(1,1245)	1:23:A:ALA:HB1	1:39:A:MET:HB2	6	0.76
(1,1245)	1:23:A:ALA:HB2	1:39:A:MET:HB2	6	0.76
(1,1245)	1:23:A:ALA:HB3	1:39:A:MET:HB2	6	0.76
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	5	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	5	0.76
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	5	0.76
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	11	0.76
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	11	0.76
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	11	0.76
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG21	9	0.75
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG22	9	0.75
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG23	9	0.75
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	7	0.75
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	7	0.75
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	7	0.75
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	2	0.75
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	4	0.75
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	4	0.75
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	4	0.75
(1,566)	1:50:A:LYS:HG3	1:50:A:LYS:H	15	0.75
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	4	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	4	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	4	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	4	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	4	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	4	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	4	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	4	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	4	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	5	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	5	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	5	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	5	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	5	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	5	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	5	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	5	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	5	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	6	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	6	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	6	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	6	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	6	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	6	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	6	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	6	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	6	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	14	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	14	0.74
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	14	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	14	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	14	0.74
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	14	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	14	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	14	0.74
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	14	0.74
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	11	0.74
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	11	0.74
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	11	0.74
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	11	0.74
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	11	0.74
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	11	0.74
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	11	0.74
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	11	0.74
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	11	0.74
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB2	1	0.74
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB3	1	0.74
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	15	0.74
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	15	0.74
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	15	0.74
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	3	0.74
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	3	0.74
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	3	0.74
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	1	0.73
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	1	0.73
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	1	0.73
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	1	0.73
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	1	0.73
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	1	0.73
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	5	0.73
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	8	0.73
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	7	0.72
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	7	0.72
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	7	0.72
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	7	0.72
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	7	0.72
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	7	0.72
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG21	14	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG22	14	0.72
(1,1716)	1:58:A:PRO:HG2	1:59:A:ILE:HG23	14	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	1	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	1	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	1	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	1	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	1	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	1	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	1	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	1	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	1	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	4	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	4	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	4	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	4	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	4	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	4	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	4	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	4	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	4	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	10	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	10	0.72
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	10	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	10	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	10	0.72
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	10	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	10	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	10	0.72
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	10	0.72
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	2	0.72
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	2	0.72
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	2	0.72
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	1	0.72
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	1	0.72
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	1	0.72
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	9	0.71
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	9	0.71
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	9	0.71
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	9	0.71
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	9	0.71
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	9	0.71
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	9	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	8	0.71
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	8	0.71
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	8	0.71
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	8	0.71
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	8	0.71
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	8	0.71
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	3	0.71
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	3	0.71
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	3	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	2	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	2	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	2	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	2	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	2	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	2	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	2	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	2	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	2	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	6	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	6	0.71
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	6	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	6	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	6	0.71
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	6	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	6	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	6	0.71
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	6	0.71
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	3	0.71
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	3	0.71
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	3	0.71
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	1	0.71
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	1	0.71
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	1	0.71
(1,566)	1:50:A:LYS:HG3	1:50:A:LYS:H	11	0.71
(1,1828)	1:66:A:LEU:HD11	1:68:A:ALA:HA	11	0.7
(1,1828)	1:66:A:LEU:HD12	1:68:A:ALA:HA	11	0.7
(1,1828)	1:66:A:LEU:HD13	1:68:A:ALA:HA	11	0.7
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	14	0.7
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	14	0.7
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	14	0.7
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	14	0.7
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	14	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	14	0.7
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	11	0.7
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	11	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	11	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	11	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	11	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	11	0.7
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	13	0.7
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	13	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	13	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	13	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	13	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	13	0.7
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	15	0.7
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	15	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	15	0.7
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	15	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	15	0.7
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	15	0.7
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	1	0.7
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	1	0.7
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	1	0.7
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	1	0.7
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	1	0.7
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	1	0.7
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	1	0.7
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	1	0.7
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	1	0.7
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	10	0.7
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	10	0.7
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	10	0.7
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	10	0.7
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	10	0.7
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	10	0.7
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	10	0.7
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	10	0.7
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	10	0.7
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	7	0.7
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	7	0.7
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	7	0.7
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	7	0.7
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	7	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	7	0.7
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	7	0.7
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	7	0.7
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	7	0.7
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	12	0.7
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	12	0.7
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	12	0.7
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	12	0.7
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	12	0.7
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	12	0.7
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	12	0.7
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	12	0.7
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	12	0.7
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	15	0.7
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	15	0.7
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	15	0.7
(1,1634)	1:50:A:LYS:HE2	1:50:A:LYS:HB3	9	0.69
(1,1634)	1:50:A:LYS:HE3	1:50:A:LYS:HB3	9	0.69
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	3	0.69
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	3	0.69
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	3	0.69
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	3	0.69
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	3	0.69
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	3	0.69
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	12	0.69
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	12	0.69
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	12	0.69
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	12	0.69
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	12	0.69
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	12	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	5	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	5	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	5	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	5	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	5	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	5	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	5	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	5	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	5	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	8	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	8	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	8	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	8	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	8	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	8	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	8	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	8	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	8	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	13	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	13	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	13	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	13	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	13	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	13	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	13	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	13	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	13	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	15	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	15	0.69
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	15	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	15	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	15	0.69
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	15	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	15	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	15	0.69
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	15	0.69
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	5	0.69
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	5	0.69
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	5	0.69
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	4	0.69
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	3	0.69
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	10	0.69
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	5	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	5	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	5	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	5	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	5	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	5	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	10	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	10	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	10	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	10	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	10	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	10	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	13	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	13	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	13	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	13	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	13	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	13	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	15	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	15	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	15	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	15	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	15	0.68
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	15	0.68
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	2	0.68
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	2	0.68
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	2	0.68
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	2	0.68
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	2	0.68
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	2	0.68
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	4	0.68
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	4	0.68
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	4	0.68
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	4	0.68
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	4	0.68
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	4	0.68
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	7	0.68
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	7	0.68
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	7	0.68
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	7	0.68
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	7	0.68
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	7	0.68
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	12	0.68
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	12	0.68
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	12	0.68
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	12	0.68
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	12	0.68
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	12	0.68
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	12	0.68
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	12	0.68
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	12	0.68
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	13	0.68
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	13	0.68
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	13	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	13	0.68
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	13	0.68
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	13	0.68
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	13	0.68
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	13	0.68
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	13	0.68
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	2	0.68
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	13	0.68
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	7	0.68
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	6	0.68
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	6	0.68
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	6	0.68
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	2	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	2	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	2	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	2	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	2	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	2	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	8	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	8	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	8	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	8	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	8	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	8	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	11	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	11	0.67
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	11	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	11	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	11	0.67
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	11	0.67
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE2	9	0.67
(1,1572)	1:46:A:THR:HG21	1:52:A:LYS:HE3	9	0.67
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE2	9	0.67
(1,1572)	1:46:A:THR:HG22	1:52:A:LYS:HE3	9	0.67
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE2	9	0.67
(1,1572)	1:46:A:THR:HG23	1:52:A:LYS:HE3	9	0.67
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	4	0.67
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	4	0.67
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	4	0.67
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	15	0.67
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	3	0.67
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	8	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	15	0.66
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	9	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	3	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	3	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	3	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	3	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	3	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	3	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	4	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	4	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	4	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	4	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	4	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	4	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	6	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	6	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	6	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	6	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	6	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	6	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	12	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	12	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	12	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	12	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	12	0.66
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	12	0.66
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	13	0.66
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	13	0.66
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	13	0.66
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	13	0.66
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	13	0.66
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	13	0.66
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	13	0.66
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	13	0.66
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	13	0.66
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	2	0.66
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	2	0.66
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	2	0.66
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	2	0.66
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	2	0.66
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	2	0.66
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	2	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	2	0.66
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	2	0.66
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	4	0.66
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	4	0.66
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	4	0.66
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	4	0.66
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	4	0.66
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	4	0.66
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	4	0.66
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	4	0.66
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	4	0.66
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD21	1	0.65
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD22	1	0.65
(1,1778)	1:63:A:LEU:HB2	1:63:A:LEU:HD23	1	0.65
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD21	1	0.65
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD22	1	0.65
(1,1778)	1:63:A:LEU:HB3	1:63:A:LEU:HD23	1	0.65
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG21	14	0.65
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG22	14	0.65
(1,1269)	1:24:A:ALA:HB1	1:81:A:VAL:HG23	14	0.65
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG21	14	0.65
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG22	14	0.65
(1,1269)	1:24:A:ALA:HB2	1:81:A:VAL:HG23	14	0.65
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG21	14	0.65
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG22	14	0.65
(1,1269)	1:24:A:ALA:HB3	1:81:A:VAL:HG23	14	0.65
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	11	0.65
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	11	0.65
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	11	0.65
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	11	0.65
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	11	0.65
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	11	0.65
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	11	0.65
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	11	0.65
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	11	0.65
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	1	0.65
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	1	0.65
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	1	0.65
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	15	0.65
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	4	0.65
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	4	0.65
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	8	0.65
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	8	0.65
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	14	0.65
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	14	0.65
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	14	0.65
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	7	0.64
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	7	0.64
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	7	0.64
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	7	0.64
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	7	0.64
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	7	0.64
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	7	0.64
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	7	0.64
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	7	0.64
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	15	0.64
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	15	0.64
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	15	0.64
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	15	0.64
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	15	0.64
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	15	0.64
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	15	0.64
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	15	0.64
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	15	0.64
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	1	0.64
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	1	0.64
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	1	0.64
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	9	0.64
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	9	0.64
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	9	0.64
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	15	0.64
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	2	0.64
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	2	0.64
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	2	0.64
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	11	0.64
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	11	0.64
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	11	0.64
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	15	0.64
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	15	0.64
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	15	0.64
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	14	0.63
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	14	0.63
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	14	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	14	0.63
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	14	0.63
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	14	0.63
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	14	0.63
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	14	0.63
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	14	0.63
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	6	0.63
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	6	0.63
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	6	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	3	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	3	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	3	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	3	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	3	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	3	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	3	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	3	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	3	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	4	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	4	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	4	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	4	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	4	0.63
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	4	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	4	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	4	0.63
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	4	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	2	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	2	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	2	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	4	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	4	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	4	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	5	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	5	0.63
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	5	0.63
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	1	0.63
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	1	0.63
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	1	0.63
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	1	0.63
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	1	0.63
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	1	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	1	0.63
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	1	0.63
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	1	0.63
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	12	0.63
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	4	0.63
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	5	0.63
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	13	0.63
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	13	0.63
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	13	0.63
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	8	0.62
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	8	0.62
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	8	0.62
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	8	0.62
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	8	0.62
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	8	0.62
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	8	0.62
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	8	0.62
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	8	0.62
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	14	0.62
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	14	0.62
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	14	0.62
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	14	0.62
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	14	0.62
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	14	0.62
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	14	0.62
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	14	0.62
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	14	0.62
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	7	0.62
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	7	0.62
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	7	0.62
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	8	0.62
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	8	0.62
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	8	0.62
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	13	0.62
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	13	0.62
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	13	0.62
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	13	0.62
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	13	0.62
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	13	0.62
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	13	0.62
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	13	0.62
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	13	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	15	0.62
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	15	0.62
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	12	0.62
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	12	0.62
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	12	0.62
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	2	0.61
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	2	0.61
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	2	0.61
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	2	0.61
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	2	0.61
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	2	0.61
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	2	0.61
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	2	0.61
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	2	0.61
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	10	0.61
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	10	0.61
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	10	0.61
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	1	0.61
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	1	0.61
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	1	0.61
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	1	0.61
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	1	0.61
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	1	0.61
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	1	0.61
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	1	0.61
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	1	0.61
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	6	0.61
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	6	0.61
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	6	0.61
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	6	0.61
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	6	0.61
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	6	0.61
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	6	0.61
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	6	0.61
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	6	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	3	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	3	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	3	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	13	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	13	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	13	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	14	0.61
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	14	0.61
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	3	0.61
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	3	0.61
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	3	0.61
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	3	0.61
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	3	0.61
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	3	0.61
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	3	0.61
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	3	0.61
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	3	0.61
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	3	0.61
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	5	0.61
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	5	0.61
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	8	0.61
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	8	0.61
(1,57)	1:4:A:SER:H	1:7:A:ASP:HB2	14	0.61
(1,57)	1:4:A:SER:H	1:7:A:ASP:HB3	14	0.61
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	3	0.6
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	3	0.6
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	3	0.6
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	3	0.6
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	3	0.6
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	3	0.6
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	3	0.6
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	3	0.6
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	3	0.6
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	12	0.6
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	12	0.6
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	12	0.6
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	12	0.6
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	12	0.6
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	12	0.6
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	12	0.6
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	12	0.6
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	12	0.6
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	11	0.6
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	11	0.6
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	11	0.6
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	4	0.6
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	2	0.6
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	5	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	5	0.6
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	5	0.6
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	3	0.6
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	3	0.6
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	3	0.6
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	11	0.59
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	6	0.59
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	6	0.59
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	6	0.59
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	6	0.59
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	6	0.59
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	6	0.59
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	6	0.59
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	6	0.59
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	6	0.59
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	5	0.59
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	5	0.59
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	5	0.59
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	9	0.59
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	9	0.59
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	9	0.59
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	9	0.59
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	9	0.59
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	9	0.59
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	9	0.59
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	9	0.59
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	9	0.59
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	12	0.59
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	12	0.59
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	12	0.59
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	15	0.59
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	15	0.59
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	15	0.59
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD11	1	0.59
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD12	1	0.59
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD13	1	0.59
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD11	1	0.59
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD12	1	0.59
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD13	1	0.59
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	10	0.59
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	10	0.59
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	10	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	5	0.59
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	5	0.59
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	5	0.59
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	13	0.59
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	13	0.59
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	13	0.59
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	15	0.58
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	4	0.58
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	4	0.58
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	4	0.58
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	4	0.58
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	4	0.58
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	4	0.58
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	4	0.58
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	4	0.58
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	4	0.58
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	8	0.58
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	8	0.58
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	8	0.58
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	8	0.58
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	8	0.58
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	8	0.58
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	8	0.58
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	8	0.58
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	8	0.58
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	9	0.58
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	9	0.58
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	9	0.58
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	9	0.58
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	9	0.58
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	9	0.58
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	9	0.58
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	9	0.58
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	9	0.58
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	1	0.58
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	1	0.58
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	1	0.58
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	10	0.58
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	10	0.58
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	10	0.58
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	10	0.58
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	10	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	10	0.58
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	10	0.58
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	10	0.58
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	10	0.58
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	9	0.58
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	9	0.58
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	9	0.58
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	9	0.58
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	9	0.58
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	9	0.58
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	9	0.58
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	9	0.58
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	9	0.58
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	7	0.58
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	8	0.58
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	10	0.58
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	15	0.58
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	2	0.58
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	2	0.58
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB2	11	0.58
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB3	11	0.58
(1,775)	1:85:A:LEU:HD11	1:85:A:LEU:H	2	0.58
(1,775)	1:85:A:LEU:HD12	1:85:A:LEU:H	2	0.58
(1,775)	1:85:A:LEU:HD13	1:85:A:LEU:H	2	0.58
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	4	0.58
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	4	0.58
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	4	0.58
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	9	0.58
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	9	0.58
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	1	0.58
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	1	0.58
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	1	0.58
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG11	5	0.57
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG12	5	0.57
(1,1201)	1:20:A:LEU:HD21	1:81:A:VAL:HG13	5	0.57
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG11	5	0.57
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG12	5	0.57
(1,1201)	1:20:A:LEU:HD22	1:81:A:VAL:HG13	5	0.57
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG11	5	0.57
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG12	5	0.57
(1,1201)	1:20:A:LEU:HD23	1:81:A:VAL:HG13	5	0.57
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	6	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	6	0.57
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	6	0.57
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB1	10	0.57
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB2	10	0.57
(1,1169)	1:20:A:LEU:HA	1:23:A:ALA:HB3	10	0.57
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	9	0.57
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	9	0.57
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	9	0.57
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	10	0.57
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	10	0.57
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	10	0.57
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	2	0.57
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	3	0.57
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	4	0.57
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	5	0.57
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	6	0.57
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	6	0.57
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	6	0.57
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	9	0.57
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	9	0.57
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	9	0.57
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	6	0.57
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	6	0.57
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	6	0.57
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	3	0.56
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	3	0.56
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	3	0.56
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	3	0.56
(1,1514)	1:42:A:VAL:HG21	1:59:A:ILE:HG21	9	0.56
(1,1514)	1:42:A:VAL:HG21	1:59:A:ILE:HG22	9	0.56
(1,1514)	1:42:A:VAL:HG21	1:59:A:ILE:HG23	9	0.56
(1,1514)	1:42:A:VAL:HG22	1:59:A:ILE:HG21	9	0.56
(1,1514)	1:42:A:VAL:HG22	1:59:A:ILE:HG22	9	0.56
(1,1514)	1:42:A:VAL:HG22	1:59:A:ILE:HG23	9	0.56
(1,1514)	1:42:A:VAL:HG23	1:59:A:ILE:HG21	9	0.56
(1,1514)	1:42:A:VAL:HG23	1:59:A:ILE:HG22	9	0.56
(1,1514)	1:42:A:VAL:HG23	1:59:A:ILE:HG23	9	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	2	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	2	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	2	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	2	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	2	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	2	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	2	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	2	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	2	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	11	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	11	0.56
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	11	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	11	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	11	0.56
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	11	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	11	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	11	0.56
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	11	0.56
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	5	0.56
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	5	0.56
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	5	0.56
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	8	0.56
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	8	0.56
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	8	0.56
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	13	0.56
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	13	0.56
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	3	0.56
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	3	0.56
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	15	0.56
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	15	0.56
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD21	14	0.56
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD22	14	0.56
(1,28)	2:16:B:ILE:H	1:20:A:LEU:HD23	14	0.56
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE2	12	0.55
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE3	12	0.55
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE2	12	0.55
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE3	12	0.55
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	11	0.55
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	11	0.55
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	11	0.55
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	11	0.55
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	15	0.55
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	15	0.55
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	15	0.55
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	15	0.55
(1,1510)	1:42:A:VAL:HG11	1:59:A:ILE:HA	14	0.55
(1,1510)	1:42:A:VAL:HG12	1:59:A:ILE:HA	14	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1510)	1:42:A:VAL:HG13	1:59:A:ILE:HA	14	0.55
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	3	0.55
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	3	0.55
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	3	0.55
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	14	0.55
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	14	0.55
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	14	0.55
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	14	0.55
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	14	0.55
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	14	0.55
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	14	0.55
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	14	0.55
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	14	0.55
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	14	0.55
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	14	0.55
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	14	0.55
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	11	0.55
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	11	0.55
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	7	0.55
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	7	0.55
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	7	0.55
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	13	0.55
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	13	0.55
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	13	0.55
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	7	0.55
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	7	0.55
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	11	0.55
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	11	0.55
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	12	0.55
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	12	0.55
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	7	0.54
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	7	0.54
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	7	0.54
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	15	0.54
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	15	0.54
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	15	0.54
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	15	0.54
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	15	0.54
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	15	0.54
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	11	0.54
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	11	0.54
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	11	0.54
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	11	0.54
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	11	0.54
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	11	0.54
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	11	0.54
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	11	0.54
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	12	0.54
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	12	0.54
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	12	0.54
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	13	0.54
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	13	0.54
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	13	0.54
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	12	0.54
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	12	0.54
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	12	0.54
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	14	0.54
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	14	0.54
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	14	0.54
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	12	0.54
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	12	0.54
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	12	0.54
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	3	0.53
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	3	0.53
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	3	0.53
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE1	6	0.53
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE2	6	0.53
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE1	6	0.53
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE2	6	0.53
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE1	6	0.53
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE2	6	0.53
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	13	0.53
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	13	0.53
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	13	0.53
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	13	0.53
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	7	0.53
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	7	0.53
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	7	0.53
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	7	0.53
(1,1353)	1:33:A:LEU:HD11	1:36:A:CYS:HB2	9	0.53
(1,1353)	1:33:A:LEU:HD12	1:36:A:CYS:HB2	9	0.53
(1,1353)	1:33:A:LEU:HD13	1:36:A:CYS:HB2	9	0.53
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	14	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	14	0.53
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	14	0.53
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	14	0.53
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	14	0.53
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	14	0.53
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	14	0.53
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	14	0.53
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	14	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	1	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	1	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	1	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	7	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	7	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	7	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	11	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	11	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	11	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	15	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	15	0.53
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	15	0.53
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	12	0.53
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	12	0.53
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	12	0.53
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	12	0.53
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	12	0.53
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	12	0.53
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	12	0.53
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	12	0.53
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	12	0.53
(1,847)	2:11:B:LEU:HD21	2:11:B:LEU:H	11	0.53
(1,847)	2:11:B:LEU:HD22	2:11:B:LEU:H	11	0.53
(1,847)	2:11:B:LEU:HD23	2:11:B:LEU:H	11	0.53
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	15	0.53
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	15	0.53
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	15	0.53
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	3	0.53
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	3	0.53
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	3	0.53
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	10	0.53
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	10	0.53
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	10	0.53
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	2	0.53
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	4	0.53
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	4	0.53
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	5	0.53
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	5	0.53
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	13	0.53
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	13	0.53
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	13	0.52
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	13	0.52
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	13	0.52
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	13	0.52
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	13	0.52
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	13	0.52
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	13	0.52
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	13	0.52
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	13	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	2	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	2	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	2	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	2	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	8	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	8	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	8	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	8	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	9	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	9	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	9	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	9	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	12	0.52
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	12	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	12	0.52
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	12	0.52
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	6	0.52
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	6	0.52
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	6	0.52
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	9	0.52
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	9	0.52
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	9	0.52
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	12	0.52
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	12	0.52
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	12	0.52
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	12	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	12	0.52
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	12	0.52
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	12	0.52
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	12	0.52
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	12	0.52
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	13	0.52
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	13	0.52
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	13	0.52
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	13	0.52
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	13	0.52
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	13	0.52
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	13	0.52
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	13	0.52
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	13	0.52
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	10	0.52
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	10	0.52
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	10	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	5	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	5	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	5	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	5	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	5	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	5	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	5	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	5	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	5	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	7	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	7	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	7	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	7	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	7	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	7	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	7	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	7	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	7	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	12	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	12	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	12	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	12	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	12	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	12	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	12	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	12	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	12	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	15	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	15	0.52
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	15	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	15	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	15	0.52
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	15	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	15	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	15	0.52
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	15	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	2	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	2	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	2	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	4	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	4	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	4	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	9	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	9	0.52
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	9	0.52
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	11	0.52
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	11	0.52
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	5	0.52
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	5	0.52
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	5	0.52
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	6	0.52
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	6	0.52
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	6	0.52
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	7	0.52
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	7	0.52
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	7	0.52
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	13	0.52
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	13	0.52
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	13	0.52
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	6	0.52
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	6	0.52
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	10	0.52
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	10	0.52
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	10	0.52
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	10	0.52
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	10	0.52
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	14	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	14	0.51
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	14	0.51
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	9	0.51
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	9	0.51
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	9	0.51
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	9	0.51
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	9	0.51
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	9	0.51
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	9	0.51
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	9	0.51
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	9	0.51
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	4	0.51
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	4	0.51
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	4	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	1	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	1	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	1	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	1	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	1	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	1	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	1	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	1	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	1	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	2	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	2	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	2	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	2	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	2	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	2	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	2	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	2	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	2	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	4	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	4	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	4	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	4	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	4	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	4	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	4	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	4	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	4	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	8	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	8	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	8	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	8	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	8	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	8	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	8	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	8	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	8	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	13	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	13	0.51
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	13	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	13	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	13	0.51
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	13	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	13	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	13	0.51
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	13	0.51
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	10	0.51
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	10	0.51
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	10	0.51
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	13	0.51
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	13	0.51
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	13	0.51
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	15	0.51
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	15	0.51
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	15	0.51
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	15	0.51
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	15	0.51
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	15	0.51
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	15	0.51
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	15	0.51
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	15	0.51
(1,1072)	1:13:A:ILE:HG21	1:17:A:ILE:HG13	11	0.51
(1,1072)	1:13:A:ILE:HG22	1:17:A:ILE:HG13	11	0.51
(1,1072)	1:13:A:ILE:HG23	1:17:A:ILE:HG13	11	0.51
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	2	0.51
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	2	0.51
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	2	0.51
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	2	0.51
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	2	0.51
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	2	0.51
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	2	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	2	0.51
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	2	0.51
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	1	0.51
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	1	0.51
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	1	0.51
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	11	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	5	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	5	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	5	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	6	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	6	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	6	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	8	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	8	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	8	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	10	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	10	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	10	0.5
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	2	0.5
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	2	0.5
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	2	0.5
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	6	0.5
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	6	0.5
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	6	0.5
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	6	0.5
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	14	0.5
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	14	0.5
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	14	0.5
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	14	0.5
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	1	0.5
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	1	0.5
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	1	0.5
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	8	0.5
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	8	0.5
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	8	0.5
(1,1353)	1:33:A:LEU:HD11	1:36:A:CYS:HB2	11	0.5
(1,1353)	1:33:A:LEU:HD12	1:36:A:CYS:HB2	11	0.5
(1,1353)	1:33:A:LEU:HD13	1:36:A:CYS:HB2	11	0.5
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	2	0.5
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	2	0.5
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	2	0.5
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	4	0.5
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	4	0.5
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	5	0.5
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	5	0.5
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	5	0.5
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	6	0.5
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	6	0.5
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	6	0.5
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	7	0.5
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	7	0.5
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	7	0.5
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	8	0.5
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	8	0.5
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	8	0.5
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	14	0.5
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	14	0.5
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	14	0.5
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	3	0.5
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	3	0.5
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	3	0.5
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	5	0.5
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	5	0.5
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	5	0.5
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	5	0.5
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	5	0.5
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	5	0.5
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	5	0.5
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	5	0.5
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	5	0.5
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	7	0.5
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	7	0.5
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	7	0.5
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	7	0.5
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	7	0.5
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	7	0.5
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	7	0.5
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	7	0.5
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	7	0.5
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	2	0.5
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	2	0.5
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	12	0.5
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	12	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	4	0.5
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	4	0.5
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	4	0.5
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	4	0.5
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	4	0.5
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	4	0.5
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	5	0.5
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	5	0.5
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	5	0.5
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	6	0.5
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	6	0.5
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	6	0.5
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	7	0.5
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	7	0.5
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	7	0.5
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	8	0.5
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	8	0.5
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	8	0.5
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	14	0.5
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	14	0.5
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	14	0.5
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	11	0.49
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	11	0.49
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	11	0.49
(1,1901)	1:76:A:GLU:HG2	1:78:A:LYS:HD2	14	0.49
(1,1901)	1:76:A:GLU:HG2	1:78:A:LYS:HD3	14	0.49
(1,1901)	1:76:A:GLU:HG3	1:78:A:LYS:HD2	14	0.49
(1,1901)	1:76:A:GLU:HG3	1:78:A:LYS:HD3	14	0.49
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	10	0.49
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	10	0.49
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	10	0.49
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	10	0.49
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	10	0.49
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	10	0.49
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	10	0.49
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	10	0.49
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	10	0.49
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	3	0.49
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	3	0.49
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	3	0.49
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	4	0.49
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	4	0.49
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	7	0.49
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	7	0.49
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	7	0.49
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	10	0.49
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	10	0.49
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	10	0.49
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	2	0.49
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	2	0.49
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	1	0.49
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	1	0.49
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	1	0.49
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	1	0.49
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	10	0.49
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	10	0.49
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	10	0.49
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	10	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	5	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	5	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	5	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	10	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	10	0.49
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	10	0.49
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	1	0.49
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	1	0.49
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	1	0.49
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	3	0.49
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	3	0.49
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	3	0.49
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	5	0.49
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	5	0.49
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	5	0.49
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	12	0.49
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	12	0.49
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	12	0.49
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	13	0.49
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	13	0.49
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	13	0.49
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	15	0.49
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	15	0.49
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	15	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	3	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	3	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	3	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	3	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	3	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	3	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	3	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	3	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	3	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	6	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	6	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	6	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	6	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	6	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	6	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	6	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	6	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	6	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	9	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	9	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	9	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	9	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	9	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	9	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	9	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	9	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	9	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	10	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	10	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	10	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	10	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	10	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	10	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	10	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	10	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	10	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE1	11	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE2	11	0.49
(1,1182)	1:20:A:LEU:HD11	1:39:A:MET:HE3	11	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE1	11	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE2	11	0.49
(1,1182)	1:20:A:LEU:HD12	1:39:A:MET:HE3	11	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE1	11	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE2	11	0.49
(1,1182)	1:20:A:LEU:HD13	1:39:A:MET:HE3	11	0.49
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	11	0.49
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	12	0.49
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	2	0.49
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	2	0.49
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	2	0.49
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	8	0.49
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	8	0.49
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	8	0.49
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	14	0.49
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	14	0.49
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	14	0.49
(1,397)	1:33:A:LEU:HD11	1:36:A:CYS:H	15	0.49
(1,397)	1:33:A:LEU:HD12	1:36:A:CYS:H	15	0.49
(1,397)	1:33:A:LEU:HD13	1:36:A:CYS:H	15	0.49
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	12	0.49
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	12	0.49
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	12	0.49
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	13	0.49
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	13	0.49
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	13	0.49
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	15	0.49
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	15	0.49
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	15	0.49
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	5	0.49
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	5	0.49
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	7	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	7	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	7	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	13	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	13	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	13	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	15	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	15	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	15	0.48
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	2	0.48
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	2	0.48
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	2	0.48
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	8	0.48
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	8	0.48
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	8	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	13	0.48
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	13	0.48
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	13	0.48
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	15	0.48
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	15	0.48
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	15	0.48
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	3	0.48
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	3	0.48
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	3	0.48
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	3	0.48
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	3	0.48
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	3	0.48
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	10	0.48
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	10	0.48
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	10	0.48
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	6	0.48
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	6	0.48
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	6	0.48
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	8	0.48
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	8	0.48
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	8	0.48
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	8	0.48
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	8	0.48
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	8	0.48
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	8	0.48
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	8	0.48
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	8	0.48
(1,1072)	1:13:A:ILE:HG21	1:17:A:ILE:HG13	7	0.48
(1,1072)	1:13:A:ILE:HG22	1:17:A:ILE:HG13	7	0.48
(1,1072)	1:13:A:ILE:HG23	1:17:A:ILE:HG13	7	0.48
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	15	0.48
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	15	0.48
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	15	0.48
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	11	0.48
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	13	0.48
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	12	0.48
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	12	0.48
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	8	0.48
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	8	0.48
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	2	0.48
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	2	0.48
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	2	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	2	0.48
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	2	0.48
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	2	0.48
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	5	0.48
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	5	0.48
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	5	0.48
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	11	0.48
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	11	0.48
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	11	0.48
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	1	0.48
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	1	0.48
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	6	0.48
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	6	0.48
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	6	0.48
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	7	0.48
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	7	0.48
(1,64)	1:5:A:PRO:HA	1:9:A:ARG:H	11	0.48
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	4	0.47
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	4	0.47
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	4	0.47
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	1	0.47
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	1	0.47
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	1	0.47
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	1	0.47
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	1	0.47
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	1	0.47
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	1	0.47
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	1	0.47
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	1	0.47
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	10	0.47
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	10	0.47
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	10	0.47
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	5	0.47
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	5	0.47
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	5	0.47
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	5	0.47
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	5	0.47
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	5	0.47
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	5	0.47
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	5	0.47
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	5	0.47
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	5	0.47
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	5	0.47
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	12	0.47
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	12	0.47
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	12	0.47
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	4	0.47
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	4	0.47
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	4	0.47
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	4	0.47
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	5	0.47
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	5	0.47
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	5	0.47
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	5	0.47
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	6	0.47
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	6	0.47
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	6	0.47
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	6	0.47
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	6	0.47
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	6	0.47
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	7	0.47
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	7	0.47
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	7	0.47
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	13	0.47
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	13	0.47
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	13	0.47
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	13	0.47
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	13	0.47
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	13	0.47
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	13	0.47
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	13	0.47
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	13	0.47
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	7	0.47
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	7	0.47
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	7	0.47
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	2	0.47
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	2	0.47
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	2	0.47
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	2	0.47
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	2	0.47
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	2	0.47
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	2	0.47
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	2	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	2	0.47
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	15	0.47
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	15	0.47
(1,847)	2:11:B:LEU:HD21	2:11:B:LEU:H	15	0.47
(1,847)	2:11:B:LEU:HD22	2:11:B:LEU:H	15	0.47
(1,847)	2:11:B:LEU:HD23	2:11:B:LEU:H	15	0.47
(1,750)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	9	0.47
(1,750)	1:75:A:GLN:HB3	1:75:A:GLN:HE21	9	0.47
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	10	0.47
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	10	0.47
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	10	0.47
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	12	0.47
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	12	0.47
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	12	0.47
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	12	0.47
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	12	0.47
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	12	0.47
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	12	0.47
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	3	0.47
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	9	0.46
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	9	0.46
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	9	0.46
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	9	0.46
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	9	0.46
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	9	0.46
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	9	0.46
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	9	0.46
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	9	0.46
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	9	0.46
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	9	0.46
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	9	0.46
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	4	0.46
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	4	0.46
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	4	0.46
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	11	0.46
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	11	0.46
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	11	0.46
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	12	0.46
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	12	0.46
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	12	0.46
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	14	0.46
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	14	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	14	0.46
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	15	0.46
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	15	0.46
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	15	0.46
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	6	0.46
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	6	0.46
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	6	0.46
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	8	0.46
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	8	0.46
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	8	0.46
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	8	0.46
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	8	0.46
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	8	0.46
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	8	0.46
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	8	0.46
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	8	0.46
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	1	0.46
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	1	0.46
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	1	0.46
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	9	0.46
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	9	0.46
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	9	0.46
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	11	0.46
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	11	0.46
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	11	0.46
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	13	0.46
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	13	0.46
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	13	0.46
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	14	0.46
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	14	0.46
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	14	0.46
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	1	0.46
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	1	0.46
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	1	0.46
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	1	0.46
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	1	0.46
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	1	0.46
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	1	0.46
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	1	0.46
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	1	0.46
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	3	0.46
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	3	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	3	0.46
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	4	0.46
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	4	0.46
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	4	0.46
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	9	0.46
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	9	0.46
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	9	0.46
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	11	0.46
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	11	0.46
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	11	0.46
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	12	0.46
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	12	0.46
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	12	0.46
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	5	0.46
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	5	0.46
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	5	0.46
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	5	0.46
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	5	0.46
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	5	0.46
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	5	0.46
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	5	0.46
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	5	0.46
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	14	0.46
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	14	0.46
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	14	0.46
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	14	0.46
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	14	0.46
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	14	0.46
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	14	0.46
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	14	0.46
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	14	0.46
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	3	0.46
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	3	0.46
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	3	0.46
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	12	0.46
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	12	0.46
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	12	0.46
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	7	0.46
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	7	0.46
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	7	0.46
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	8	0.46
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	8	0.46
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	9	0.46
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	9	0.46
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	9	0.46
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	11	0.46
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	11	0.46
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	11	0.46
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	12	0.46
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	12	0.46
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	12	0.46
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	13	0.46
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	13	0.46
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	13	0.46
(1,1072)	1:13:A:ILE:HG21	1:17:A:ILE:HG13	8	0.46
(1,1072)	1:13:A:ILE:HG22	1:17:A:ILE:HG13	8	0.46
(1,1072)	1:13:A:ILE:HG23	1:17:A:ILE:HG13	8	0.46
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	10	0.46
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	10	0.46
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	10	0.46
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	15	0.46
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	15	0.46
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	15	0.46
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	15	0.46
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	15	0.46
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	15	0.46
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	15	0.46
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	15	0.46
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	15	0.46
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	7	0.46
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	7	0.46
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	13	0.46
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	13	0.46
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	13	0.46
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	6	0.46
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	4	0.46
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	4	0.46
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	4	0.46
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	11	0.46
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	11	0.46
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	11	0.46
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	12	0.46
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	12	0.46
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	14	0.46
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	14	0.46
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	14	0.46
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	15	0.46
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	15	0.46
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	15	0.46
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	4	0.46
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	4	0.46
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	4	0.46
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	3	0.46
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	3	0.46
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	7	0.46
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	7	0.46
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	13	0.46
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	13	0.46
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	1	0.46
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	1	0.46
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	1	0.46
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	7	0.46
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	7	0.46
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	7	0.46
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	8	0.46
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	8	0.46
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	8	0.46
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	7	0.46
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	7	0.46
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	7	0.46
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	8	0.46
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	8	0.46
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	8	0.46
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	9	0.46
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	9	0.46
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	9	0.46
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	11	0.46
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	11	0.46
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	11	0.46
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	12	0.46
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	12	0.46
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	12	0.46
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	13	0.46
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	13	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	13	0.46
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	1	0.46
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	1	0.46
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	1	0.46
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	10	0.46
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	10	0.46
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	10	0.46
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	2	0.46
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	2	0.46
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	13	0.46
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	13	0.46
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD11	7	0.46
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD12	7	0.46
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD13	7	0.46
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	4	0.45
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	12	0.45
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	12	0.45
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	12	0.45
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	1	0.45
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	1	0.45
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	1	0.45
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	3	0.45
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	3	0.45
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	3	0.45
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	5	0.45
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	5	0.45
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	5	0.45
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	6	0.45
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	6	0.45
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	6	0.45
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	8	0.45
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	8	0.45
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	8	0.45
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	1	0.45
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	1	0.45
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	1	0.45
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	1	0.45
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	1	0.45
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	1	0.45
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	1	0.45
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	1	0.45
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	11	0.45
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	11	0.45
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	11	0.45
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	11	0.45
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	11	0.45
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	11	0.45
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	11	0.45
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	11	0.45
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	11	0.45
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	15	0.45
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	15	0.45
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	15	0.45
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	15	0.45
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	15	0.45
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	2	0.45
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	2	0.45
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	2	0.45
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	12	0.45
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	12	0.45
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	12	0.45
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	7	0.45
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	7	0.45
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	7	0.45
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	7	0.45
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	7	0.45
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	7	0.45
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	2	0.45
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	2	0.45
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	2	0.45
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	12	0.45
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	12	0.45
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	12	0.45
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	14	0.45
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	14	0.45
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	14	0.45
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	1	0.45
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	1	0.45
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	1	0.45
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	11	0.45
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	11	0.45
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	11	0.45
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	1	0.45
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	1	0.45
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	1	0.45
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	1	0.45
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	1	0.45
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	1	0.45
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	1	0.45
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	1	0.45
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	2	0.45
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	2	0.45
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	2	0.45
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	6	0.45
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	6	0.45
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	6	0.45
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	7	0.45
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	7	0.45
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	7	0.45
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	14	0.45
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	14	0.45
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	14	0.45
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	4	0.45
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	4	0.45
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	4	0.45
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	1	0.45
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	1	0.45
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	1	0.45
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	2	0.45
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	2	0.45
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	2	0.45
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	4	0.45
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	4	0.45
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	4	0.45
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	10	0.45
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	10	0.45
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	10	0.45
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	14	0.45
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	14	0.45
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	14	0.45
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	2	0.45
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	2	0.45
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	2	0.45
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD11	14	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD12	14	0.45
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD13	14	0.45
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	10	0.45
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	8	0.45
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	7	0.45
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	7	0.45
(1,776)	1:85:A:LEU:HD21	1:85:A:LEU:H	2	0.45
(1,776)	1:85:A:LEU:HD22	1:85:A:LEU:H	2	0.45
(1,776)	1:85:A:LEU:HD23	1:85:A:LEU:H	2	0.45
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	1	0.45
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	1	0.45
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	1	0.45
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	3	0.45
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	3	0.45
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	3	0.45
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	5	0.45
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	5	0.45
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	5	0.45
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	6	0.45
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	6	0.45
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	6	0.45
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	8	0.45
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	8	0.45
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	8	0.45
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	8	0.45
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	8	0.45
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	8	0.45
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	3	0.45
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	3	0.45
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	3	0.45
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	13	0.45
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	13	0.45
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	13	0.45
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	6	0.45
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	6	0.45
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	13	0.45
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	13	0.45
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	13	0.45
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	1	0.45
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	1	0.45
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	1	0.45
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	11	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	11	0.45
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	11	0.45
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	1	0.45
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	1	0.45
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	1	0.45
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	2	0.45
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	2	0.45
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	2	0.45
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	4	0.45
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	4	0.45
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	4	0.45
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	10	0.45
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	10	0.45
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	10	0.45
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	14	0.45
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	14	0.45
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	14	0.45
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	5	0.45
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	5	0.45
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	5	0.45
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	15	0.45
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	15	0.45
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	15	0.45
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	7	0.45
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	7	0.45
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	10	0.45
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	10	0.45
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	4	0.45
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	7	0.44
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	7	0.44
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	7	0.44
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	9	0.44
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	9	0.44
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	9	0.44
(1,1814)	1:65:A:ALA:HB1	1:65:A:ALA:H	13	0.44
(1,1814)	1:65:A:ALA:HB2	1:65:A:ALA:H	13	0.44
(1,1814)	1:65:A:ALA:HB3	1:65:A:ALA:H	13	0.44
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	2	0.44
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	2	0.44
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	2	0.44
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	2	0.44
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	2	0.44
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	2	0.44
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	2	0.44
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	2	0.44
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	3	0.44
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	3	0.44
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	3	0.44
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	3	0.44
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	3	0.44
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	3	0.44
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	3	0.44
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	3	0.44
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	3	0.44
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	4	0.44
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	4	0.44
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	4	0.44
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	4	0.44
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	4	0.44
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	4	0.44
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	4	0.44
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	4	0.44
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	4	0.44
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE2	13	0.44
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE3	13	0.44
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE2	13	0.44
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE3	13	0.44
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	12	0.44
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	10	0.44
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	10	0.44
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	10	0.44
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	10	0.44
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	10	0.44
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	10	0.44
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	10	0.44
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	10	0.44
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	10	0.44
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	10	0.44
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	10	0.44
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	10	0.44
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	11	0.44
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	11	0.44
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	11	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	14	0.44
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	14	0.44
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	14	0.44
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	15	0.44
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	15	0.44
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	15	0.44
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	3	0.44
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	3	0.44
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	3	0.44
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	9	0.44
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	9	0.44
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	9	0.44
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	3	0.44
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	3	0.44
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	3	0.44
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	3	0.44
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	3	0.44
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	3	0.44
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	3	0.44
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	3	0.44
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	3	0.44
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	7	0.44
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	7	0.44
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	7	0.44
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	7	0.44
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	7	0.44
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	7	0.44
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	7	0.44
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	7	0.44
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	7	0.44
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	1	0.44
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	1	0.44
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	1	0.44
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	10	0.44
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	10	0.44
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	10	0.44
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	3	0.44
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	3	0.44
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	3	0.44
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	5	0.44
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	5	0.44
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1095)	1:16:A:ALA:HB1	1:16:A:ALA:H	15	0.44
(1,1095)	1:16:A:ALA:HB2	1:16:A:ALA:H	15	0.44
(1,1095)	1:16:A:ALA:HB3	1:16:A:ALA:H	15	0.44
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	9	0.44
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	9	0.44
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	9	0.44
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD11	9	0.44
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD12	9	0.44
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD13	9	0.44
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	12	0.44
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	7	0.44
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	7	0.44
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	7	0.44
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	9	0.44
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	9	0.44
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	9	0.44
(1,721)	1:65:A:ALA:HB1	1:65:A:ALA:H	13	0.44
(1,721)	1:65:A:ALA:HB2	1:65:A:ALA:H	13	0.44
(1,721)	1:65:A:ALA:HB3	1:65:A:ALA:H	13	0.44
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	5	0.44
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	5	0.44
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	14	0.44
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	14	0.44
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	2	0.44
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	2	0.44
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	2	0.44
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	3	0.44
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	3	0.44
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	3	0.44
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	14	0.44
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	14	0.44
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	14	0.44
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	3	0.44
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	3	0.44
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	3	0.44
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	9	0.44
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	9	0.44
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	9	0.44
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	3	0.44
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	3	0.44
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	3	0.44
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	5	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	5	0.44
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	5	0.44
(1,158)	1:16:A:ALA:HB1	1:16:A:ALA:H	15	0.44
(1,158)	1:16:A:ALA:HB2	1:16:A:ALA:H	15	0.44
(1,158)	1:16:A:ALA:HB3	1:16:A:ALA:H	15	0.44
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	2	0.44
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	2	0.44
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	2	0.44
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	4	0.44
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	4	0.44
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	13	0.44
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	13	0.44
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	15	0.44
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	15	0.44
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	4	0.44
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	4	0.44
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	8	0.44
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	8	0.44
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	10	0.44
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	10	0.44
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	1	0.43
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	1	0.43
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	1	0.43
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	1	0.43
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	1	0.43
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	1	0.43
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	1	0.43
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	1	0.43
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	1	0.43
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	11	0.43
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	11	0.43
(1,1630)	1:50:A:LYS:HA	1:50:A:LYS:HG2	9	0.43
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	3	0.43
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	3	0.43
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	3	0.43
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD21	11	0.43
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD22	11	0.43
(1,1541)	1:43:A:VAL:HA	1:63:A:LEU:HD23	11	0.43
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	5	0.43
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	5	0.43
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	5	0.43
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	5	0.43
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	5	0.43
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	5	0.43
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	5	0.43
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	5	0.43
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	9	0.43
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	9	0.43
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	9	0.43
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	15	0.43
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	15	0.43
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	13	0.43
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	13	0.43
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	13	0.43
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	1	0.43
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	1	0.43
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	1	0.43
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	4	0.43
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	4	0.43
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	4	0.43
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	8	0.43
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	8	0.43
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	8	0.43
(1,1258)	1:24:A:ALA:HB1	1:24:A:ALA:H	2	0.43
(1,1258)	1:24:A:ALA:HB2	1:24:A:ALA:H	2	0.43
(1,1258)	1:24:A:ALA:HB3	1:24:A:ALA:H	2	0.43
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	1	0.43
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	1	0.43
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	1	0.43
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	11	0.43
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	11	0.43
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	11	0.43
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	3	0.43
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	3	0.43
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	3	0.43
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	6	0.43
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	6	0.43
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	6	0.43
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	4	0.43
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	4	0.43
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	4	0.43
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	4	0.43
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	4	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	4	0.43
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	9	0.43
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	9	0.43
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	9	0.43
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	13	0.43
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	13	0.43
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	13	0.43
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	15	0.43
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	15	0.43
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	15	0.43
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD11	6	0.43
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD12	6	0.43
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD13	6	0.43
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	7	0.43
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	7	0.43
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	7	0.43
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	7	0.43
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	7	0.43
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	7	0.43
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	7	0.43
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	7	0.43
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	7	0.43
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	11	0.43
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	11	0.43
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	11	0.43
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	11	0.43
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	11	0.43
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	11	0.43
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	11	0.43
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	11	0.43
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	11	0.43
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	1	0.43
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	1	0.43
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	1	0.43
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	10	0.43
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	11	0.43
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	3	0.43
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	3	0.43
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	4	0.43
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	4	0.43
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	5	0.43
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	5	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	10	0.43
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	10	0.43
(1,847)	2:11:B:LEU:HD21	2:11:B:LEU:H	6	0.43
(1,847)	2:11:B:LEU:HD22	2:11:B:LEU:H	6	0.43
(1,847)	2:11:B:LEU:HD23	2:11:B:LEU:H	6	0.43
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	6	0.43
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	6	0.43
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	6	0.43
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	6	0.43
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	6	0.43
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	15	0.43
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	15	0.43
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	15	0.43
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	10	0.43
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	10	0.43
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	6	0.43
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	6	0.43
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	6	0.43
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	9	0.43
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	9	0.43
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	9	0.43
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	11	0.43
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	11	0.43
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	11	0.43
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	12	0.43
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	12	0.43
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	12	0.43
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	15	0.43
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	15	0.43
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	15	0.43
(1,253)	1:24:A:ALA:HB1	1:24:A:ALA:H	2	0.43
(1,253)	1:24:A:ALA:HB2	1:24:A:ALA:H	2	0.43
(1,253)	1:24:A:ALA:HB3	1:24:A:ALA:H	2	0.43
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	4	0.43
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	4	0.43
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	4	0.43
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	13	0.43
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	13	0.43
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	13	0.43
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	3	0.43
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	7	0.43
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	8	0.43
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	8	0.43
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	1	0.43
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	1	0.43
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	3	0.43
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	3	0.43
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	11	0.43
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	11	0.43
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	15	0.43
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	15	0.43
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	6	0.42
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	3	0.42
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	3	0.42
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	3	0.42
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	7	0.42
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	9	0.42
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	6	0.42
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	6	0.42
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	6	0.42
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	6	0.42
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	6	0.42
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	6	0.42
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	6	0.42
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	6	0.42
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	6	0.42
(1,1584)	1:46:A:THR:HG21	1:60:A:CYS:HB3	1	0.42
(1,1584)	1:46:A:THR:HG22	1:60:A:CYS:HB3	1	0.42
(1,1584)	1:46:A:THR:HG23	1:60:A:CYS:HB3	1	0.42
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	8	0.42
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	8	0.42
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	8	0.42
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	8	0.42
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	8	0.42
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	8	0.42
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	8	0.42
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	8	0.42
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	8	0.42
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	8	0.42
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	8	0.42
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	8	0.42
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	13	0.42
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	13	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	13	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	1	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	1	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	5	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	5	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	7	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	7	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	11	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	11	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	12	0.42
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	12	0.42
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	3	0.42
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	3	0.42
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	3	0.42
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	6	0.42
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	6	0.42
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	6	0.42
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	13	0.42
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	13	0.42
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	13	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	4	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	4	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	4	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	4	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	4	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	4	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	4	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	4	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	4	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	6	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	6	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	6	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	6	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	6	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	6	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	6	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	6	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	6	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	8	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	8	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	8	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	8	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	8	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	8	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	8	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	8	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	8	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	12	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	12	0.42
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	12	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	12	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	12	0.42
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	12	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	12	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	12	0.42
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	12	0.42
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	8	0.42
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	8	0.42
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	8	0.42
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	6	0.42
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	6	0.42
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	6	0.42
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	6	0.42
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	6	0.42
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	6	0.42
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	6	0.42
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	6	0.42
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	6	0.42
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	3	0.42
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	3	0.42
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	3	0.42
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	12	0.42
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	12	0.42
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	12	0.42
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG2	13	0.42
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG3	13	0.42
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	5	0.42
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	10	0.42
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	11	0.42
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	11	0.42
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	5	0.42
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	5	0.42
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	5	0.42
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	11	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	11	0.42
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	11	0.42
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	9	0.42
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	9	0.42
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	4	0.42
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	4	0.42
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	4	0.42
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	10	0.42
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	10	0.42
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	10	0.42
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	7	0.42
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	7	0.42
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	7	0.42
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	8	0.42
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	8	0.42
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	8	0.42
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	12	0.42
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	12	0.42
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	12	0.42
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	3	0.42
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	3	0.42
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	11	0.42
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	11	0.42
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	12	0.42
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	12	0.42
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	2	0.42
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	2	0.42
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	6	0.42
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	6	0.42
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	5	0.42
(1,57)	1:4:A:SER:H	1:7:A:ASP:HB2	9	0.42
(1,57)	1:4:A:SER:H	1:7:A:ASP:HB3	9	0.42
(1,1938)	1:81:A:VAL:HG11	1:84:A:CYS:HB3	3	0.41
(1,1938)	1:81:A:VAL:HG12	1:84:A:CYS:HB3	3	0.41
(1,1938)	1:81:A:VAL:HG13	1:84:A:CYS:HB3	3	0.41
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	1	0.41
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	1	0.41
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	1	0.41
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	7	0.41
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	9	0.41
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	9	0.41
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	9	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	9	0.41
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	9	0.41
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	9	0.41
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	7	0.41
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	7	0.41
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	7	0.41
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	9	0.41
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	9	0.41
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	9	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	2	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	2	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	3	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	3	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	4	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	4	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	8	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	8	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	10	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	10	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	14	0.41
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	14	0.41
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	1	0.41
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	1	0.41
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	6	0.41
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	6	0.41
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	6	0.41
(1,1265)	1:24:A:ALA:HB1	1:80:A:PRO:HB2	7	0.41
(1,1265)	1:24:A:ALA:HB2	1:80:A:PRO:HB2	7	0.41
(1,1265)	1:24:A:ALA:HB3	1:80:A:PRO:HB2	7	0.41
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	9	0.41
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	9	0.41
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	9	0.41
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	15	0.41
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	15	0.41
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	15	0.41
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	15	0.41
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	15	0.41
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	15	0.41
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	15	0.41
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	15	0.41
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	15	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	4	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	4	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	4	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	4	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	4	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	4	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	4	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	4	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	8	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	8	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	8	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	8	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	8	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	8	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	8	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	8	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	8	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	10	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	10	0.41
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	10	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	10	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	10	0.41
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	10	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	10	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	10	0.41
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	10	0.41
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	10	0.41
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	10	0.41
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	9	0.41
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	9	0.41
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	13	0.41
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	13	0.41
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	2	0.41
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	2	0.41
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	2	0.41
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	12	0.41
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	12	0.41
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	12	0.41
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	6	0.41
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	6	0.41
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	5	0.41
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	5	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	7	0.41
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	10	0.41
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	3	0.4
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	5	0.4
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	4	0.4
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	4	0.4
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	4	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	4	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	4	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	4	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	4	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	4	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	4	0.4
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	7	0.4
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	7	0.4
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	7	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	7	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	7	0.4
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	7	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	7	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	7	0.4
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	7	0.4
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	11	0.4
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	11	0.4
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	3	0.4
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	13	0.4
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	9	0.4
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	9	0.4
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	13	0.4
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	13	0.4
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	9	0.4
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	9	0.4
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	9	0.4
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	11	0.4
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	11	0.4
(1,1332)	1:33:A:LEU:HD11	1:33:A:LEU:HB2	11	0.4
(1,1332)	1:33:A:LEU:HD12	1:33:A:LEU:HB2	11	0.4
(1,1332)	1:33:A:LEU:HD13	1:33:A:LEU:HB2	11	0.4
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	3	0.4
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	3	0.4
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	3	0.4
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	3	0.4
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	3	0.4
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	3	0.4
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	3	0.4
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	3	0.4
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	3	0.4
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	3	0.4
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	3	0.4
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	14	0.4
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	14	0.4
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	14	0.4
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	15	0.4
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	15	0.4
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	15	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	1	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	1	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	1	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	2	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	2	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	2	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	4	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	4	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	4	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	12	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	12	0.4
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	12	0.4
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	2	0.4
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	2	0.4
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	2	0.4
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	2	0.4
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	2	0.4
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	2	0.4
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	2	0.4
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	2	0.4
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	2	0.4
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	9	0.4
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	9	0.4
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	9	0.4
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	9	0.4
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	9	0.4
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	9	0.4
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	9	0.4
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	9	0.4
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	9	0.4
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	9	0.4
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	9	0.4
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	12	0.4
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	12	0.4
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	12	0.4
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	13	0.4
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	13	0.4
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	13	0.4
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	5	0.4
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	5	0.4
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	5	0.4
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	5	0.4
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	5	0.4
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	5	0.4
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	5	0.4
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	5	0.4
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	5	0.4
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	7	0.4
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	7	0.4
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	7	0.4
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	7	0.4
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	7	0.4
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	7	0.4
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	7	0.4
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	7	0.4
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	7	0.4
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	10	0.4
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	10	0.4
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	10	0.4
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	10	0.4
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	10	0.4
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	10	0.4
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	10	0.4
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	10	0.4
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	10	0.4
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	6	0.4
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	6	0.4
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	6	0.4
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	13	0.4
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	13	0.4
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD11	5	0.4
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD12	5	0.4
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD13	5	0.4
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	7	0.4
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	6	0.4
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	6	0.4
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	2	0.4
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	2	0.4
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	2	0.4
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	2	0.4
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	4	0.4
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	4	0.4
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	8	0.4
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	8	0.4
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	8	0.4
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	8	0.4
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	8	0.4
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	14	0.4
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	14	0.4
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	14	0.4
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	12	0.4
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	12	0.4
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	12	0.4
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	1	0.4
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	4	0.4
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	4	0.4
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	9	0.4
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	9	0.4
(1,259)	1:24:A:ALA:HB1	1:25:A:GLN:H	5	0.4
(1,259)	1:24:A:ALA:HB2	1:25:A:GLN:H	5	0.4
(1,259)	1:24:A:ALA:HB3	1:25:A:GLN:H	5	0.4
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	11	0.4
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	11	0.4
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	1	0.4
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	1	0.4
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	8	0.4
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	9	0.4
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	9	0.4
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	7	0.4
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	8	0.39
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	5	0.39
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	5	0.39
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	5	0.39
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	5	0.39
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	5	0.39
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	5	0.39
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	5	0.39
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	5	0.39
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	5	0.39
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	13	0.39
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	13	0.39
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	13	0.39
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	12	0.39
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	12	0.39
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	12	0.39
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	12	0.39
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	12	0.39
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	12	0.39
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	12	0.39
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	12	0.39
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	12	0.39
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	7	0.39
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	7	0.39
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	6	0.39
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	6	0.39
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	15	0.39
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	15	0.39
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	2	0.39
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	11	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	1	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	1	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	1	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	4	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	4	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	4	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	5	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	5	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	5	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	6	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	6	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	14	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	14	0.39
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	14	0.39
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	13	0.39
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	13	0.39
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD2	6	0.39
(1,1459)	1:40:A:LYS:HB2	1:40:A:LYS:HD3	6	0.39
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	8	0.39
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	8	0.39
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	8	0.39
(1,1332)	1:33:A:LEU:HD11	1:33:A:LEU:HB2	9	0.39
(1,1332)	1:33:A:LEU:HD12	1:33:A:LEU:HB2	9	0.39
(1,1332)	1:33:A:LEU:HD13	1:33:A:LEU:HB2	9	0.39
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	11	0.39
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	11	0.39
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	11	0.39
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	1	0.39
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	1	0.39
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	1	0.39
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	1	0.39
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	1	0.39
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	1	0.39
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	1	0.39
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	1	0.39
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	1	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	3	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	3	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	3	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	6	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	6	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	6	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	8	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	8	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	8	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	10	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	10	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	10	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	11	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	11	0.39
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	11	0.39
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	11	0.39
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	11	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	11	0.39
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	11	0.39
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	11	0.39
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	11	0.39
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	11	0.39
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	11	0.39
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	11	0.39
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	14	0.39
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	14	0.39
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	14	0.39
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	14	0.39
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	14	0.39
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	14	0.39
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	14	0.39
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	14	0.39
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	14	0.39
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	11	0.39
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	11	0.39
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	11	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	1	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	1	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	1	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	1	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	1	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	1	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	1	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	1	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	1	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	5	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	5	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	5	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	5	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	5	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	5	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	5	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	5	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	5	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	13	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	13	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	13	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	13	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	13	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	13	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	13	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	13	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	15	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	15	0.39
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	15	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	15	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	15	0.39
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	15	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	15	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	15	0.39
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	15	0.39
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	14	0.39
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	14	0.39
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	5	0.39
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	5	0.39
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	3	0.39
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	3	0.39
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	11	0.39
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	11	0.39
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	15	0.39
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	15	0.39
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	3	0.39
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE2	9	0.39
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE3	9	0.39
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	8	0.39
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	8	0.39
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	14	0.39
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	14	0.39
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	1	0.39
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	1	0.39
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	5	0.39
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	5	0.39
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	11	0.39
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	15	0.39
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	3	0.39
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	13	0.39
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	10	0.39
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	11	0.38
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	2	0.38
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	2	0.38
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	2	0.38
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	2	0.38
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	2	0.38
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	2	0.38
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	2	0.38
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	2	0.38
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	11	0.38
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	11	0.38
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	11	0.38
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	11	0.38
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	11	0.38
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	11	0.38
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	11	0.38
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	11	0.38
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	11	0.38
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	4	0.38
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	4	0.38
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	4	0.38
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	12	0.38
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	12	0.38
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	3	0.38
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	3	0.38
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	14	0.38
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	14	0.38
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	15	0.38
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	4	0.38
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	13	0.38
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	1	0.38
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	1	0.38
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	1	0.38
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	1	0.38
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	10	0.38
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	10	0.38
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	10	0.38
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	1	0.38
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	1	0.38
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	2	0.38
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	2	0.38
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	7	0.38
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	7	0.38
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	2	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	2	0.38
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	5	0.38
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	5	0.38
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	12	0.38
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	12	0.38
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	15	0.38
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	15	0.38
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	1	0.38
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	1	0.38
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	11	0.38
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	11	0.38
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	11	0.38
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	9	0.38
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	9	0.38
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	9	0.38
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	9	0.38
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	9	0.38
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	9	0.38
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	9	0.38
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	9	0.38
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	9	0.38
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	14	0.38
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	14	0.38
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	14	0.38
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	14	0.38
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	14	0.38
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	14	0.38
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	14	0.38
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	14	0.38
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	14	0.38
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	15	0.38
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	15	0.38
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	15	0.38
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD21	10	0.38
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD22	10	0.38
(1,1193)	1:20:A:LEU:HD21	1:66:A:LEU:HD23	10	0.38
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD21	10	0.38
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD22	10	0.38
(1,1193)	1:20:A:LEU:HD22	1:66:A:LEU:HD23	10	0.38
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD21	10	0.38
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD22	10	0.38
(1,1193)	1:20:A:LEU:HD23	1:66:A:LEU:HD23	10	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	6	0.38
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	6	0.38
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	6	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	2	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	2	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	2	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	2	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	2	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	2	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	2	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	2	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	2	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	3	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	3	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	3	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	3	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	3	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	3	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	3	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	3	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	3	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	9	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	9	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	9	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	9	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	9	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	9	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	9	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	9	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	9	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	12	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	12	0.38
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	12	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	12	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	12	0.38
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	12	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	12	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	12	0.38
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	12	0.38
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD11	11	0.38
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD12	11	0.38
(1,1078)	1:13:A:ILE:HG21	1:66:A:LEU:HD13	11	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD11	11	0.38
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD12	11	0.38
(1,1078)	1:13:A:ILE:HG22	1:66:A:LEU:HD13	11	0.38
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD11	11	0.38
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD12	11	0.38
(1,1078)	1:13:A:ILE:HG23	1:66:A:LEU:HD13	11	0.38
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	4	0.38
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	4	0.38
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	4	0.38
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	6	0.38
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	6	0.38
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	6	0.38
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD11	2	0.38
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD12	2	0.38
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD13	2	0.38
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD11	2	0.38
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD12	2	0.38
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD13	2	0.38
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	2	0.38
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	4	0.38
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	10	0.38
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	13	0.38
(1,847)	2:11:B:LEU:HD21	2:11:B:LEU:H	8	0.38
(1,847)	2:11:B:LEU:HD22	2:11:B:LEU:H	8	0.38
(1,847)	2:11:B:LEU:HD23	2:11:B:LEU:H	8	0.38
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	7	0.38
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	7	0.38
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	12	0.38
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	12	0.38
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	14	0.38
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	14	0.38
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	14	0.38
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	14	0.38
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	11	0.38
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	11	0.38
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	11	0.38
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	15	0.38
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	15	0.38
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	15	0.38
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE2	3	0.38
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE3	3	0.38
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	3	0.38
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	8	0.38
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	8	0.38
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	12	0.38
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	12	0.38
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	3	0.38
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	3	0.38
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	4	0.38
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	11	0.38
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	2	0.38
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	1	0.38
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	4	0.38
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	2	0.37
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	13	0.37
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	13	0.37
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	13	0.37
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	13	0.37
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	13	0.37
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	13	0.37
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	13	0.37
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	13	0.37
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	13	0.37
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	3	0.37
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	3	0.37
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	3	0.37
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	3	0.37
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	3	0.37
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	3	0.37
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	3	0.37
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	3	0.37
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	3	0.37
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	11	0.37
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	11	0.37
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	11	0.37
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	11	0.37
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	11	0.37
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	11	0.37
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	11	0.37
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	11	0.37
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	11	0.37
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	15	0.37
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	15	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	5	0.37
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	12	0.37
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	15	0.37
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	8	0.37
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	8	0.37
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	8	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	4	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	4	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	5	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	5	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	8	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	8	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	11	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	11	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	12	0.37
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	12	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	3	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	3	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	4	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	4	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	6	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	6	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	13	0.37
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	13	0.37
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	3	0.37
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	3	0.37
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	4	0.37
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	4	0.37
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	4	0.37
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	15	0.37
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	15	0.37
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	15	0.37
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	5	0.37
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	5	0.37
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	5	0.37
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	2	0.37
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	2	0.37
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	2	0.37
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	2	0.37
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	2	0.37
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	2	0.37
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	2	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	2	0.37
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	2	0.37
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	15	0.37
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	15	0.37
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	15	0.37
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	15	0.37
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	15	0.37
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	15	0.37
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	15	0.37
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	15	0.37
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	15	0.37
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	13	0.37
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	13	0.37
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	13	0.37
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG21	14	0.37
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG22	14	0.37
(1,1123)	1:17:A:ILE:HG21	1:21:A:VAL:HG23	14	0.37
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG21	14	0.37
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG22	14	0.37
(1,1123)	1:17:A:ILE:HG22	1:21:A:VAL:HG23	14	0.37
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG21	14	0.37
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG22	14	0.37
(1,1123)	1:17:A:ILE:HG23	1:21:A:VAL:HG23	14	0.37
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	4	0.37
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	4	0.37
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	4	0.37
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	14	0.37
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	14	0.37
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	14	0.37
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	9	0.37
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	9	0.37
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	9	0.37
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	14	0.37
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	14	0.37
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	14	0.37
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	3	0.37
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	15	0.37
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	5	0.37
(1,781)	1:85:A:LEU:HD11	1:86:A:ASN:H	4	0.37
(1,781)	1:85:A:LEU:HD12	1:86:A:ASN:H	4	0.37
(1,781)	1:85:A:LEU:HD13	1:86:A:ASN:H	4	0.37
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	8	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	8	0.37
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	11	0.37
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	11	0.37
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	7	0.37
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	14	0.37
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	14	0.37
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	1	0.37
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	7	0.37
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	7	0.37
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	7	0.37
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	13	0.37
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	13	0.37
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	14	0.37
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	15	0.37
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	1	0.37
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	1	0.37
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	6	0.37
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	6	0.37
(1,70)	1:7:A:ASP:HB2	1:7:A:ASP:H	14	0.37
(1,70)	1:7:A:ASP:HB3	1:7:A:ASP:H	14	0.37
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	10	0.37
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	15	0.37
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	12	0.37
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	15	0.37
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	5	0.37
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	14	0.37
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD11	10	0.36
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD12	10	0.36
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD13	10	0.36
(1,1870)	1:71:A:ALA:HB1	1:88:A:LYS:HD2	1	0.36
(1,1870)	1:71:A:ALA:HB1	1:88:A:LYS:HD3	1	0.36
(1,1870)	1:71:A:ALA:HB2	1:88:A:LYS:HD2	1	0.36
(1,1870)	1:71:A:ALA:HB2	1:88:A:LYS:HD3	1	0.36
(1,1870)	1:71:A:ALA:HB3	1:88:A:LYS:HD2	1	0.36
(1,1870)	1:71:A:ALA:HB3	1:88:A:LYS:HD3	1	0.36
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	8	0.36
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	8	0.36
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	8	0.36
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	8	0.36
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	8	0.36
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	8	0.36
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	8	0.36
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	8	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	9	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	9	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	9	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	9	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	9	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	9	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	9	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	9	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	9	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	14	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	14	0.36
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	14	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	14	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	14	0.36
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	14	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	14	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	14	0.36
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	14	0.36
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	6	0.36
(1,1647)	1:50:A:LYS:HG2	1:53:A:THR:HA	14	0.36
(1,1584)	1:46:A:THR:HG21	1:60:A:CYS:HB3	4	0.36
(1,1584)	1:46:A:THR:HG22	1:60:A:CYS:HB3	4	0.36
(1,1584)	1:46:A:THR:HG23	1:60:A:CYS:HB3	4	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	3	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	3	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	6	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	6	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	10	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	10	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	15	0.36
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	15	0.36
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	4	0.36
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	4	0.36
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	8	0.36
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	8	0.36
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	12	0.36
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	12	0.36
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	14	0.36
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	14	0.36
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	3	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	3	0.36
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	2	0.36
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	2	0.36
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	7	0.36
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	7	0.36
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	6	0.36
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	10	0.36
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	15	0.36
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	4	0.36
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	4	0.36
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	7	0.36
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	7	0.36
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	9	0.36
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	9	0.36
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	9	0.36
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	10	0.36
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	10	0.36
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	10	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	5	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	5	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	5	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	5	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	5	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	5	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	5	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	5	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	5	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	8	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	8	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	8	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	8	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	8	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	8	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	8	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	8	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	8	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	13	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	13	0.36
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	13	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	13	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	13	0.36
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	13	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	13	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	13	0.36
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	13	0.36
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	8	0.36
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	8	0.36
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	8	0.36
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	9	0.36
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	5	0.36
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	1	0.36
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	1	0.36
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	1	0.36
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	1	0.36
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	9	0.36
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	9	0.36
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	10	0.36
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	10	0.36
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	5	0.36
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	5	0.36
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	10	0.36
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	10	0.36
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	13	0.36
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	3	0.36
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	1	0.36
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	6	0.36
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	6	0.36
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	3	0.36
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	3	0.36
(1,274)	1:25:A:GLN:HB2	1:25:A:GLN:HE21	1	0.36
(1,274)	1:25:A:GLN:HB3	1:25:A:GLN:HE21	1	0.36
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	7	0.36
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	7	0.36
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	3	0.36
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	3	0.36
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	2	0.36
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	6	0.36
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	9	0.36
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	8	0.36
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	14	0.36
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	14	0.36
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	15	0.35
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	11	0.35
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	11	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	11	0.35
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	14	0.35
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	14	0.35
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	14	0.35
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	10	0.35
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	10	0.35
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	10	0.35
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	10	0.35
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	10	0.35
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	10	0.35
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	10	0.35
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	10	0.35
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	10	0.35
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	15	0.35
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	15	0.35
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	15	0.35
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	15	0.35
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	15	0.35
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	15	0.35
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	15	0.35
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	15	0.35
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	15	0.35
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	14	0.35
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	14	0.35
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	14	0.35
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	13	0.35
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	13	0.35
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	15	0.35
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	15	0.35
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	5	0.35
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	5	0.35
(1,1607)	1:47:A:LYS:HD2	1:82:A:PRO:HB3	7	0.35
(1,1607)	1:47:A:LYS:HD3	1:82:A:PRO:HB3	7	0.35
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	13	0.35
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	13	0.35
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	13	0.35
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	10	0.35
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	10	0.35
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	13	0.35
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	13	0.35
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	15	0.35
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	6	0.35
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	6	0.35
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	6	0.35
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	1	0.35
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	1	0.35
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	7	0.35
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	7	0.35
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	11	0.35
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	11	0.35
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	5	0.35
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	5	0.35
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	8	0.35
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	8	0.35
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	10	0.35
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	10	0.35
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	12	0.35
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	13	0.35
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	13	0.35
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	14	0.35
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	14	0.35
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	9	0.35
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	9	0.35
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	9	0.35
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	4	0.35
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	4	0.35
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	4	0.35
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	4	0.35
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	4	0.35
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	4	0.35
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	4	0.35
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	4	0.35
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	4	0.35
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	1	0.35
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	1	0.35
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	1	0.35
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	13	0.35
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	13	0.35
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	13	0.35
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD11	11	0.35
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD12	11	0.35
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD13	11	0.35
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	1	0.35
(1,776)	1:85:A:LEU:HD21	1:85:A:LEU:H	12	0.35
(1,776)	1:85:A:LEU:HD22	1:85:A:LEU:H	12	0.35
(1,776)	1:85:A:LEU:HD23	1:85:A:LEU:H	12	0.35
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	3	0.35
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	3	0.35
(1,710)	1:63:A:LEU:HB2	1:63:A:LEU:H	1	0.35
(1,710)	1:63:A:LEU:HB3	1:63:A:LEU:H	1	0.35
(1,700)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	4	0.35
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	2	0.35
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	11	0.35
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	6	0.35
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	6	0.35
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	9	0.35
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	5	0.35
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	5	0.35
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	4	0.35
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	4	0.35
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	10	0.35
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	10	0.35
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	11	0.35
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	11	0.35
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	11	0.35
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	15	0.35
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	15	0.35
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	1	0.35
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	7	0.35
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	10	0.35
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	12	0.35
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	9	0.35
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	9	0.35
(1,73)	1:7:A:ASP:HB2	1:8:A:SER:H	14	0.35
(1,73)	1:7:A:ASP:HB3	1:8:A:SER:H	14	0.35
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	3	0.35
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	4	0.35
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	10	0.35
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	7	0.35
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	7	0.35
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	1	0.34
(1,1977)	2:9:B:LEU:HB2	2:9:B:LEU:HD21	6	0.34
(1,1977)	2:9:B:LEU:HB2	2:9:B:LEU:HD22	6	0.34
(1,1977)	2:9:B:LEU:HB2	2:9:B:LEU:HD23	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1977)	2:9:B:LEU:HB3	2:9:B:LEU:HD21	6	0.34
(1,1977)	2:9:B:LEU:HB3	2:9:B:LEU:HD22	6	0.34
(1,1977)	2:9:B:LEU:HB3	2:9:B:LEU:HD23	6	0.34
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	15	0.34
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	15	0.34
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	15	0.34
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	15	0.34
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	15	0.34
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	15	0.34
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	15	0.34
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	15	0.34
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	15	0.34
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	12	0.34
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	12	0.34
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	12	0.34
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	12	0.34
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	12	0.34
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	12	0.34
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	12	0.34
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	12	0.34
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	12	0.34
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	6	0.34
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	6	0.34
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD11	7	0.34
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD12	7	0.34
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD13	7	0.34
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	14	0.34
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	14	0.34
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	14	0.34
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	15	0.34
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	15	0.34
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	15	0.34
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	7	0.34
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	7	0.34
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	7	0.34
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	7	0.34
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	7	0.34
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	7	0.34
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	7	0.34
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	7	0.34
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	7	0.34
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	3	0.34
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	9	0.34
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	9	0.34
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	11	0.34
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	11	0.34
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	4	0.34
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	4	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	3	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	3	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	4	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	4	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	8	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	8	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	9	0.34
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	9	0.34
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	2	0.34
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	14	0.34
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	14	0.34
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	7	0.34
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	7	0.34
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	7	0.34
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	7	0.34
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	7	0.34
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	7	0.34
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	7	0.34
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	7	0.34
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	7	0.34
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	5	0.34
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	5	0.34
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	5	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	2	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	2	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	2	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	3	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	3	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	3	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	7	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	7	0.34
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	7	0.34
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	9	0.34
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	9	0.34
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	7	0.34
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	5	0.34
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	5	0.34
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	8	0.34
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	8	0.34
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	9	0.34
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	9	0.34
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	9	0.34
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	9	0.34
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	8	0.34
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	4	0.34
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	4	0.34
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	4	0.34
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	8	0.34
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	8	0.34
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	8	0.34
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	10	0.34
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	10	0.34
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	10	0.34
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	14	0.34
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	14	0.34
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	14	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	6	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	6	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	6	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	6	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	6	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	6	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	6	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	6	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	6	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	7	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	7	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	7	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	7	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	7	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	7	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	7	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	7	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	7	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	10	0.34
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	10	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	10	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	10	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	10	0.34
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	10	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	10	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	10	0.34
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	10	0.34
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	11	0.34
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	11	0.34
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	11	0.34
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	15	0.34
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	15	0.34
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	15	0.34
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	8	0.34
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	8	0.34
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	8	0.34
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	8	0.34
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	8	0.34
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	8	0.34
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	8	0.34
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	8	0.34
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	8	0.34
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	9	0.34
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	9	0.34
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	9	0.34
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	9	0.34
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	9	0.34
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	9	0.34
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	9	0.34
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	9	0.34
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	9	0.34
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	14	0.34
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	14	0.34
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	14	0.34
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	6	0.34
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	6	0.34
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	6	0.34
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	2	0.34
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	2	0.34
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	2	0.34
(1,979)	1:4:A:SER:HB2	1:5:A:PRO:HB2	3	0.34
(1,979)	1:4:A:SER:HB3	1:5:A:PRO:HB2	3	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	6	0.34
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	6	0.34
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	4	0.34
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	4	0.34
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	6	0.34
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	6	0.34
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	7	0.34
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	7	0.34
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	10	0.34
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	10	0.34
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	11	0.34
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	11	0.34
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	14	0.34
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	14	0.34
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	15	0.34
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	15	0.34
(1,655)	1:59:A:ILE:HD11	1:60:A:CYS:H	14	0.34
(1,655)	1:59:A:ILE:HD12	1:60:A:CYS:H	14	0.34
(1,655)	1:59:A:ILE:HD13	1:60:A:CYS:H	14	0.34
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	8	0.34
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	12	0.34
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	15	0.34
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	8	0.34
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	7	0.34
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	7	0.34
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	15	0.34
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	15	0.34
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	11	0.34
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	11	0.34
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	13	0.34
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	13	0.34
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE2	1	0.34
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE3	1	0.34
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	1	0.34
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	1	0.34
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	6	0.34
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	6	0.34
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	4	0.34
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	4	0.34
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	2	0.34
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	2	0.34
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	15	0.34
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	5	0.34
(1,74)	1:7:A:ASP:HA	1:9:A:ARG:H	13	0.34
(1,65)	1:6:A:GLY:H	1:7:A:ASP:H	6	0.34
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	4	0.34
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	12	0.34
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	12	0.34
(1,1953)	1:85:A:LEU:HD11	1:85:A:LEU:HB3	2	0.33
(1,1953)	1:85:A:LEU:HD12	1:85:A:LEU:HB3	2	0.33
(1,1953)	1:85:A:LEU:HD13	1:85:A:LEU:HB3	2	0.33
(1,1938)	1:81:A:VAL:HG11	1:84:A:CYS:HB3	4	0.33
(1,1938)	1:81:A:VAL:HG12	1:84:A:CYS:HB3	4	0.33
(1,1938)	1:81:A:VAL:HG13	1:84:A:CYS:HB3	4	0.33
(1,1900)	1:76:A:GLU:HG2	1:78:A:LYS:HE2	6	0.33
(1,1900)	1:76:A:GLU:HG2	1:78:A:LYS:HE3	6	0.33
(1,1900)	1:76:A:GLU:HG3	1:78:A:LYS:HE2	6	0.33
(1,1900)	1:76:A:GLU:HG3	1:78:A:LYS:HE3	6	0.33
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	14	0.33
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	14	0.33
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	14	0.33
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	14	0.33
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	14	0.33
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	14	0.33
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	14	0.33
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	14	0.33
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	14	0.33
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	2	0.33
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	2	0.33
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	2	0.33
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	10	0.33
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	10	0.33
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	10	0.33
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	9	0.33
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	9	0.33
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	14	0.33
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	14	0.33
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	15	0.33
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	2	0.33
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	2	0.33
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	1	0.33
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	1	0.33
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	11	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	1	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	1	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	2	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	2	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	6	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	6	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	11	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	11	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	12	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	12	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	15	0.33
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	15	0.33
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	3	0.33
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	15	0.33
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	9	0.33
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	9	0.33
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	12	0.33
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	12	0.33
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB2	14	0.33
(1,1490)	1:41:A:ARG:HA	1:44:A:GLN:HB3	14	0.33
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	6	0.33
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	6	0.33
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	14	0.33
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	14	0.33
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	14	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	2	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	2	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	6	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	6	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	10	0.33
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	10	0.33
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD2	14	0.33
(1,1402)	1:37:A:GLN:HA	1:40:A:LYS:HD3	14	0.33
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	2	0.33
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	8	0.33
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	8	0.33
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	8	0.33
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	2	0.33
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	2	0.33
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	2	0.33
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	1	0.33
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	1	0.33
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	12	0.33
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	12	0.33
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	12	0.33
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	12	0.33
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	12	0.33
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	12	0.33
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	12	0.33
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	12	0.33
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	12	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	1	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	1	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	1	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	4	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	4	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	4	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	6	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	6	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	6	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	7	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	7	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	7	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	13	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	13	0.33
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	13	0.33
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	8	0.33
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	8	0.33
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	8	0.33
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	10	0.33
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	10	0.33
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	10	0.33
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	10	0.33
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	10	0.33
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	10	0.33
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	10	0.33
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	10	0.33
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	10	0.33
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	6	0.33
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	12	0.33
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	11	0.33
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	11	0.33
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	12	0.33
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	12	0.33
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	12	0.33
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	12	0.33
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	12	0.33
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	12	0.33
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	12	0.33
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	12	0.33
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	12	0.33
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	3	0.33
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	3	0.33
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	3	0.33
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	11	0.33
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG2	12	0.33
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG3	12	0.33
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	3	0.33
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	4	0.33
(1,847)	2:11:B:LEU:HD21	2:11:B:LEU:H	10	0.33
(1,847)	2:11:B:LEU:HD22	2:11:B:LEU:H	10	0.33
(1,847)	2:11:B:LEU:HD23	2:11:B:LEU:H	10	0.33
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	1	0.33
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	1	0.33
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	12	0.33
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	12	0.33
(1,750)	1:75:A:GLN:HB2	1:75:A:GLN:HE21	12	0.33
(1,750)	1:75:A:GLN:HB3	1:75:A:GLN:HE21	12	0.33
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	4	0.33
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	4	0.33
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	6	0.33
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	6	0.33
(1,679)	1:61:A:LYS:HB2	1:61:A:LYS:H	15	0.33
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	5	0.33
(1,647)	1:59:A:ILE:HB	1:59:A:ILE:H	9	0.33
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	6	0.33
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	12	0.33
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	13	0.33
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	15	0.33
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	9	0.33
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	9	0.33
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	12	0.33
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	2	0.33
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	2	0.33
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	10	0.33
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	10	0.33
(1,90)	1:10:A:ARG:HD2	1:10:A:ARG:H	10	0.33
(1,90)	1:10:A:ARG:HD3	1:10:A:ARG:H	10	0.33
(1,65)	1:6:A:GLY:H	1:7:A:ASP:H	1	0.33
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	13	0.33
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	8	0.33
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	3	0.33
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	4	0.33
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	9	0.33
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE1	8	0.33
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE2	8	0.33
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	1	0.33
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	1	0.32
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	9	0.32
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	10	0.32
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD11	14	0.32
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD12	14	0.32
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD13	14	0.32
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	15	0.32
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	15	0.32
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	15	0.32
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	15	0.32
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	15	0.32
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	15	0.32
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	15	0.32
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	15	0.32
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	15	0.32
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	15	0.32
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	15	0.32
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	15	0.32
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	15	0.32
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	15	0.32
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	15	0.32
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	15	0.32
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	15	0.32
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	15	0.32
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	11	0.32
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	11	0.32
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	5	0.32
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	5	0.32
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	5	0.32
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	5	0.32
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	5	0.32
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	5	0.32
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	5	0.32
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	5	0.32
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	5	0.32
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	7	0.32
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	7	0.32
(1,1607)	1:47:A:LYS:HD2	1:82:A:PRO:HB3	3	0.32
(1,1607)	1:47:A:LYS:HD3	1:82:A:PRO:HB3	3	0.32
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	2	0.32
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	2	0.32
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	7	0.32
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	7	0.32
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	12	0.32
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	12	0.32
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	7	0.32
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	9	0.32
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	13	0.32
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD11	7	0.32
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD12	7	0.32
(1,1511)	1:42:A:VAL:HG11	1:59:A:ILE:HD13	7	0.32
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD11	7	0.32
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD12	7	0.32
(1,1511)	1:42:A:VAL:HG12	1:59:A:ILE:HD13	7	0.32
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD11	7	0.32
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD12	7	0.32
(1,1511)	1:42:A:VAL:HG13	1:59:A:ILE:HD13	7	0.32
(1,1509)	1:42:A:VAL:HG11	1:59:A:ILE:HG13	15	0.32
(1,1509)	1:42:A:VAL:HG12	1:59:A:ILE:HG13	15	0.32
(1,1509)	1:42:A:VAL:HG13	1:59:A:ILE:HG13	15	0.32
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	13	0.32
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	13	0.32
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	13	0.32
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	4	0.32
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	4	0.32
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	12	0.32
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	12	0.32
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	2	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	2	0.32
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	9	0.32
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	9	0.32
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	11	0.32
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	11	0.32
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	8	0.32
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	8	0.32
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	8	0.32
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	6	0.32
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	12	0.32
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	12	0.32
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	12	0.32
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	15	0.32
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	15	0.32
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	15	0.32
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	5	0.32
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	5	0.32
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	5	0.32
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	12	0.32
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	12	0.32
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	12	0.32
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	15	0.32
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	15	0.32
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	15	0.32
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	4	0.32
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	5	0.32
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	10	0.32
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	9	0.32
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	9	0.32
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	9	0.32
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	5	0.32
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	10	0.32
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	11	0.32
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	13	0.32
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	14	0.32
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	3	0.32
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	3	0.32
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	3	0.32
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	12	0.32
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	12	0.32
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	12	0.32
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	7	0.32
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	7	0.32
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	9	0.32
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	9	0.32
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	9	0.32
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	9	0.32
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	9	0.32
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	9	0.32
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	9	0.32
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	9	0.32
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	9	0.32
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	12	0.32
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	12	0.32
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	12	0.32
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	15	0.32
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	15	0.32
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	15	0.32
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB2	11	0.32
(1,971)	1:3:A:GLN:HB3	1:7:A:ASP:HB3	11	0.32
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	2	0.32
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	2	0.32
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	4	0.32
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	4	0.32
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	12	0.32
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	12	0.32
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	4	0.32
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	4	0.32
(1,751)	1:75:A:GLN:HG2	1:75:A:GLN:HE21	13	0.32
(1,751)	1:75:A:GLN:HG3	1:75:A:GLN:HE21	13	0.32
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	2	0.32
(1,673)	1:60:A:CYS:HB2	1:61:A:LYS:H	15	0.32
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	10	0.32
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	14	0.32
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	15	0.32
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	14	0.32
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	3	0.32
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	3	0.32
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	11	0.32
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	11	0.32
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	11	0.32
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	11	0.32
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	1	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	1	0.32
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	3	0.32
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	2	0.32
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	2	0.32
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	2	0.32
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	4	0.32
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	4	0.32
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	9	0.32
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	9	0.32
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	11	0.32
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	11	0.32
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	3	0.32
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	3	0.32
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	8	0.32
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	8	0.32
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	9	0.32
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	9	0.32
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	11	0.32
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	11	0.32
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	12	0.32
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	12	0.32
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	14	0.32
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	14	0.32
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	4	0.32
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	4	0.32
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	7	0.32
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	7	0.32
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	4	0.32
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	15	0.32
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	5	0.32
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	12	0.32
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	13	0.32
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	9	0.32
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	9	0.32
(2,81)	1:81:A:VAL:O	1:85:A:LEU:H	12	0.31
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	7	0.31
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	1	0.31
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD11	8	0.31
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD12	8	0.31
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD13	8	0.31
(1,1967)	1:90:A:LYS:HE2	1:90:A:LYS:HA	15	0.31
(1,1967)	1:90:A:LYS:HE3	1:90:A:LYS:HA	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1938)	1:81:A:VAL:HG11	1:84:A:CYS:HB3	6	0.31
(1,1938)	1:81:A:VAL:HG12	1:84:A:CYS:HB3	6	0.31
(1,1938)	1:81:A:VAL:HG13	1:84:A:CYS:HB3	6	0.31
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	14	0.31
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	7	0.31
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	7	0.31
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	7	0.31
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	7	0.31
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	7	0.31
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	7	0.31
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	7	0.31
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	7	0.31
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	7	0.31
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	1	0.31
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	1	0.31
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	7	0.31
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	7	0.31
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	12	0.31
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	12	0.31
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	13	0.31
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	13	0.31
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	13	0.31
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	13	0.31
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	13	0.31
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	13	0.31
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	13	0.31
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	13	0.31
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	13	0.31
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	7	0.31
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	7	0.31
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	7	0.31
(1,1607)	1:47:A:LYS:HD2	1:82:A:PRO:HB3	15	0.31
(1,1607)	1:47:A:LYS:HD3	1:82:A:PRO:HB3	15	0.31
(1,1584)	1:46:A:THR:HG21	1:60:A:CYS:HB3	8	0.31
(1,1584)	1:46:A:THR:HG22	1:60:A:CYS:HB3	8	0.31
(1,1584)	1:46:A:THR:HG23	1:60:A:CYS:HB3	8	0.31
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	11	0.31
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	3	0.31
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	3	0.31
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	15	0.31
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	15	0.31
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	12	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	12	0.31
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	12	0.31
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	12	0.31
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	12	0.31
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	12	0.31
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	13	0.31
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	13	0.31
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	14	0.31
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	14	0.31
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD2	15	0.31
(1,1415)	1:38:A:LYS:HB2	1:38:A:LYS:HD3	15	0.31
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	11	0.31
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	1	0.31
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	1	0.31
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	9	0.31
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	9	0.31
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	5	0.31
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	7	0.31
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	7	0.31
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	7	0.31
(1,1251)	1:23:A:ALA:HB1	1:40:A:LYS:HB2	13	0.31
(1,1251)	1:23:A:ALA:HB2	1:40:A:LYS:HB2	13	0.31
(1,1251)	1:23:A:ALA:HB3	1:40:A:LYS:HB2	13	0.31
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	14	0.31
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	14	0.31
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	14	0.31
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	14	0.31
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	15	0.31
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	8	0.31
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	8	0.31
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	8	0.31
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	12	0.31
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	12	0.31
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	12	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	4	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	4	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	4	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	4	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	4	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	4	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	4	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	4	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	6	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	6	0.31
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	6	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	6	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	6	0.31
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	6	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	6	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	6	0.31
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	6	0.31
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	1	0.31
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	2	0.31
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	4	0.31
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	5	0.31
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	5	0.31
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	5	0.31
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	10	0.31
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	10	0.31
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	10	0.31
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	15	0.31
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	15	0.31
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	15	0.31
(1,1135)	1:17:A:ILE:HD11	1:70:A:HIS:HB2	5	0.31
(1,1135)	1:17:A:ILE:HD12	1:70:A:HIS:HB2	5	0.31
(1,1135)	1:17:A:ILE:HD13	1:70:A:HIS:HB2	5	0.31
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	2	0.31
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	2	0.31
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	2	0.31
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	8	0.31
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	8	0.31
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	8	0.31
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	11	0.31
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	11	0.31
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	11	0.31
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD11	8	0.31
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD12	8	0.31
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD13	8	0.31
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	8	0.31
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	8	0.31
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	9	0.31
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	9	0.31
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	8	0.31
(1,776)	1:85:A:LEU:HD21	1:85:A:LEU:H	1	0.31
(1,776)	1:85:A:LEU:HD22	1:85:A:LEU:H	1	0.31
(1,776)	1:85:A:LEU:HD23	1:85:A:LEU:H	1	0.31
(1,700)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	7	0.31
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	3	0.31
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	3	0.31
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	11	0.31
(1,637)	1:57:A:CYS:H	1:60:A:CYS:HB2	6	0.31
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	4	0.31
(1,578)	1:51:A:ARG:HB2	1:55:A:GLY:H	2	0.31
(1,578)	1:51:A:ARG:HB3	1:55:A:GLY:H	2	0.31
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	2	0.31
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	2	0.31
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	8	0.31
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	8	0.31
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	14	0.31
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	14	0.31
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	13	0.31
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	13	0.31
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	13	0.31
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	1	0.31
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	1	0.31
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	13	0.31
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	13	0.31
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	4	0.31
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	1	0.31
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	1	0.31
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	2	0.31
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	2	0.31
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	13	0.31
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	13	0.31
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	2	0.31
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE1	6	0.31
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE2	6	0.31
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	2	0.31
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	1	0.3
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	9	0.3
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	6	0.3
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	6	0.3
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD11	15	0.3
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD12	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD13	15	0.3
(1,1967)	1:90:A:LYS:HE2	1:90:A:LYS:HA	2	0.3
(1,1967)	1:90:A:LYS:HE3	1:90:A:LYS:HA	2	0.3
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	12	0.3
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	6	0.3
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE2	2	0.3
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE3	2	0.3
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE2	4	0.3
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE3	4	0.3
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	4	0.3
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	4	0.3
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	4	0.3
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	3	0.3
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	3	0.3
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	10	0.3
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	10	0.3
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	13	0.3
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	13	0.3
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	3	0.3
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	3	0.3
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	3	0.3
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	9	0.3
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	7	0.3
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	7	0.3
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	12	0.3
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	12	0.3
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	10	0.3
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	10	0.3
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	15	0.3
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	15	0.3
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	7	0.3
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	7	0.3
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	7	0.3
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	7	0.3
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	6	0.3
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	6	0.3
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	6	0.3
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	6	0.3
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	14	0.3
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	14	0.3
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	14	0.3
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	12	0.3
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	11	0.3
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	11	0.3
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	11	0.3
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	14	0.3
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	14	0.3
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	11	0.3
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	11	0.3
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	11	0.3
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	13	0.3
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	14	0.3
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	5	0.3
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	5	0.3
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	12	0.3
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	12	0.3
(1,1335)	1:33:A:LEU:HD21	1:33:A:LEU:HB3	11	0.3
(1,1335)	1:33:A:LEU:HD22	1:33:A:LEU:HB3	11	0.3
(1,1335)	1:33:A:LEU:HD23	1:33:A:LEU:HB3	11	0.3
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	3	0.3
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	3	0.3
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	6	0.3
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	6	0.3
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	11	0.3
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	11	0.3
(1,1266)	1:24:A:ALA:HB1	1:80:A:PRO:HG2	2	0.3
(1,1266)	1:24:A:ALA:HB2	1:80:A:PRO:HG2	2	0.3
(1,1266)	1:24:A:ALA:HB3	1:80:A:PRO:HG2	2	0.3
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	7	0.3
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	2	0.3
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	2	0.3
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	2	0.3
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	3	0.3
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	7	0.3
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	8	0.3
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	12	0.3
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	13	0.3
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	10	0.3
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	10	0.3
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	10	0.3
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	14	0.3
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	14	0.3
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	14	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	12	0.3
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	12	0.3
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	12	0.3
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	15	0.3
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	15	0.3
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	15	0.3
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	13	0.3
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	13	0.3
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	13	0.3
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	13	0.3
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	13	0.3
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	13	0.3
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	13	0.3
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	13	0.3
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	13	0.3
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	7	0.3
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	8	0.3
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	15	0.3
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	2	0.3
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	2	0.3
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	2	0.3
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	7	0.3
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	7	0.3
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	7	0.3
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	9	0.3
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	9	0.3
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	9	0.3
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	14	0.3
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	14	0.3
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	14	0.3
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	6	0.3
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	6	0.3
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	6	0.3
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	6	0.3
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	6	0.3
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	6	0.3
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	6	0.3
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	6	0.3
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	6	0.3
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	2	0.3
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	2	0.3
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	3	0.3
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	3	0.3
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	7	0.3
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	14	0.3
(1,931)	2:21:B:THR:HG21	2:21:B:THR:H	1	0.3
(1,931)	2:21:B:THR:HG22	2:21:B:THR:H	1	0.3
(1,931)	2:21:B:THR:HG23	2:21:B:THR:H	1	0.3
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	9	0.3
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	9	0.3
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	2	0.3
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	2	0.3
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	13	0.3
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	13	0.3
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	3	0.3
(1,736)	1:72:A:LYS:HG2	1:72:A:LYS:H	13	0.3
(1,736)	1:72:A:LYS:HG3	1:72:A:LYS:H	13	0.3
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	2	0.3
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	2	0.3
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	13	0.3
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	13	0.3
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	10	0.3
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	2	0.3
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	2	0.3
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	4	0.3
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	4	0.3
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	15	0.3
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	15	0.3
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	14	0.3
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	14	0.3
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	14	0.3
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	14	0.3
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	1	0.3
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	1	0.3
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	7	0.3
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	7	0.3
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	15	0.3
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	15	0.3
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	8	0.3
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	3	0.3
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	3	0.3
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	7	0.3
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	7	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	14	0.3
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	14	0.3
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	2	0.3
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	8	0.3
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	15	0.3
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	6	0.3
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	6	0.3
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	9	0.3
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	9	0.3
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	15	0.3
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	15	0.3
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	11	0.3
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	11	0.3
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	5	0.3
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	5	0.3
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	3	0.3
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	13	0.3
(1,65)	1:6:A:GLY:H	1:7:A:ASP:H	14	0.3
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	2	0.3
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	15	0.3
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	2	0.3
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	7	0.3
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	15	0.3
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	2	0.29
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	12	0.29
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	14	0.29
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	4	0.29
(1,1967)	1:90:A:LYS:HE2	1:90:A:LYS:HA	7	0.29
(1,1967)	1:90:A:LYS:HE3	1:90:A:LYS:HA	7	0.29
(1,1967)	1:90:A:LYS:HE2	1:90:A:LYS:HA	9	0.29
(1,1967)	1:90:A:LYS:HE3	1:90:A:LYS:HA	9	0.29
(1,1938)	1:81:A:VAL:HG11	1:84:A:CYS:HB3	8	0.29
(1,1938)	1:81:A:VAL:HG12	1:84:A:CYS:HB3	8	0.29
(1,1938)	1:81:A:VAL:HG13	1:84:A:CYS:HB3	8	0.29
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE2	10	0.29
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE3	10	0.29
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	3	0.29
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	15	0.29
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	15	0.29
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	10	0.29
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	10	0.29
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	10	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	10	0.29
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	10	0.29
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	10	0.29
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	10	0.29
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	10	0.29
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	10	0.29
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	6	0.29
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	6	0.29
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	6	0.29
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	12	0.29
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	12	0.29
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	12	0.29
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	2	0.29
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	2	0.29
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	4	0.29
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	4	0.29
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	8	0.29
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	8	0.29
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	3	0.29
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	3	0.29
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	14	0.29
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	14	0.29
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	14	0.29
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	14	0.29
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	14	0.29
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	14	0.29
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	3	0.29
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	3	0.29
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	10	0.29
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	10	0.29
(1,1464)	1:40:A:LYS:HG2	1:40:A:LYS:HE3	1	0.29
(1,1464)	1:40:A:LYS:HG3	1:40:A:LYS:HE3	1	0.29
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	4	0.29
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	5	0.29
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	8	0.29
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	8	0.29
(1,1335)	1:33:A:LEU:HD21	1:33:A:LEU:HB3	9	0.29
(1,1335)	1:33:A:LEU:HD22	1:33:A:LEU:HB3	9	0.29
(1,1335)	1:33:A:LEU:HD23	1:33:A:LEU:HB3	9	0.29
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	2	0.29
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	2	0.29
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	2	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	4	0.29
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	4	0.29
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	4	0.29
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	5	0.29
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	5	0.29
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	7	0.29
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	7	0.29
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	12	0.29
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	12	0.29
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	7	0.29
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	10	0.29
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	10	0.29
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	10	0.29
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	12	0.29
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	12	0.29
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	12	0.29
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	13	0.29
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	9	0.29
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	9	0.29
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	9	0.29
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	2	0.29
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	6	0.29
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	3	0.29
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	3	0.29
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	3	0.29
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	1	0.29
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	1	0.29
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	1	0.29
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	3	0.29
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	3	0.29
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	3	0.29
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	6	0.29
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	6	0.29
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	6	0.29
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	8	0.29
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	8	0.29
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	8	0.29
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	12	0.29
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	12	0.29
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	12	0.29
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	13	0.29
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	13	0.29
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	5	0.29
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	5	0.29
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	5	0.29
(1,1136)	1:17:A:ILE:HG21	1:70:A:HIS:HB2	5	0.29
(1,1136)	1:17:A:ILE:HG22	1:70:A:HIS:HB2	5	0.29
(1,1136)	1:17:A:ILE:HG23	1:70:A:HIS:HB2	5	0.29
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	15	0.29
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	15	0.29
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	15	0.29
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	8	0.29
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	8	0.29
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	8	0.29
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	8	0.29
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	8	0.29
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	8	0.29
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	8	0.29
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	8	0.29
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	8	0.29
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	10	0.29
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	10	0.29
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	10	0.29
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	10	0.29
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	10	0.29
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	10	0.29
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	10	0.29
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	10	0.29
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	10	0.29
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	10	0.29
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	10	0.29
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	10	0.29
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	15	0.29
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	15	0.29
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	3	0.29
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	9	0.29
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	3	0.29
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	3	0.29
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	3	0.29
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	6	0.29
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	6	0.29
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	12	0.29
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	15	0.29
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	15	0.29
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	7	0.29
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	14	0.29
(1,700)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	3	0.29
(1,700)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	6	0.29
(1,700)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	8	0.29
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	8	0.29
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	8	0.29
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	11	0.29
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	11	0.29
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	5	0.29
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	2	0.29
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	4	0.29
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	8	0.29
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	3	0.29
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	3	0.29
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	7	0.29
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	7	0.29
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	10	0.29
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	10	0.29
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	3	0.29
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	3	0.29
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	8	0.29
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	8	0.29
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	15	0.29
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	15	0.29
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	7	0.29
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	8	0.29
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	6	0.29
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	6	0.29
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	9	0.29
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	9	0.29
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	10	0.29
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	10	0.29
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	11	0.29
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	11	0.29
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	12	0.29
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	12	0.29
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	2	0.29
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	2	0.29
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	5	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	5	0.29
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	9	0.29
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	9	0.29
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	10	0.29
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	10	0.29
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	11	0.29
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	11	0.29
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	12	0.29
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	12	0.29
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	13	0.29
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	13	0.29
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	5	0.29
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	13	0.29
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	2	0.29
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	2	0.29
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	5	0.29
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	5	0.29
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	6	0.29
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	6	0.29
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	8	0.29
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	8	0.29
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	9	0.29
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	11	0.29
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	14	0.29
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	1	0.29
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	1	0.29
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	2	0.29
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	2	0.29
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	14	0.29
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	14	0.29
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	5	0.29
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	5	0.29
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	10	0.29
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	10	0.29
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	9	0.29
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	9	0.29
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	7	0.29
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	7	0.29
(1,133)	1:14:A:GLN:HG2	1:14:A:GLN:H	9	0.29
(1,133)	1:14:A:GLN:HG3	1:14:A:GLN:H	9	0.29
(1,133)	1:14:A:GLN:HG2	1:14:A:GLN:H	14	0.29
(1,133)	1:14:A:GLN:HG3	1:14:A:GLN:H	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	12	0.29
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	12	0.29
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	13	0.29
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	13	0.29
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	12	0.29
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	1	0.29
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	12	0.29
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	11	0.29
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE1	5	0.29
(1,24)	2:11:B:LEU:H	1:69:A:TYR:HE2	5	0.29
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	1	0.29
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	1	0.29
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	2	0.28
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	15	0.28
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	11	0.28
(1,1915)	1:78:A:LYS:HE2	1:78:A:LYS:HB3	5	0.28
(1,1915)	1:78:A:LYS:HE3	1:78:A:LYS:HB3	5	0.28
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE2	8	0.28
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE3	8	0.28
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	10	0.28
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	10	0.28
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	10	0.28
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	10	0.28
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	10	0.28
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	10	0.28
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	10	0.28
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	10	0.28
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	10	0.28
(1,1753)	1:61:A:LYS:HE2	1:61:A:LYS:HB2	5	0.28
(1,1753)	1:61:A:LYS:HE3	1:61:A:LYS:HB2	5	0.28
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	4	0.28
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	4	0.28
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	4	0.28
(1,1697)	1:53:A:THR:HG21	1:61:A:LYS:HG3	6	0.28
(1,1697)	1:53:A:THR:HG22	1:61:A:LYS:HG3	6	0.28
(1,1697)	1:53:A:THR:HG23	1:61:A:LYS:HG3	6	0.28
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	13	0.28
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	13	0.28
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	14	0.28
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	11	0.28
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	11	0.28
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	13	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	1	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	1	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	1	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	4	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	4	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	4	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	8	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	8	0.28
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	8	0.28
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD11	15	0.28
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD12	15	0.28
(1,1516)	1:42:A:VAL:HG21	1:59:A:ILE:HD13	15	0.28
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD11	15	0.28
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD12	15	0.28
(1,1516)	1:42:A:VAL:HG22	1:59:A:ILE:HD13	15	0.28
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD11	15	0.28
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD12	15	0.28
(1,1516)	1:42:A:VAL:HG23	1:59:A:ILE:HD13	15	0.28
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	4	0.28
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	4	0.28
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	9	0.28
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	9	0.28
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	15	0.28
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	15	0.28
(1,1464)	1:40:A:LYS:HG2	1:40:A:LYS:HE3	9	0.28
(1,1464)	1:40:A:LYS:HG3	1:40:A:LYS:HE3	9	0.28
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	7	0.28
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	7	0.28
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	7	0.28
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	11	0.28
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	11	0.28
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	11	0.28
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	3	0.28
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	6	0.28
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	6	0.28
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	10	0.28
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	10	0.28
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	13	0.28
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	13	0.28
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	3	0.28
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	14	0.28
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	15	0.28
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	7	0.28
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	7	0.28
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	7	0.28
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	10	0.28
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	1	0.28
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	5	0.28
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	5	0.28
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	5	0.28
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	2	0.28
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	2	0.28
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	2	0.28
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	14	0.28
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	14	0.28
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	14	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	1	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	1	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	1	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	1	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	1	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	1	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	1	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	1	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	1	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	2	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	2	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	2	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	2	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	2	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	2	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	2	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	2	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	2	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	15	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	15	0.28
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	15	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	15	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	15	0.28
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	15	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	15	0.28
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	15	0.28
(1,1161)	1:20:A:LEU:HD21	1:20:A:LEU:HB3	4	0.28
(1,1161)	1:20:A:LEU:HD22	1:20:A:LEU:HB3	4	0.28
(1,1161)	1:20:A:LEU:HD23	1:20:A:LEU:HB3	4	0.28
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	7	0.28
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	7	0.28
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	7	0.28
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	1	0.28
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	1	0.28
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	1	0.28
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	1	0.28
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	1	0.28
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	1	0.28
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	1	0.28
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	1	0.28
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	1	0.28
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	13	0.28
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	13	0.28
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	13	0.28
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	15	0.28
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	15	0.28
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	15	0.28
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	14	0.28
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD11	7	0.28
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD12	7	0.28
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD13	7	0.28
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	12	0.28
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	12	0.28
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	15	0.28
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	15	0.28
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	13	0.28
(1,942)	2:22:B:GLU:HA	2:23:B:ASP:H	13	0.28
(1,796)	2:3:B:SER:HB2	2:4:B:GLN:H	7	0.28
(1,796)	2:3:B:SER:HB3	2:4:B:GLN:H	7	0.28
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	8	0.28
(1,700)	1:62:A:GLN:HB3	1:62:A:GLN:HE21	15	0.28
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	1	0.28
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	1	0.28
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	4	0.28
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	4	0.28
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	12	0.28
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	1	0.28
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	4	0.28
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	5	0.28
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	5	0.28
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	5	0.28
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	9	0.28
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	9	0.28
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	13	0.28
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	13	0.28
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	4	0.28
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	4	0.28
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	7	0.28
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	7	0.28
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	9	0.28
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	9	0.28
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	11	0.28
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	11	0.28
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	13	0.28
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	13	0.28
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	5	0.28
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	10	0.28
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	11	0.28
(1,571)	1:51:A:ARG:HG2	1:51:A:ARG:H	8	0.28
(1,571)	1:51:A:ARG:HG3	1:51:A:ARG:H	8	0.28
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	13	0.28
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	13	0.28
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	13	0.28
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	13	0.28
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	10	0.28
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	10	0.28
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	3	0.28
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	3	0.28
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	3	0.28
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	6	0.28
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	6	0.28
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	9	0.28
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	9	0.28
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	14	0.28
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	14	0.28
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	1	0.28
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	1	0.28
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	3	0.28
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	4	0.28
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	4	0.28
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	6	0.28
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	6	0.28
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	8	0.28
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	8	0.28
(1,515)	1:44:A:GLN:HB2	1:44:A:GLN:H	14	0.28
(1,515)	1:44:A:GLN:HB3	1:44:A:GLN:H	14	0.28
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	2	0.28
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	3	0.28
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	12	0.28
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	12	0.28
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	15	0.28
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	15	0.28
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	12	0.28
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	3	0.28
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	3	0.28
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	4	0.28
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	4	0.28
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	5	0.28
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	5	0.28
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	7	0.28
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	7	0.28
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	11	0.28
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	11	0.28
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	12	0.28
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	12	0.28
(1,143)	1:15:A:ARG:HG2	1:15:A:ARG:H	15	0.28
(1,143)	1:15:A:ARG:HG3	1:15:A:ARG:H	15	0.28
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	2	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	2	0.28
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	6	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	6	0.28
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	8	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	8	0.28
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	12	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	12	0.28
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	13	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	13	0.28
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	14	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	15	0.28
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	15	0.28
(1,101)	1:11:A:LEU:HD11	1:11:A:LEU:H	3	0.28
(1,101)	1:11:A:LEU:HD12	1:11:A:LEU:H	3	0.28
(1,101)	1:11:A:LEU:HD13	1:11:A:LEU:H	3	0.28
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	2	0.28
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	2	0.28
(1,64)	1:5:A:PRO:HA	1:9:A:ARG:H	12	0.28
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	8	0.28
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	14	0.28
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	8	0.28
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	12	0.28
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	2	0.28
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	4	0.28
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	4	0.28
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	6	0.27
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	11	0.27
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	13	0.27
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	13	0.27
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	9	0.27
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD11	11	0.27
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD12	11	0.27
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD13	11	0.27
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	4	0.27
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	2	0.27
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	2	0.27
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	5	0.27
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	5	0.27
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	11	0.27
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	11	0.27
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	13	0.27
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	13	0.27
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	13	0.27
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	13	0.27
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	13	0.27
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	13	0.27
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	13	0.27
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	13	0.27
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	13	0.27
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG11	12	0.27
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG12	12	0.27
(1,1840)	1:67:A:ALA:HB1	1:81:A:VAL:HG13	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG11	12	0.27
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG12	12	0.27
(1,1840)	1:67:A:ALA:HB2	1:81:A:VAL:HG13	12	0.27
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG11	12	0.27
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG12	12	0.27
(1,1840)	1:67:A:ALA:HB3	1:81:A:VAL:HG13	12	0.27
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE1	8	0.27
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE2	8	0.27
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE1	8	0.27
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE2	8	0.27
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE1	8	0.27
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE2	8	0.27
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	11	0.27
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	3	0.27
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	3	0.27
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	3	0.27
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	8	0.27
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	8	0.27
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	8	0.27
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	6	0.27
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	6	0.27
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	6	0.27
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	9	0.27
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	9	0.27
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	9	0.27
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	1	0.27
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	14	0.27
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	13	0.27
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	13	0.27
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	13	0.27
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	15	0.27
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	15	0.27
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	15	0.27
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	15	0.27
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	6	0.27
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	6	0.27
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	6	0.27
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	12	0.27
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	12	0.27
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	12	0.27
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	12	0.27
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1464)	1:40:A:LYS:HG2	1:40:A:LYS:HE3	3	0.27
(1,1464)	1:40:A:LYS:HG3	1:40:A:LYS:HE3	3	0.27
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	11	0.27
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	11	0.27
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	4	0.27
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	4	0.27
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	4	0.27
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	5	0.27
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	5	0.27
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	5	0.27
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	7	0.27
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	12	0.27
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	13	0.27
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	15	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	5	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	5	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	5	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	10	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	10	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	10	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	12	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	12	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	12	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	14	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	14	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	14	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	15	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	15	0.27
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	15	0.27
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	14	0.27
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	14	0.27
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	2	0.27
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	8	0.27
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	10	0.27
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	13	0.27
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	13	0.27
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	13	0.27
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	9	0.27
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	2	0.27
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	2	0.27
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	2	0.27
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	12	0.27
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	12	0.27
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	12	0.27
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	12	0.27
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	12	0.27
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	12	0.27
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	12	0.27
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	12	0.27
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	3	0.27
(1,1165)	1:20:A:LEU:HA	1:22:A:HIS:HB3	9	0.27
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	9	0.27
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	9	0.27
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	9	0.27
(1,1129)	1:17:A:ILE:HG13	1:66:A:LEU:HD21	6	0.27
(1,1129)	1:17:A:ILE:HG13	1:66:A:LEU:HD22	6	0.27
(1,1129)	1:17:A:ILE:HG13	1:66:A:LEU:HD23	6	0.27
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	5	0.27
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	5	0.27
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	5	0.27
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	9	0.27
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	9	0.27
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	9	0.27
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	7	0.27
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	7	0.27
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	7	0.27
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	7	0.27
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	7	0.27
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	7	0.27
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	7	0.27
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	7	0.27
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	7	0.27
(1,1097)	1:16:A:ALA:HB1	1:17:A:ILE:HG12	11	0.27
(1,1097)	1:16:A:ALA:HB2	1:17:A:ILE:HG12	11	0.27
(1,1097)	1:16:A:ALA:HB3	1:17:A:ILE:HG12	11	0.27
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	5	0.27
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	5	0.27
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	5	0.27
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	12	0.27
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	12	0.27
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	12	0.27
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB2	9	0.27
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB3	9	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	2:11:B:LEU:HD11	2:12:B:SER:H	1	0.27
(1,851)	2:11:B:LEU:HD12	2:12:B:SER:H	1	0.27
(1,851)	2:11:B:LEU:HD13	2:12:B:SER:H	1	0.27
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	8	0.27
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	8	0.27
(1,830)	2:9:B:LEU:HD21	2:9:B:LEU:H	6	0.27
(1,830)	2:9:B:LEU:HD22	2:9:B:LEU:H	6	0.27
(1,830)	2:9:B:LEU:HD23	2:9:B:LEU:H	6	0.27
(1,787)	1:87:A:ILE:HG12	1:87:A:ILE:H	9	0.27
(1,787)	1:87:A:ILE:HG13	1:87:A:ILE:H	9	0.27
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	5	0.27
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	14	0.27
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	14	0.27
(1,649)	1:59:A:ILE:HG21	1:59:A:ILE:H	10	0.27
(1,649)	1:59:A:ILE:HG22	1:59:A:ILE:H	10	0.27
(1,649)	1:59:A:ILE:HG23	1:59:A:ILE:H	10	0.27
(1,647)	1:59:A:ILE:HB	1:59:A:ILE:H	7	0.27
(1,643)	1:58:A:PRO:HA	1:61:A:LYS:H	10	0.27
(1,628)	1:55:A:GLY:H	1:57:A:CYS:H	1	0.27
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	3	0.27
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	15	0.27
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	6	0.27
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	6	0.27
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	1	0.27
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	1	0.27
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	8	0.27
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	8	0.27
(1,616)	1:54:A:ASN:HB2	1:54:A:ASN:HD21	12	0.27
(1,616)	1:54:A:ASN:HB3	1:54:A:ASN:HD21	12	0.27
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	2	0.27
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	2	0.27
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	5	0.27
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	5	0.27
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	11	0.27
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	11	0.27
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	12	0.27
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	12	0.27
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	1	0.27
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	1	0.27
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	10	0.27
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	10	0.27
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	5	0.27
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	6	0.27
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	6	0.27
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	14	0.27
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	4	0.27
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	4	0.27
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	10	0.27
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	10	0.27
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	12	0.27
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	12	0.27
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	15	0.27
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	15	0.27
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	6	0.27
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	1	0.27
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	7	0.27
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	10	0.27
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	13	0.27
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	13	0.27
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	1	0.27
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	1	0.27
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	3	0.27
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	3	0.27
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	14	0.27
(1,89)	1:10:A:ARG:HG2	1:10:A:ARG:H	9	0.27
(1,89)	1:10:A:ARG:HG3	1:10:A:ARG:H	9	0.27
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	8	0.27
(1,79)	1:8:A:SER:HB2	1:8:A:SER:H	6	0.27
(1,79)	1:8:A:SER:HB3	1:8:A:SER:H	6	0.27
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	2	0.27
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	5	0.27
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	6	0.27
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	10	0.27
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	3	0.27
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	3	0.27
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	3	0.26
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	8	0.26
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	7	0.26
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	12	0.26
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD11	6	0.26
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD12	6	0.26
(1,1980)	2:11:B:LEU:HA	2:11:B:LEU:HD13	6	0.26
(1,1967)	1:90:A:LYS:HE2	1:90:A:LYS:HA	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1967)	1:90:A:LYS:HE3	1:90:A:LYS:HA	4	0.26
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	1	0.26
(1,1911)	1:78:A:LYS:HA	1:78:A:LYS:HD2	10	0.26
(1,1911)	1:78:A:LYS:HA	1:78:A:LYS:HD3	10	0.26
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	3	0.26
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE2	15	0.26
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE3	15	0.26
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	6	0.26
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	9	0.26
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB1	6	0.26
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB2	6	0.26
(1,1796)	1:63:A:LEU:HD11	1:67:A:ALA:HB3	6	0.26
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB1	6	0.26
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB2	6	0.26
(1,1796)	1:63:A:LEU:HD12	1:67:A:ALA:HB3	6	0.26
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB1	6	0.26
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB2	6	0.26
(1,1796)	1:63:A:LEU:HD13	1:67:A:ALA:HB3	6	0.26
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	9	0.26
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	9	0.26
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	9	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	8	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	8	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	8	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	11	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	11	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	11	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	14	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	14	0.26
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	14	0.26
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD11	2	0.26
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD12	2	0.26
(1,1700)	1:53:A:THR:HG21	1:64:A:ILE:HD13	2	0.26
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD11	2	0.26
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD12	2	0.26
(1,1700)	1:53:A:THR:HG22	1:64:A:ILE:HD13	2	0.26
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD11	2	0.26
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD12	2	0.26
(1,1700)	1:53:A:THR:HG23	1:64:A:ILE:HD13	2	0.26
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	10	0.26
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	10	0.26
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD2	14	0.26
(1,1649)	1:51:A:ARG:HA	1:51:A:ARG:HD3	14	0.26
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	6	0.26
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	6	0.26
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	6	0.26
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	6	0.26
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	6	0.26
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	6	0.26
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	6	0.26
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	13	0.26
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	13	0.26
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	13	0.26
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	13	0.26
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	13	0.26
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	13	0.26
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	15	0.26
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	15	0.26
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	15	0.26
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	15	0.26
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	15	0.26
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	15	0.26
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	15	0.26
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	15	0.26
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	15	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	2	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	2	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	8	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	8	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	11	0.26
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	11	0.26
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	2	0.26
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	2	0.26
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	2	0.26
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	13	0.26
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	13	0.26
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	13	0.26
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	15	0.26
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	15	0.26
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	15	0.26
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	7	0.26
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	1	0.26
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	5	0.26
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	7	0.26
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	7	0.26
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	7	0.26
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	7	0.26
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	2	0.26
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	2	0.26
(1,1301)	1:28:A:ASN:HB2	1:30:A:ASN:HB2	6	0.26
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	5	0.26
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	5	0.26
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	5	0.26
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	2	0.26
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	2	0.26
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	2	0.26
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	12	0.26
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	12	0.26
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	12	0.26
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	4	0.26
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	8	0.26
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	14	0.26
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	4	0.26
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	4	0.26
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	4	0.26
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG21	11	0.26
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG22	11	0.26
(1,1222)	1:21:A:VAL:HG21	1:81:A:VAL:HG23	11	0.26
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG21	11	0.26
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG22	11	0.26
(1,1222)	1:21:A:VAL:HG22	1:81:A:VAL:HG23	11	0.26
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG21	11	0.26
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG22	11	0.26
(1,1222)	1:21:A:VAL:HG23	1:81:A:VAL:HG23	11	0.26
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	3	0.26
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	3	0.26
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	3	0.26
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	3	0.26
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	3	0.26
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	3	0.26
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	3	0.26
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	3	0.26
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	3	0.26
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD11	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD12	11	0.26
(1,1185)	1:20:A:LEU:HD21	1:63:A:LEU:HD13	11	0.26
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD11	11	0.26
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD12	11	0.26
(1,1185)	1:20:A:LEU:HD22	1:63:A:LEU:HD13	11	0.26
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD11	11	0.26
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD12	11	0.26
(1,1185)	1:20:A:LEU:HD23	1:63:A:LEU:HD13	11	0.26
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	7	0.26
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	7	0.26
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	7	0.26
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	8	0.26
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	8	0.26
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	8	0.26
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	3	0.26
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	3	0.26
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	3	0.26
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	3	0.26
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	3	0.26
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	3	0.26
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	3	0.26
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	3	0.26
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	3	0.26
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	5	0.26
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	5	0.26
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	5	0.26
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	5	0.26
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	5	0.26
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	5	0.26
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	5	0.26
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	5	0.26
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	5	0.26
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG21	11	0.26
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG22	11	0.26
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG23	11	0.26
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	11	0.26
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	11	0.26
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	11	0.26
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD11	10	0.26
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD12	10	0.26
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD13	10	0.26
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD11	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD12	10	0.26
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD13	10	0.26
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	6	0.26
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	6	0.26
(1,1017)	1:9:A:ARG:HA	1:9:A:ARG:HG2	5	0.26
(1,1017)	1:9:A:ARG:HA	1:9:A:ARG:HG3	5	0.26
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	3	0.26
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	3	0.26
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	10	0.26
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	10	0.26
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	12	0.26
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	5	0.26
(1,868)	2:15:B:ASP:H	2:16:B:ILE:H	10	0.26
(1,851)	2:11:B:LEU:HD11	2:12:B:SER:H	14	0.26
(1,851)	2:11:B:LEU:HD12	2:12:B:SER:H	14	0.26
(1,851)	2:11:B:LEU:HD13	2:12:B:SER:H	14	0.26
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	7	0.26
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	7	0.26
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	11	0.26
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	11	0.26
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	3	0.26
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	5	0.26
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	3	0.26
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	5	0.26
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	4	0.26
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	4	0.26
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	2	0.26
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	2	0.26
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	8	0.26
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	8	0.26
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	4	0.26
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	4	0.26
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	7	0.26
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	7	0.26
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	6	0.26
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	1	0.26
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	1	0.26
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	2	0.26
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	2	0.26
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	3	0.26
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	3	0.26
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	8	0.26
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	11	0.26
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	11	0.26
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	13	0.26
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	13	0.26
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	1	0.26
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	9	0.26
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	10	0.26
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	5	0.26
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	5	0.26
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	12	0.26
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	13	0.26
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	6	0.26
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	3	0.26
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	3	0.26
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	3	0.26
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	9	0.26
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	4	0.26
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	4	0.26
(1,65)	1:6:A:GLY:H	1:7:A:ASP:H	9	0.26
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	3	0.26
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	13	0.26
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	8	0.26
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	9	0.26
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	12	0.26
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	9	0.25
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	5	0.25
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	10	0.25
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	4	0.25
(1,1967)	1:90:A:LYS:HE2	1:90:A:LYS:HA	1	0.25
(1,1967)	1:90:A:LYS:HE3	1:90:A:LYS:HA	1	0.25
(1,1953)	1:85:A:LEU:HD11	1:85:A:LEU:HB3	1	0.25
(1,1953)	1:85:A:LEU:HD12	1:85:A:LEU:HB3	1	0.25
(1,1953)	1:85:A:LEU:HD13	1:85:A:LEU:HB3	1	0.25
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	7	0.25
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	10	0.25
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	10	0.25
(1,1855)	1:69:A:TYR:HB3	1:72:A:LYS:HB2	10	0.25
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	4	0.25
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	5	0.25
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	12	0.25
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	7	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	7	0.25
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	7	0.25
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	13	0.25
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	13	0.25
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	13	0.25
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	5	0.25
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	5	0.25
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	2	0.25
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	5	0.25
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	9	0.25
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	2	0.25
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	2	0.25
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	2	0.25
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	2	0.25
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	2	0.25
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	2	0.25
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	2	0.25
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	2	0.25
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	2	0.25
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG21	15	0.25
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG22	15	0.25
(1,1496)	1:42:A:VAL:HA	1:42:A:VAL:HG23	15	0.25
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	15	0.25
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	1	0.25
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	1	0.25
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD2	11	0.25
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD3	11	0.25
(1,1464)	1:40:A:LYS:HG2	1:40:A:LYS:HE3	11	0.25
(1,1464)	1:40:A:LYS:HG3	1:40:A:LYS:HE3	11	0.25
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	3	0.25
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	3	0.25
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	3	0.25
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	10	0.25
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	10	0.25
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	10	0.25
(1,1396)	1:37:A:GLN:HA	1:38:A:LYS:HB3	9	0.25
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	10	0.25
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	4	0.25
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	4	0.25
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	1	0.25
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	4	0.25
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	8	0.25
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	8	0.25
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	8	0.25
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	13	0.25
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	13	0.25
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	13	0.25
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	1	0.25
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	8	0.25
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	8	0.25
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	8	0.25
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG21	3	0.25
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG22	3	0.25
(1,1218)	1:21:A:VAL:HA	1:81:A:VAL:HG23	3	0.25
(1,1214)	1:21:A:VAL:HG21	1:74:A:CYS:HB2	10	0.25
(1,1214)	1:21:A:VAL:HG22	1:74:A:CYS:HB2	10	0.25
(1,1214)	1:21:A:VAL:HG23	1:74:A:CYS:HB2	10	0.25
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	5	0.25
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	5	0.25
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	5	0.25
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	10	0.25
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	10	0.25
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	10	0.25
(1,1188)	1:20:A:LEU:HD21	1:66:A:LEU:HG	11	0.25
(1,1188)	1:20:A:LEU:HD22	1:66:A:LEU:HG	11	0.25
(1,1188)	1:20:A:LEU:HD23	1:66:A:LEU:HG	11	0.25
(1,1072)	1:13:A:ILE:HG21	1:17:A:ILE:HG13	14	0.25
(1,1072)	1:13:A:ILE:HG22	1:17:A:ILE:HG13	14	0.25
(1,1072)	1:13:A:ILE:HG23	1:17:A:ILE:HG13	14	0.25
(1,1041)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	6	0.25
(1,1041)	1:11:A:LEU:HD12	1:11:A:LEU:HB2	6	0.25
(1,1041)	1:11:A:LEU:HD13	1:11:A:LEU:HB2	6	0.25
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	1	0.25
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	1	0.25
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	1	0.25
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	4	0.25
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	4	0.25
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	4	0.25
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	1	0.25
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	5	0.25
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	3	0.25
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	3	0.25
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	3	0.25
(1,787)	1:87:A:ILE:HG12	1:87:A:ILE:H	3	0.25
(1,787)	1:87:A:ILE:HG13	1:87:A:ILE:H	3	0.25
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	13	0.25
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	4	0.25
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	7	0.25
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	10	0.25
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	1	0.25
(1,701)	1:62:A:GLN:HG2	1:62:A:GLN:HE21	9	0.25
(1,701)	1:62:A:GLN:HG3	1:62:A:GLN:HE21	9	0.25
(1,699)	1:62:A:GLN:HB2	1:62:A:GLN:HE21	12	0.25
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	15	0.25
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	15	0.25
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	1	0.25
(1,628)	1:55:A:GLY:H	1:57:A:CYS:H	8	0.25
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	2	0.25
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	12	0.25
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	13	0.25
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	2	0.25
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	3	0.25
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	10	0.25
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	4	0.25
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	4	0.25
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	15	0.25
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	15	0.25
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	1	0.25
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	5	0.25
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	5	0.25
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	9	0.25
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	12	0.25
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	7	0.25
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	13	0.25
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	15	0.25
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	4	0.25
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	7	0.25
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	14	0.25
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	15	0.25
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	8	0.25
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	13	0.25
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	1	0.25
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	4	0.25
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	7	0.25
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	5	0.25
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	10	0.25
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	2	0.25
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	10	0.25
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	10	0.25
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	10	0.25
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	6	0.25
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	6	0.25
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	6	0.25
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	4	0.25
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	4	0.25
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	7	0.25
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	7	0.25
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	9	0.25
(1,89)	1:10:A:ARG:HG2	1:10:A:ARG:H	8	0.25
(1,89)	1:10:A:ARG:HG3	1:10:A:ARG:H	8	0.25
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	4	0.25
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	7	0.25
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	11	0.25
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	15	0.25
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	5	0.25
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	4	0.25
(2,60)	1:58:A:PRO:O	1:62:A:GLN:N	4	0.24
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	3	0.24
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	3	0.24
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	3	0.24
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	3	0.24
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	3	0.24
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	3	0.24
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	5	0.24
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	5	0.24
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	5	0.24
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	5	0.24
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	5	0.24
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	5	0.24
(1,1969)	1:90:A:LYS:HE2	1:90:A:LYS:HB2	3	0.24
(1,1969)	1:90:A:LYS:HE3	1:90:A:LYS:HB2	3	0.24
(1,1969)	1:90:A:LYS:HE2	1:90:A:LYS:HB2	14	0.24
(1,1969)	1:90:A:LYS:HE3	1:90:A:LYS:HB2	14	0.24
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	5	0.24
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	13	0.24
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	9	0.24
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	13	0.24
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	14	0.24
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	8	0.24
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	8	0.24
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	2	0.24
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	2	0.24
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	2	0.24
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	2	0.24
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	2	0.24
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	2	0.24
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	2	0.24
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	2	0.24
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	2	0.24
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	3	0.24
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	13	0.24
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	1	0.24
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	1	0.24
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	1	0.24
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE2	15	0.24
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE3	15	0.24
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	8	0.24
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	6	0.24
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	6	0.24
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE2	7	0.24
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE3	7	0.24
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE2	7	0.24
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE3	7	0.24
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	7	0.24
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	11	0.24
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	4	0.24
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	4	0.24
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	5	0.24
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	5	0.24
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	3	0.24
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	3	0.24
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	12	0.24
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	12	0.24
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	12	0.24
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	14	0.24
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	14	0.24
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	2	0.24
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	2	0.24
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	4	0.24
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	8	0.24
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	14	0.24
(1,1350)	1:33:A:LEU:HB2	1:36:A:CYS:HB2	9	0.24
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	6	0.24
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	6	0.24
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	6	0.24
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	6	0.24
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	6	0.24
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	6	0.24
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	10	0.24
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	10	0.24
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	10	0.24
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	5	0.24
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	6	0.24
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	15	0.24
(1,1246)	1:23:A:ALA:HB1	1:39:A:MET:HB3	7	0.24
(1,1246)	1:23:A:ALA:HB2	1:39:A:MET:HB3	7	0.24
(1,1246)	1:23:A:ALA:HB3	1:39:A:MET:HB3	7	0.24
(1,1235)	1:23:A:ALA:HA	1:26:A:CYS:HB2	11	0.24
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	15	0.24
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	15	0.24
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	15	0.24
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	1	0.24
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	11	0.24
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	14	0.24
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	14	0.24
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	14	0.24
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	14	0.24
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	14	0.24
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	14	0.24
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	14	0.24
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	14	0.24
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	14	0.24
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	14	0.24
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	14	0.24
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	14	0.24
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	4	0.24
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	4	0.24
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	4	0.24
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	4	0.24
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	4	0.24
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	4	0.24
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	4	0.24
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	4	0.24
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	8	0.24
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	8	0.24
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	8	0.24
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	11	0.24
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	4	0.24
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	4	0.24
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	2	0.24
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	2	0.24
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	2	0.24
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	2	0.24
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	6	0.24
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	10	0.24
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	12	0.24
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	13	0.24
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	15	0.24
(1,865)	2:14:B:ASP:H	2:15:B:ASP:H	10	0.24
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	10	0.24
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	10	0.24
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	14	0.24
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	5	0.24
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	5	0.24
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	15	0.24
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	15	0.24
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	1	0.24
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	9	0.24
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	11	0.24
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	13	0.24
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	9	0.24
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	13	0.24
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	15	0.24
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	8	0.24
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	6	0.24
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	2	0.24
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	6	0.24
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	2	0.24
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	2	0.24
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	2	0.24
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	2	0.24
(1,554)	1:49:A:CYS:HA	1:50:A:LYS:H	9	0.24
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	13	0.24
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	4	0.24
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	13	0.24
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	14	0.24
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	8	0.24
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	8	0.24
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	5	0.24
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	5	0.24
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	10	0.24
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	15	0.24
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	4	0.24
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	12	0.24
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	11	0.24
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	2	0.24
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	5	0.24
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	6	0.24
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	15	0.24
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	12	0.24
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	12	0.24
(1,381)	1:33:A:LEU:HD11	1:33:A:LEU:H	9	0.24
(1,381)	1:33:A:LEU:HD12	1:33:A:LEU:H	9	0.24
(1,381)	1:33:A:LEU:HD13	1:33:A:LEU:H	9	0.24
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	12	0.24
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	13	0.24
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	7	0.24
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	2	0.24
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	8	0.24
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	10	0.24
(1,340)	1:29:A:ALA:HB1	1:30:A:ASN:HD21	15	0.24
(1,340)	1:29:A:ALA:HB2	1:30:A:ASN:HD21	15	0.24
(1,340)	1:29:A:ALA:HB3	1:30:A:ASN:HD21	15	0.24
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	3	0.24
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	4	0.24
(1,119)	1:13:A:ILE:HG12	1:13:A:ILE:H	6	0.24
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	10	0.24
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	11	0.24
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	7	0.24
(1,12)	1:62:A:GLN:HE22	2:11:B:LEU:HG	2	0.24
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	5	0.23
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	15	0.23
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	10	0.23
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	2	0.23
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	7	0.23
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	8	0.23
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	6	0.23
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	8	0.23
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	9	0.23
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	14	0.23
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	15	0.23
(1,1929)	1:81:A:VAL:HG21	1:80:A:PRO:HD2	12	0.23
(1,1929)	1:81:A:VAL:HG22	1:80:A:PRO:HD2	12	0.23
(1,1929)	1:81:A:VAL:HG23	1:80:A:PRO:HD2	12	0.23
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG21	2	0.23
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG22	2	0.23
(1,1926)	1:80:A:PRO:HG2	1:81:A:VAL:HG23	2	0.23
(1,1915)	1:78:A:LYS:HE2	1:78:A:LYS:HB3	1	0.23
(1,1915)	1:78:A:LYS:HE3	1:78:A:LYS:HB3	1	0.23
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	8	0.23
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	9	0.23
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	9	0.23
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	7	0.23
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	8	0.23
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	3	0.23
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	3	0.23
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	3	0.23
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	7	0.23
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	7	0.23
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	7	0.23
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	8	0.23
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	8	0.23
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	8	0.23
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	7	0.23
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	7	0.23
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	7	0.23
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	9	0.23
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	9	0.23
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	9	0.23
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	12	0.23
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	12	0.23
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	1	0.23
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE2	1	0.23
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE3	1	0.23
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE2	14	0.23
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE3	14	0.23
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	8	0.23
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	8	0.23
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	8	0.23
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	3	0.23
(1,1629)	1:50:A:LYS:HA	1:50:A:LYS:HE2	12	0.23
(1,1629)	1:50:A:LYS:HA	1:50:A:LYS:HE3	12	0.23
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG21	7	0.23
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG22	7	0.23
(1,1626)	1:49:A:CYS:HB2	1:59:A:ILE:HG23	7	0.23
(1,1623)	1:49:A:CYS:HB2	1:57:A:CYS:HB3	9	0.23
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	1	0.23
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	4	0.23
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	8	0.23
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	13	0.23
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	7	0.23
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	7	0.23
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	1	0.23
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	1	0.23
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	10	0.23
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	3	0.23
(1,1413)	1:38:A:LYS:HE2	1:38:A:LYS:HB2	4	0.23
(1,1413)	1:38:A:LYS:HE3	1:38:A:LYS:HB2	4	0.23
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	4	0.23
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	10	0.23
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	15	0.23
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	15	0.23
(1,1352)	1:33:A:LEU:HD11	1:36:A:CYS:HB3	3	0.23
(1,1352)	1:33:A:LEU:HD12	1:36:A:CYS:HB3	3	0.23
(1,1352)	1:33:A:LEU:HD13	1:36:A:CYS:HB3	3	0.23
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	6	0.23
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	12	0.23
(1,1350)	1:33:A:LEU:HB2	1:36:A:CYS:HB2	11	0.23
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	10	0.23
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	10	0.23
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	13	0.23
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	13	0.23
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	13	0.23
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	8	0.23
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	8	0.23
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	15	0.23
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	15	0.23
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	15	0.23
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	5	0.23
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	5	0.23
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	5	0.23
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	14	0.23
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	14	0.23
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	14	0.23
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	1	0.23
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	1	0.23
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	1	0.23
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	5	0.23
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	13	0.23
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	10	0.23
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	10	0.23
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	10	0.23
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	11	0.23
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	11	0.23
(1,1041)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	14	0.23
(1,1041)	1:11:A:LEU:HD12	1:11:A:LEU:HB2	14	0.23
(1,1041)	1:11:A:LEU:HD13	1:11:A:LEU:HB2	14	0.23
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	5	0.23
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	5	0.23
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	5	0.23
(1,1038)	1:11:A:LEU:HD21	1:11:A:LEU:HB3	7	0.23
(1,1038)	1:11:A:LEU:HD22	1:11:A:LEU:HB3	7	0.23
(1,1038)	1:11:A:LEU:HD23	1:11:A:LEU:HB3	7	0.23
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD11	7	0.23
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD12	7	0.23
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD13	7	0.23
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD11	7	0.23
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD12	7	0.23
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD13	7	0.23
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD11	11	0.23
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD12	11	0.23
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD13	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD11	11	0.23
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD12	11	0.23
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD13	11	0.23
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	5	0.23
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	7	0.23
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	7	0.23
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	3	0.23
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	7	0.23
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	11	0.23
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	11	0.23
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	8	0.23
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	8	0.23
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	9	0.23
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	9	0.23
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	11	0.23
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	11	0.23
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	14	0.23
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	14	0.23
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	2	0.23
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	3	0.23
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	12	0.23
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	12	0.23
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	12	0.23
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	15	0.23
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	3	0.23
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	4	0.23
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	7	0.23
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	1	0.23
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	3	0.23
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	9	0.23
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	12	0.23
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	14	0.23
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	7	0.23
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	7	0.23
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	7	0.23
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	3	0.23
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	5	0.23
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	13	0.23
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	15	0.23
(1,701)	1:62:A:GLN:HG2	1:62:A:GLN:HE21	14	0.23
(1,701)	1:62:A:GLN:HG3	1:62:A:GLN:HE21	14	0.23
(1,699)	1:62:A:GLN:HB2	1:62:A:GLN:HE21	5	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	6	0.23
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	6	0.23
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	10	0.23
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	14	0.23
(1,577)	1:51:A:ARG:HA	1:54:A:ASN:HD21	14	0.23
(1,567)	1:50:A:LYS:H	1:51:A:ARG:H	1	0.23
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	3	0.23
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	4	0.23
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	7	0.23
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	11	0.23
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	15	0.23
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	5	0.23
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	6	0.23
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	14	0.23
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	14	0.23
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	5	0.23
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	9	0.23
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	2	0.23
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	3	0.23
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	6	0.23
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	8	0.23
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	9	0.23
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	14	0.23
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	2	0.23
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	5	0.23
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	12	0.23
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	13	0.23
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	3	0.23
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	7	0.23
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	10	0.23
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	11	0.23
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	12	0.23
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	14	0.23
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	9	0.23
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	9	0.23
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	9	0.23
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	11	0.23
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	3	0.23
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	4	0.23
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	5	0.23
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	6	0.23
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	2	0.23
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	4	0.23
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	5	0.23
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	8	0.23
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	12	0.23
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	3	0.23
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	14	0.23
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	15	0.23
(1,362)	1:31:A:CYS:HB3	1:36:A:CYS:H	13	0.23
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	6	0.23
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	6	0.23
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	6	0.23
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	8	0.23
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	8	0.23
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	8	0.23
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	5	0.23
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	13	0.23
(1,185)	1:18:A:GLN:HG2	1:18:A:GLN:HE21	8	0.23
(1,185)	1:18:A:GLN:HG3	1:18:A:GLN:HE21	8	0.23
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	7	0.23
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	13	0.23
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	7	0.23
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	12	0.23
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	2	0.23
(1,122)	1:13:A:ILE:HG12	1:14:A:GLN:H	5	0.23
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	1	0.23
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	2	0.23
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	6	0.23
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	9	0.22
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	14	0.22
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	2	0.22
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	2	0.22
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	2	0.22
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	2	0.22
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	2	0.22
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	2	0.22
(1,1969)	1:90:A:LYS:HE2	1:90:A:LYS:HB2	6	0.22
(1,1969)	1:90:A:LYS:HE3	1:90:A:LYS:HB2	6	0.22
(1,1969)	1:90:A:LYS:HE2	1:90:A:LYS:HB2	10	0.22
(1,1969)	1:90:A:LYS:HE3	1:90:A:LYS:HB2	10	0.22
(1,1968)	1:90:A:LYS:HE2	1:90:A:LYS:HB3	5	0.22
(1,1968)	1:90:A:LYS:HE3	1:90:A:LYS:HB3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	12	0.22
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	12	0.22
(1,1868)	1:71:A:ALA:HB1	1:88:A:LYS:HE2	3	0.22
(1,1868)	1:71:A:ALA:HB1	1:88:A:LYS:HE3	3	0.22
(1,1868)	1:71:A:ALA:HB2	1:88:A:LYS:HE2	3	0.22
(1,1868)	1:71:A:ALA:HB2	1:88:A:LYS:HE3	3	0.22
(1,1868)	1:71:A:ALA:HB3	1:88:A:LYS:HE2	3	0.22
(1,1868)	1:71:A:ALA:HB3	1:88:A:LYS:HE3	3	0.22
(1,1855)	1:69:A:TYR:HB3	1:72:A:LYS:HB2	15	0.22
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	10	0.22
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	10	0.22
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	10	0.22
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	14	0.22
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	14	0.22
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	14	0.22
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	6	0.22
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	1	0.22
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	1	0.22
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	1	0.22
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	2	0.22
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	2	0.22
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	2	0.22
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	14	0.22
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	2	0.22
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	12	0.22
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	12	0.22
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	12	0.22
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	12	0.22
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	12	0.22
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	12	0.22
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	11	0.22
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	11	0.22
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	11	0.22
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	11	0.22
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	11	0.22
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	11	0.22
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	12	0.22
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	12	0.22
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	12	0.22
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	12	0.22
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	12	0.22
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	7	0.22
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	9	0.22
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	6	0.22
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	6	0.22
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	2	0.22
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	8	0.22
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	1	0.22
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	1	0.22
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	1	0.22
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	9	0.22
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	5	0.22
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	8	0.22
(1,1352)	1:33:A:LEU:HD11	1:36:A:CYS:HB3	1	0.22
(1,1352)	1:33:A:LEU:HD12	1:36:A:CYS:HB3	1	0.22
(1,1352)	1:33:A:LEU:HD13	1:36:A:CYS:HB3	1	0.22
(1,1351)	1:33:A:LEU:HG	1:36:A:CYS:HB2	13	0.22
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	9	0.22
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	3	0.22
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	3	0.22
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	3	0.22
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	12	0.22
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	12	0.22
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	12	0.22
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	14	0.22
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	14	0.22
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	14	0.22
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	11	0.22
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	14	0.22
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	4	0.22
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	4	0.22
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	4	0.22
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	5	0.22
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	5	0.22
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	5	0.22
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	6	0.22
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	6	0.22
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	6	0.22
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	14	0.22
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	14	0.22
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	14	0.22
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	7	0.22
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1106)	1:17:A:ILE:HG21	1:17:A:ILE:HA	1	0.22
(1,1106)	1:17:A:ILE:HG22	1:17:A:ILE:HA	1	0.22
(1,1106)	1:17:A:ILE:HG23	1:17:A:ILE:HA	1	0.22
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	1	0.22
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	1	0.22
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD11	6	0.22
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD12	6	0.22
(1,1013)	1:8:A:SER:HA	1:11:A:LEU:HD13	6	0.22
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	10	0.22
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	14	0.22
(1,981)	1:4:A:SER:HA	1:7:A:ASP:HB2	14	0.22
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	4	0.22
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	8	0.22
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	15	0.22
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB2	14	0.22
(1,968)	1:3:A:GLN:HA	1:7:A:ASP:HB3	14	0.22
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	14	0.22
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	7	0.22
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	7	0.22
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	5	0.22
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	5	0.22
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	4	0.22
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	5	0.22
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	6	0.22
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	6	0.22
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	6	0.22
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	1	0.22
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	10	0.22
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	15	0.22
(1,654)	1:59:A:ILE:H	1:60:A:CYS:H	6	0.22
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	14	0.22
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	4	0.22
(1,629)	1:56:A:GLY:H	1:57:A:CYS:H	1	0.22
(1,629)	1:56:A:GLY:H	1:57:A:CYS:H	3	0.22
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	4	0.22
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	12	0.22
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	1	0.22
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	9	0.22
(1,570)	1:51:A:ARG:HB2	1:51:A:ARG:H	1	0.22
(1,570)	1:51:A:ARG:HB3	1:51:A:ARG:H	1	0.22
(1,567)	1:50:A:LYS:H	1:51:A:ARG:H	8	0.22
(1,567)	1:50:A:LYS:H	1:51:A:ARG:H	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:49:A:CYS:H	1:50:A:LYS:HD2	11	0.22
(1,555)	1:49:A:CYS:H	1:50:A:LYS:HD3	11	0.22
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	2	0.22
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	5	0.22
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	10	0.22
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	12	0.22
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	14	0.22
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	7	0.22
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	12	0.22
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	8	0.22
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	1	0.22
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	10	0.22
(1,458)	1:39:A:MET:HB2	1:39:A:MET:H	8	0.22
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	4	0.22
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	11	0.22
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	10	0.22
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	14	0.22
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	6	0.22
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	10	0.22
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	14	0.22
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	15	0.22
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	5	0.22
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	9	0.22
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	9	0.22
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	9	0.22
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	11	0.22
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	11	0.22
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	11	0.22
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	7	0.22
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	10	0.22
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	10	0.22
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	6	0.22
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	2	0.22
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	4	0.22
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	4	0.22
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	11	0.22
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	1	0.22
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	12	0.22
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	13	0.22
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	9	0.22
(1,29)	2:16:B:ILE:H	1:17:A:ILE:H	11	0.22
(1,12)	1:62:A:GLN:HE22	2:11:B:LEU:HG	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	3	0.21
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	5	0.21
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	6	0.21
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	6	0.21
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	6	0.21
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	6	0.21
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	6	0.21
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	6	0.21
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	14	0.21
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	14	0.21
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	14	0.21
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	14	0.21
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	14	0.21
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	14	0.21
(1,1969)	1:90:A:LYS:HE2	1:90:A:LYS:HB2	8	0.21
(1,1969)	1:90:A:LYS:HE3	1:90:A:LYS:HB2	8	0.21
(1,1953)	1:85:A:LEU:HD11	1:85:A:LEU:HB3	5	0.21
(1,1953)	1:85:A:LEU:HD12	1:85:A:LEU:HB3	5	0.21
(1,1953)	1:85:A:LEU:HD13	1:85:A:LEU:HB3	5	0.21
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	3	0.21
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	4	0.21
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	1	0.21
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	1	0.21
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	1	0.21
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	1	0.21
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	1	0.21
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	1	0.21
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	1	0.21
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	1	0.21
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	1	0.21
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	2	0.21
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	2	0.21
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	2	0.21
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	10	0.21
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	15	0.21
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	6	0.21
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	6	0.21
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	6	0.21
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	5	0.21
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	5	0.21
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	5	0.21
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1681)	1:52:A:LYS:HD3	1:60:A:CYS:HB2	7	0.21
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	4	0.21
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	4	0.21
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	6	0.21
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	3	0.21
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	5	0.21
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	9	0.21
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE2	3	0.21
(1,1596)	1:47:A:LYS:HG2	1:47:A:LYS:HE3	3	0.21
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE2	3	0.21
(1,1596)	1:47:A:LYS:HG3	1:47:A:LYS:HE3	3	0.21
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	7	0.21
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	7	0.21
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	10	0.21
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	10	0.21
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	10	0.21
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	10	0.21
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	10	0.21
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	10	0.21
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	1	0.21
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	10	0.21
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	11	0.21
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	10	0.21
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	10	0.21
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	10	0.21
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	10	0.21
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	10	0.21
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	10	0.21
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	10	0.21
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	10	0.21
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	10	0.21
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD2	15	0.21
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD3	15	0.21
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	12	0.21
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	12	0.21
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	14	0.21
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	8	0.21
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	8	0.21
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	8	0.21
(1,1437)	1:39:A:MET:HE1	1:39:A:MET:HA	9	0.21
(1,1437)	1:39:A:MET:HE2	1:39:A:MET:HA	9	0.21
(1,1437)	1:39:A:MET:HE3	1:39:A:MET:HA	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	11	0.21
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	3	0.21
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	3	0.21
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	3	0.21
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD2	15	0.21
(1,1326)	1:32:A:SER:HA	1:34:A:PRO:HD3	15	0.21
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	10	0.21
(1,1272)	1:24:A:ALA:HB1	1:81:A:VAL:HA	2	0.21
(1,1272)	1:24:A:ALA:HB2	1:81:A:VAL:HA	2	0.21
(1,1272)	1:24:A:ALA:HB3	1:81:A:VAL:HA	2	0.21
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	3	0.21
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	3	0.21
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	3	0.21
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	9	0.21
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	9	0.21
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	9	0.21
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	11	0.21
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	11	0.21
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	11	0.21
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	12	0.21
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	2	0.21
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	8	0.21
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	15	0.21
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	8	0.21
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	8	0.21
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	13	0.21
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	13	0.21
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	13	0.21
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	13	0.21
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	13	0.21
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	13	0.21
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	13	0.21
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	13	0.21
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	13	0.21
(1,1041)	1:11:A:LEU:HD11	1:11:A:LEU:HB2	9	0.21
(1,1041)	1:11:A:LEU:HD12	1:11:A:LEU:HB2	9	0.21
(1,1041)	1:11:A:LEU:HD13	1:11:A:LEU:HB2	9	0.21
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	8	0.21
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	4	0.21
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	8	0.21
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	8	0.21
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	11	0.21
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	11	0.21
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	11	0.21
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	15	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	4	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	4	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	4	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	4	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	8	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	8	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	8	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	8	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	15	0.21
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	15	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	15	0.21
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	15	0.21
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	9	0.21
(1,983)	1:5:A:PRO:HD2	1:5:A:PRO:HA	1	0.21
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	11	0.21
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	9	0.21
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	9	0.21
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	14	0.21
(1,787)	1:87:A:ILE:HG12	1:87:A:ILE:H	5	0.21
(1,787)	1:87:A:ILE:HG13	1:87:A:ILE:H	5	0.21
(1,764)	1:77:A:ASN:HB2	1:77:A:ASN:HD21	1	0.21
(1,764)	1:77:A:ASN:HB3	1:77:A:ASN:HD21	1	0.21
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	14	0.21
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	4	0.21
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	7	0.21
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	12	0.21
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	8	0.21
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	15	0.21
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	14	0.21
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	8	0.21
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	10	0.21
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	12	0.21
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	5	0.21
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	7	0.21
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	11	0.21
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	9	0.21
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	9	0.21
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	2	0.21
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	2	0.21
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	2	0.21
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	8	0.21
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	8	0.21
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	8	0.21
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	14	0.21
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	14	0.21
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	14	0.21
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	4	0.21
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	12	0.21
(1,699)	1:62:A:GLN:HB2	1:62:A:GLN:HE21	1	0.21
(1,665)	1:59:A:ILE:HA	1:63:A:LEU:H	9	0.21
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	15	0.21
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	3	0.21
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	9	0.21
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	13	0.21
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	5	0.21
(1,534)	1:47:A:LYS:HG2	1:47:A:LYS:H	3	0.21
(1,534)	1:47:A:LYS:HG3	1:47:A:LYS:H	3	0.21
(1,516)	1:44:A:GLN:HG2	1:44:A:GLN:H	7	0.21
(1,516)	1:44:A:GLN:HG3	1:44:A:GLN:H	7	0.21
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	14	0.21
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	5	0.21
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	1	0.21
(1,446)	1:38:A:LYS:HB2	1:39:A:MET:H	9	0.21
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	1	0.21
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	2	0.21
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	3	0.21
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	12	0.21
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	14	0.21
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	4	0.21
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	4	0.21
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	15	0.21
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	15	0.21
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	9	0.21
(1,381)	1:33:A:LEU:HD11	1:33:A:LEU:H	11	0.21
(1,381)	1:33:A:LEU:HD12	1:33:A:LEU:H	11	0.21
(1,381)	1:33:A:LEU:HD13	1:33:A:LEU:H	11	0.21
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	2	0.21
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	8	0.21
(1,378)	1:33:A:LEU:HB3	1:33:A:LEU:H	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	13	0.21
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	4	0.21
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	4	0.21
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	4	0.21
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	12	0.21
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	12	0.21
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	12	0.21
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE2	11	0.21
(1,334)	1:28:A:ASN:H	1:40:A:LYS:HE3	11	0.21
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	12	0.21
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	15	0.21
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	8	0.21
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	9	0.21
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	13	0.21
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	13	0.21
(1,132)	1:14:A:GLN:HB2	1:14:A:GLN:H	6	0.21
(1,132)	1:14:A:GLN:HB3	1:14:A:GLN:H	6	0.21
(1,89)	1:10:A:ARG:HG2	1:10:A:ARG:H	4	0.21
(1,89)	1:10:A:ARG:HG3	1:10:A:ARG:H	4	0.21
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	7	0.21
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	10	0.21
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	4	0.2
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	8	0.2
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	4	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	1	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	1	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	1	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	1	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	1	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	1	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	9	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	9	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	9	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	9	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	9	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	9	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	12	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	12	0.2
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	12	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	12	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	12	0.2
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE2	2	0.2
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE3	2	0.2
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE2	12	0.2
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE3	12	0.2
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	7	0.2
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	10	0.2
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE2	13	0.2
(1,1892)	1:75:A:GLN:HA	1:88:A:LYS:HE3	13	0.2
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	12	0.2
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	6	0.2
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	6	0.2
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	3	0.2
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	3	0.2
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	6	0.2
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	6	0.2
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	6	0.2
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	2	0.2
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	10	0.2
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	10	0.2
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	10	0.2
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	15	0.2
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	15	0.2
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	15	0.2
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	15	0.2
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	15	0.2
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	15	0.2
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	6	0.2
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD11	15	0.2
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD12	15	0.2
(1,1747)	1:60:A:CYS:HA	1:63:A:LEU:HD13	15	0.2
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD11	1	0.2
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD12	1	0.2
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD13	1	0.2
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	6	0.2
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	6	0.2
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	5	0.2
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	4	0.2
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	4	0.2
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	4	0.2
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	8	0.2
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	8	0.2
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	10	0.2
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	4	0.2
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	15	0.2
(1,1605)	1:47:A:LYS:HE2	1:82:A:PRO:HB3	11	0.2
(1,1605)	1:47:A:LYS:HE3	1:82:A:PRO:HB3	11	0.2
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	10	0.2
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	10	0.2
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	10	0.2
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	10	0.2
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD21	12	0.2
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD22	12	0.2
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD23	12	0.2
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD21	12	0.2
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD22	12	0.2
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD23	12	0.2
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD21	12	0.2
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD22	12	0.2
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD23	12	0.2
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	10	0.2
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	10	0.2
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	8	0.2
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	8	0.2
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	8	0.2
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	8	0.2
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	8	0.2
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	8	0.2
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	3	0.2
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	5	0.2
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	6	0.2
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	7	0.2
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	8	0.2
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	14	0.2
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	15	0.2
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	5	0.2
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	5	0.2
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	5	0.2
(1,1508)	1:42:A:VAL:HG11	1:59:A:ILE:HG12	15	0.2
(1,1508)	1:42:A:VAL:HG12	1:59:A:ILE:HG12	15	0.2
(1,1508)	1:42:A:VAL:HG13	1:59:A:ILE:HG12	15	0.2
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	12	0.2
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	1	0.2
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	15	0.2
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG11	2	0.2
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG12	2	0.2
(1,1434)	1:38:A:LYS:HG2	1:42:A:VAL:HG13	2	0.2
(1,1381)	1:35:A:SER:HA	1:38:A:LYS:HA	10	0.2
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	1	0.2
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	1	0.2
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	1	0.2
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	4	0.2
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	4	0.2
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	4	0.2
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	5	0.2
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	5	0.2
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	5	0.2
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	7	0.2
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	7	0.2
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	7	0.2
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	13	0.2
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	13	0.2
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	13	0.2
(1,1315)	1:30:A:ASN:HA	1:34:A:PRO:HG2	9	0.2
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	14	0.2
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB1	3	0.2
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB2	3	0.2
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB3	3	0.2
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB1	3	0.2
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB2	3	0.2
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB3	3	0.2
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB1	3	0.2
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB2	3	0.2
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB3	3	0.2
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD21	7	0.2
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD22	7	0.2
(1,1194)	1:20:A:LEU:HB2	1:66:A:LEU:HD23	7	0.2
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	4	0.2
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	4	0.2
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	4	0.2
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	3	0.2
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	4	0.2
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	12	0.2
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	13	0.2
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	8	0.2
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	8	0.2
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	1	0.2
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	1	0.2
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	1	0.2
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	15	0.2
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	10	0.2
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	10	0.2
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	10	0.2
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	7	0.2
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	9	0.2
(1,943)	2:22:B:GLU:HG2	2:23:B:ASP:H	6	0.2
(1,943)	2:22:B:GLU:HG3	2:23:B:ASP:H	6	0.2
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	10	0.2
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	3	0.2
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	3	0.2
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	1	0.2
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	8	0.2
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	7	0.2
(1,787)	1:87:A:ILE:HG12	1:87:A:ILE:H	14	0.2
(1,787)	1:87:A:ILE:HG13	1:87:A:ILE:H	14	0.2
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	6	0.2
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	13	0.2
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	2	0.2
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	14	0.2
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	15	0.2
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	4	0.2
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	7	0.2
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	7	0.2
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	11	0.2
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	6	0.2
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	10	0.2
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	4	0.2
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	14	0.2
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	5	0.2
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	2	0.2
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	8	0.2
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	13	0.2
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	14	0.2
(1,664)	1:59:A:ILE:HA	1:62:A:GLN:HE22	4	0.2
(1,562)	1:50:A:LYS:HB2	1:50:A:LYS:H	5	0.2
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	9	0.2
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	2	0.2
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	4	0.2
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	11	0.2
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	12	0.2
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	15	0.2
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	9	0.2
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	11	0.2
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	15	0.2
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	1	0.2
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	1	0.2
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	3	0.2
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	3	0.2
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	7	0.2
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	7	0.2
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	13	0.2
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	13	0.2
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	14	0.2
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	14	0.2
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	12	0.2
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	1	0.2
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	1	0.2
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	1	0.2
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	10	0.2
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	10	0.2
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	10	0.2
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	13	0.2
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	13	0.2
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	13	0.2
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	6	0.2
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	11	0.2
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	14	0.2
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	3	0.2
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	5	0.2
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	7	0.2
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	12	0.2
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	3	0.2
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	8	0.2
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	10	0.2
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	10	0.2
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	10	0.2
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:13:A:ILE:HG12	1:14:A:GLN:H	8	0.2
(1,122)	1:13:A:ILE:HG12	1:14:A:GLN:H	11	0.2
(1,108)	1:11:A:LEU:HD11	1:14:A:GLN:HE22	11	0.2
(1,108)	1:11:A:LEU:HD12	1:14:A:GLN:HE22	11	0.2
(1,108)	1:11:A:LEU:HD13	1:14:A:GLN:HE22	11	0.2
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	8	0.2
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	8	0.2
(1,58)	1:4:A:SER:HA	1:8:A:SER:H	1	0.2
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	12	0.2
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	15	0.19
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	7	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	7	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	7	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	7	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	7	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	7	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	7	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	8	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	8	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	8	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	8	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	8	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	8	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	10	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	10	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	10	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	10	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	10	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	10	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	13	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	13	0.19
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	13	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	13	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	13	0.19
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	13	0.19
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	11	0.19
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	8	0.19
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	13	0.19
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	13	0.19
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	2	0.19
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	2	0.19
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	9	0.19
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	9	0.19
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	9	0.19
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	13	0.19
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	13	0.19
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	13	0.19
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD11	7	0.19
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD12	7	0.19
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD13	7	0.19
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	5	0.19
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	5	0.19
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	5	0.19
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	13	0.19
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	13	0.19
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	13	0.19
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	14	0.19
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	14	0.19
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	14	0.19
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD11	5	0.19
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD12	5	0.19
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD13	5	0.19
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD11	5	0.19
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD12	5	0.19
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD13	5	0.19
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	13	0.19
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	15	0.19
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	8	0.19
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	11	0.19
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	13	0.19
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	2	0.19
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	2	0.19
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	2	0.19
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	1	0.19
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	3	0.19
(1,1681)	1:52:A:LYS:HD3	1:60:A:CYS:HB2	4	0.19
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	8	0.19
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	8	0.19
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	9	0.19
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	2	0.19
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	12	0.19
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	10	0.19
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	11	0.19
(1,1550)	1:44:A:GLN:HA	1:47:A:LYS:HG2	4	0.19
(1,1550)	1:44:A:GLN:HA	1:47:A:LYS:HG3	4	0.19
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	1	0.19
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	1	0.19
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	1	0.19
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	1	0.19
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	1	0.19
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	1	0.19
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	13	0.19
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	13	0.19
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	13	0.19
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	14	0.19
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	14	0.19
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	14	0.19
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	2	0.19
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	4	0.19
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	12	0.19
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	13	0.19
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	13	0.19
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	13	0.19
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	13	0.19
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	13	0.19
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	13	0.19
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	13	0.19
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	13	0.19
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	13	0.19
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	13	0.19
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	12	0.19
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	8	0.19
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	4	0.19
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	7	0.19
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	5	0.19
(1,1413)	1:38:A:LYS:HE2	1:38:A:LYS:HB2	1	0.19
(1,1413)	1:38:A:LYS:HE3	1:38:A:LYS:HB2	1	0.19
(1,1413)	1:38:A:LYS:HE2	1:38:A:LYS:HB2	9	0.19
(1,1413)	1:38:A:LYS:HE3	1:38:A:LYS:HB2	9	0.19
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	4	0.19
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	7	0.19
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	14	0.19
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	15	0.19
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	15	0.19
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD11	1	0.19
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD12	1	0.19
(1,1329)	1:33:A:LEU:HA	1:33:A:LEU:HD13	1	0.19
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	2	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	3	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	3	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	3	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	6	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	6	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	6	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	10	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	10	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	10	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	13	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	13	0.19
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	13	0.19
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	9	0.19
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	14	0.19
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	3	0.19
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	4	0.19
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	14	0.19
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	4	0.19
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	4	0.19
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	4	0.19
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	4	0.19
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	4	0.19
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	4	0.19
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	4	0.19
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	4	0.19
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	4	0.19
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	7	0.19
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	7	0.19
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	7	0.19
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	2	0.19
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	2	0.19
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	2	0.19
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	11	0.19
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	13	0.19
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	13	0.19
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	13	0.19
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	6	0.19
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	5	0.19
(1,972)	1:3:A:GLN:HB3	1:8:A:SER:HA	2	0.19
(1,913)	2:19:B:TRP:HA	2:19:B:TRP:HE1	9	0.19
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	14	0.19
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	15	0.19
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	7	0.19
(1,767)	1:78:A:LYS:HB3	1:78:A:LYS:H	5	0.19
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	14	0.19
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	7	0.19
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	10	0.19
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	4	0.19
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	6	0.19
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	4	0.19
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	4	0.19
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	4	0.19
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	11	0.19
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	11	0.19
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	11	0.19
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	13	0.19
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	13	0.19
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	13	0.19
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	9	0.19
(1,701)	1:62:A:GLN:HG2	1:62:A:GLN:HE21	10	0.19
(1,701)	1:62:A:GLN:HG3	1:62:A:GLN:HE21	10	0.19
(1,699)	1:62:A:GLN:HB2	1:62:A:GLN:HE21	2	0.19
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	9	0.19
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	6	0.19
(1,622)	1:54:A:ASN:HA	1:56:A:GLY:H	3	0.19
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	10	0.19
(1,571)	1:51:A:ARG:HG2	1:51:A:ARG:H	12	0.19
(1,571)	1:51:A:ARG:HG3	1:51:A:ARG:H	12	0.19
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	6	0.19
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	4	0.19
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	10	0.19
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	1	0.19
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	13	0.19
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	2	0.19
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	12	0.19
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	14	0.19
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	4	0.19
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	9	0.19
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	10	0.19
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	13	0.19
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	11	0.19
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	11	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	4	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	7	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	8	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	10	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	12	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	13	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	14	0.19
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	15	0.19
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	15	0.19
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	8	0.19
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	8	0.19
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	6	0.19
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	4	0.19
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	11	0.19
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	14	0.19
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	7	0.19
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	7	0.19
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	7	0.19
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	14	0.19
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	14	0.19
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	14	0.19
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	8	0.19
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	9	0.19
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	8	0.19
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	14	0.19
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	15	0.19
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	6	0.19
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	15	0.19
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	5	0.19
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	5	0.19
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	3	0.19
(1,89)	1:10:A:ARG:HG2	1:10:A:ARG:H	14	0.19
(1,89)	1:10:A:ARG:HG3	1:10:A:ARG:H	14	0.19
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	9	0.19
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	8	0.19
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD11	13	0.19
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD12	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD13	13	0.19
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	6	0.18
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	12	0.18
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	6	0.18
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	11	0.18
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	1	0.18
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	8	0.18
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	14	0.18
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	8	0.18
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	15	0.18
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	11	0.18
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	11	0.18
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	11	0.18
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	11	0.18
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	11	0.18
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	11	0.18
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	4	0.18
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	15	0.18
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	8	0.18
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	12	0.18
(1,1855)	1:69:A:TYR:HB3	1:72:A:LYS:HB2	2	0.18
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	1	0.18
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	1	0.18
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	1	0.18
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	14	0.18
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	14	0.18
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	14	0.18
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	15	0.18
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	15	0.18
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	15	0.18
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD11	13	0.18
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD12	13	0.18
(1,1820)	1:66:A:LEU:HA	1:66:A:LEU:HD13	13	0.18
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	4	0.18
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	4	0.18
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	4	0.18
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	12	0.18
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	12	0.18
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	12	0.18
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	7	0.18
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	7	0.18
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB1	13	0.18
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB2	13	0.18
(1,1773)	1:62:A:GLN:HA	1:65:A:ALA:HB3	13	0.18
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	1	0.18
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	5	0.18
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD21	2	0.18
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD22	2	0.18
(1,1744)	1:60:A:CYS:HA	1:63:A:LEU:HD23	2	0.18
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	2	0.18
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	2	0.18
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	2	0.18
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	5	0.18
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	5	0.18
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	5	0.18
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	11	0.18
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	11	0.18
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	11	0.18
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	3	0.18
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	8	0.18
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	10	0.18
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE2	10	0.18
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE3	10	0.18
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	3	0.18
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	10	0.18
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	9	0.18
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	9	0.18
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	9	0.18
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	15	0.18
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	1	0.18
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	7	0.18
(1,1643)	1:50:A:LYS:HB3	1:52:A:LYS:HD2	1	0.18
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	1	0.18
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	7	0.18
(1,1623)	1:49:A:CYS:HB2	1:57:A:CYS:HB3	7	0.18
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	2	0.18
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD21	11	0.18
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD22	11	0.18
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD23	11	0.18
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD21	11	0.18
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD22	11	0.18
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD23	11	0.18
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD21	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD22	11	0.18
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD23	11	0.18
(1,1550)	1:44:A:GLN:HA	1:47:A:LYS:HG2	5	0.18
(1,1550)	1:44:A:GLN:HA	1:47:A:LYS:HG3	5	0.18
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	3	0.18
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	3	0.18
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	3	0.18
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	5	0.18
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	5	0.18
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	5	0.18
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	15	0.18
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	15	0.18
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	15	0.18
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	14	0.18
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	14	0.18
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	14	0.18
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	14	0.18
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	14	0.18
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	14	0.18
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	14	0.18
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	14	0.18
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	14	0.18
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	2	0.18
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	12	0.18
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	4	0.18
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	4	0.18
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	14	0.18
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	14	0.18
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	5	0.18
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	13	0.18
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	15	0.18
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	1	0.18
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	7	0.18
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	14	0.18
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	13	0.18
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	14	0.18
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	2	0.18
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	2	0.18
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	2	0.18
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	8	0.18
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	9	0.18
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	15	0.18
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	6	0.18
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	10	0.18
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD11	6	0.18
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD12	6	0.18
(1,1127)	1:17:A:ILE:HG13	1:66:A:LEU:HD13	6	0.18
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	5	0.18
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	7	0.18
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	15	0.18
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	12	0.18
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	12	0.18
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	12	0.18
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	12	0.18
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	12	0.18
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	12	0.18
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	12	0.18
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	12	0.18
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	12	0.18
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	7	0.18
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	7	0.18
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	3	0.18
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	3	0.18
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	3	0.18
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	3	0.18
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	3	0.18
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	3	0.18
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	3	0.18
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	3	0.18
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	3	0.18
(1,1062)	1:13:A:ILE:HA	1:13:A:ILE:HG13	6	0.18
(1,1048)	1:11:A:LEU:HA	1:14:A:GLN:HB2	8	0.18
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	3	0.18
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	10	0.18
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	8	0.18
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	8	0.18
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	2	0.18
(1,977)	1:4:A:SER:HA	1:5:A:PRO:HG3	2	0.18
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	1	0.18
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	1	0.18
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	2	0.18
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	4	0.18
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	3	0.18
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	9	0.18
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	12	0.18
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	1	0.18
(1,851)	2:11:B:LEU:HD11	2:12:B:SER:H	7	0.18
(1,851)	2:11:B:LEU:HD12	2:12:B:SER:H	7	0.18
(1,851)	2:11:B:LEU:HD13	2:12:B:SER:H	7	0.18
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	3	0.18
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	3	0.18
(1,838)	2:10:B:MET:HG2	2:10:B:MET:H	7	0.18
(1,812)	2:6:B:MET:HG2	2:6:B:MET:H	6	0.18
(1,812)	2:6:B:MET:HG3	2:6:B:MET:H	6	0.18
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	3	0.18
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	3	0.18
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	8	0.18
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	9	0.18
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	14	0.18
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	2	0.18
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	13	0.18
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	3	0.18
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	12	0.18
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	3	0.18
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	7	0.18
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	8	0.18
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	1	0.18
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	10	0.18
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	15	0.18
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	3	0.18
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	3	0.18
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	3	0.18
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	15	0.18
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	15	0.18
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	15	0.18
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	5	0.18
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	5	0.18
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	8	0.18
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	11	0.18
(1,652)	1:59:A:ILE:HG21	1:60:A:CYS:H	10	0.18
(1,652)	1:59:A:ILE:HG22	1:60:A:CYS:H	10	0.18
(1,652)	1:59:A:ILE:HG23	1:60:A:CYS:H	10	0.18
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	12	0.18
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	14	0.18
(1,629)	1:56:A:GLY:H	1:57:A:CYS:H	8	0.18
(1,628)	1:55:A:GLY:H	1:57:A:CYS:H	3	0.18
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	5	0.18
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	5	0.18
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	10	0.18
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	10	0.18
(1,577)	1:51:A:ARG:HA	1:54:A:ASN:HD21	6	0.18
(1,570)	1:51:A:ARG:HB2	1:51:A:ARG:H	14	0.18
(1,570)	1:51:A:ARG:HB3	1:51:A:ARG:H	14	0.18
(1,554)	1:49:A:CYS:HA	1:50:A:LYS:H	11	0.18
(1,554)	1:49:A:CYS:HA	1:50:A:LYS:H	15	0.18
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	6	0.18
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	6	0.18
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	5	0.18
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	14	0.18
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	3	0.18
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	7	0.18
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	8	0.18
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	15	0.18
(1,470)	1:40:A:LYS:HB2	1:40:A:LYS:H	11	0.18
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	3	0.18
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	4	0.18
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	7	0.18
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	5	0.18
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	8	0.18
(1,432)	1:37:A:GLN:HB2	1:38:A:LYS:H	10	0.18
(1,432)	1:37:A:GLN:HB3	1:38:A:LYS:H	10	0.18
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	8	0.18
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	8	0.18
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	2	0.18
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	5	0.18
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	6	0.18
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	2	0.18
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	5	0.18
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	6	0.18
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	7	0.18
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	8	0.18
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	13	0.18
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	5	0.18
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	7	0.18
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	12	0.18
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	13	0.18
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	11	0.18
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	9	0.18
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	15	0.18
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	15	0.18
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	15	0.18
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	2	0.18
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	11	0.18
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	14	0.18
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	11	0.18
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	1	0.18
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	13	0.18
(1,136)	1:14:A:GLN:HB2	1:14:A:GLN:HE21	15	0.18
(1,136)	1:14:A:GLN:HB3	1:14:A:GLN:HE21	15	0.18
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	11	0.18
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	6	0.18
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	6	0.18
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	15	0.18
(1,16)	1:69:A:TYR:HA	2:10:B:MET:HB2	8	0.18
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	3	0.17
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	5	0.17
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	2	0.17
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	2	0.17
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	4	0.17
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	7	0.17
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	13	0.17
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	4	0.17
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	4	0.17
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	4	0.17
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	4	0.17
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	4	0.17
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	4	0.17
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD11	15	0.17
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD12	15	0.17
(1,1976)	2:9:B:LEU:HB2	2:9:B:LEU:HD13	15	0.17
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD11	15	0.17
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD12	15	0.17
(1,1976)	2:9:B:LEU:HB3	2:9:B:LEU:HD13	15	0.17
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD2	6	0.17
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD3	6	0.17
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	7	0.17
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	1	0.17
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	4	0.17
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	7	0.17
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	1	0.17
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	1	0.17
(1,1852)	1:69:A:TYR:HA	1:72:A:LYS:HA	13	0.17
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	6	0.17
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	6	0.17
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	6	0.17
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	10	0.17
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	10	0.17
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	10	0.17
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE1	5	0.17
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE2	5	0.17
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE1	5	0.17
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE2	5	0.17
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE1	5	0.17
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE2	5	0.17
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	1	0.17
(1,1782)	1:63:A:LEU:HD21	1:63:A:LEU:HB2	11	0.17
(1,1782)	1:63:A:LEU:HD22	1:63:A:LEU:HB2	11	0.17
(1,1782)	1:63:A:LEU:HD23	1:63:A:LEU:HB2	11	0.17
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	14	0.17
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	14	0.17
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	14	0.17
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD11	9	0.17
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD12	9	0.17
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD13	9	0.17
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD11	9	0.17
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD12	9	0.17
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD13	9	0.17
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	5	0.17
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	12	0.17
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	12	0.17
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	12	0.17
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	8	0.17
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	11	0.17
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	4	0.17
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	13	0.17
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	13	0.17
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	4	0.17
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	7	0.17
(1,1679)	1:52:A:LYS:HA	1:60:A:CYS:HB2	7	0.17
(1,1679)	1:52:A:LYS:HA	1:60:A:CYS:HB2	15	0.17
(1,1677)	1:52:A:LYS:HA	1:57:A:CYS:HB3	3	0.17
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	1	0.17
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	1	0.17
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	10	0.17
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	10	0.17
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	12	0.17
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	13	0.17
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	2	0.17
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	7	0.17
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	1	0.17
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	1	0.17
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	12	0.17
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	12	0.17
(1,1630)	1:50:A:LYS:HA	1:50:A:LYS:HG2	10	0.17
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	8	0.17
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	8	0.17
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	14	0.17
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD21	4	0.17
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD22	4	0.17
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD23	4	0.17
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD21	4	0.17
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD22	4	0.17
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD23	4	0.17
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD21	4	0.17
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD22	4	0.17
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD23	4	0.17
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	13	0.17
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	13	0.17
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	10	0.17
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	10	0.17
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	10	0.17
(1,1526)	1:43:A:VAL:HB	1:44:A:GLN:HA	9	0.17
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	14	0.17
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	14	0.17
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	14	0.17
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	2	0.17
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	15	0.17
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	15	0.17
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	5	0.17
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	11	0.17
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	14	0.17
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	6	0.17
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	7	0.17
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	7	0.17
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	10	0.17
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	10	0.17
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	12	0.17
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	4	0.17
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	15	0.17
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	3	0.17
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	4	0.17
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	5	0.17
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	10	0.17
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	15	0.17
(1,1333)	1:33:A:LEU:HD21	1:33:A:LEU:HB2	8	0.17
(1,1333)	1:33:A:LEU:HD22	1:33:A:LEU:HB2	8	0.17
(1,1333)	1:33:A:LEU:HD23	1:33:A:LEU:HB2	8	0.17
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	7	0.17
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	8	0.17
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	15	0.17
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	3	0.17
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	11	0.17
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	2	0.17
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	2	0.17
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	2	0.17
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	12	0.17
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	12	0.17
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	12	0.17
(1,1143)	1:18:A:GLN:HB2	1:19:A:SER:HA	12	0.17
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	2	0.17
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	10	0.17
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB1	11	0.17
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB2	11	0.17
(1,1069)	1:13:A:ILE:HA	1:16:A:ALA:HB3	11	0.17
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG21	9	0.17
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG22	9	0.17
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG23	9	0.17
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	2	0.17
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	6	0.17
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	6	0.17
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD2	9	0.17
(1,1016)	1:9:A:ARG:HA	1:9:A:ARG:HD3	9	0.17
(1,1010)	1:8:A:SER:HA	1:11:A:LEU:HA	6	0.17
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	1	0.17
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	1	0.17
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	1	0.17
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	13	0.17
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	13	0.17
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	13	0.17
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	10	0.17
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	13	0.17
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	10	0.17
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	10	0.17
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	10	0.17
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	10	0.17
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	6	0.17
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	1	0.17
(1,984)	1:5:A:PRO:HD3	1:5:A:PRO:HA	6	0.17
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	9	0.17
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	9	0.17
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	15	0.17
(1,824)	2:8:B:ASP:H	2:9:B:LEU:HG	6	0.17
(1,812)	2:6:B:MET:HG2	2:6:B:MET:H	4	0.17
(1,812)	2:6:B:MET:HG3	2:6:B:MET:H	4	0.17
(1,790)	1:90:A:LYS:HB2	1:90:A:LYS:H	10	0.17
(1,790)	1:90:A:LYS:HB3	1:90:A:LYS:H	10	0.17
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	13	0.17
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	10	0.17
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	3	0.17
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	11	0.17
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	6	0.17
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	11	0.17
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	1	0.17
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	13	0.17
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	6	0.17
(1,744)	1:74:A:CYS:HB3	1:74:A:CYS:H	15	0.17
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	1	0.17
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	2	0.17
(1,734)	1:72:A:LYS:HB2	1:72:A:LYS:H	15	0.17
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	11	0.17
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	1	0.17
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	4	0.17
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	6	0.17
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	13	0.17
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	14	0.17
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	3	0.17
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	11	0.17
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	5	0.17
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	5	0.17
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	5	0.17
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	10	0.17
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	10	0.17
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	10	0.17
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	12	0.17
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	12	0.17
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	12	0.17
(1,722)	1:66:A:LEU:HB3	1:67:A:ALA:H	11	0.17
(1,711)	1:63:A:LEU:H	1:64:A:ILE:H	7	0.17
(1,711)	1:63:A:LEU:H	1:64:A:ILE:H	9	0.17
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	4	0.17
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	1	0.17
(1,665)	1:59:A:ILE:HA	1:63:A:LEU:H	7	0.17
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	13	0.17
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	10	0.17
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	15	0.17
(1,630)	1:56:A:GLY:HA2	1:57:A:CYS:H	8	0.17
(1,630)	1:56:A:GLY:HA3	1:57:A:CYS:H	8	0.17
(1,628)	1:55:A:GLY:H	1:57:A:CYS:H	15	0.17
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	7	0.17
(1,622)	1:54:A:ASN:HA	1:56:A:GLY:H	8	0.17
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	13	0.17
(1,570)	1:51:A:ARG:HB2	1:51:A:ARG:H	6	0.17
(1,570)	1:51:A:ARG:HB3	1:51:A:ARG:H	6	0.17
(1,536)	1:47:A:LYS:HB2	1:47:A:LYS:H	9	0.17
(1,536)	1:47:A:LYS:HB3	1:47:A:LYS:H	9	0.17
(1,532)	1:46:A:THR:HB	1:47:A:LYS:H	6	0.17
(1,530)	1:46:A:THR:HG21	1:46:A:THR:H	9	0.17
(1,530)	1:46:A:THR:HG22	1:46:A:THR:H	9	0.17
(1,530)	1:46:A:THR:HG23	1:46:A:THR:H	9	0.17
(1,529)	1:46:A:THR:HB	1:46:A:THR:H	8	0.17
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	6	0.17
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	13	0.17
(1,445)	1:38:A:LYS:HB3	1:39:A:MET:H	6	0.17
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	6	0.17
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	6	0.17
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	1	0.17
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	4	0.17
(1,388)	1:33:A:LEU:HB3	1:35:A:SER:H	11	0.17
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	3	0.17
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	8	0.17
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	14	0.17
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	15	0.17
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	8	0.17
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	6	0.17
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	4	0.17
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	13	0.17
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	1	0.17
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	10	0.17
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	2	0.17
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	5	0.17
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	9	0.17
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	7	0.17
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	14	0.17
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	4	0.17
(1,122)	1:13:A:ILE:HG12	1:14:A:GLN:H	7	0.17
(1,119)	1:13:A:ILE:HG12	1:13:A:ILE:H	10	0.17
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	10	0.17
(1,79)	1:8:A:SER:HB2	1:8:A:SER:H	3	0.17
(1,79)	1:8:A:SER:HB3	1:8:A:SER:H	3	0.17
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	5	0.17
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	11	0.17
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	14	0.17
(1,18)	2:5:B:ALA:H	1:17:A:ILE:H	10	0.17
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	13	0.16
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	2	0.16
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	9	0.16
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	14	0.16
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	2	0.16
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD2	8	0.16
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD3	8	0.16
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	6	0.16
(1,1953)	1:85:A:LEU:HD11	1:85:A:LEU:HB3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1953)	1:85:A:LEU:HD12	1:85:A:LEU:HB3	9	0.16
(1,1953)	1:85:A:LEU:HD13	1:85:A:LEU:HB3	9	0.16
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE2	11	0.16
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE3	11	0.16
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE2	13	0.16
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE3	13	0.16
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	11	0.16
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	4	0.16
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	4	0.16
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	4	0.16
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	4	0.16
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	4	0.16
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	4	0.16
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	4	0.16
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	4	0.16
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	4	0.16
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	4	0.16
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	4	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	12	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	12	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	12	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	15	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	15	0.16
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	15	0.16
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	11	0.16
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	11	0.16
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	11	0.16
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB1	1	0.16
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB2	1	0.16
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB3	1	0.16
(1,1807)	1:64:A:ILE:HA	1:67:A:ALA:HA	14	0.16
(1,1780)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	5	0.16
(1,1780)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	5	0.16
(1,1780)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	5	0.16
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	2	0.16
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	1	0.16
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	9	0.16
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	10	0.16
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	14	0.16
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	13	0.16
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	3	0.16
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	12	0.16
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE2	3	0.16
(1,1721)	1:58:A:PRO:HB3	1:61:A:LYS:HE3	3	0.16
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	4	0.16
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	2	0.16
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	9	0.16
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE2	14	0.16
(1,1670)	1:52:A:LYS:HG2	1:52:A:LYS:HE3	14	0.16
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	7	0.16
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	11	0.16
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	2	0.16
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	3	0.16
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	8	0.16
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	2	0.16
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	14	0.16
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	1	0.16
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	3	0.16
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	10	0.16
(1,1630)	1:50:A:LYS:HA	1:50:A:LYS:HG2	2	0.16
(1,1630)	1:50:A:LYS:HA	1:50:A:LYS:HG2	3	0.16
(1,1629)	1:50:A:LYS:HA	1:50:A:LYS:HE2	4	0.16
(1,1629)	1:50:A:LYS:HA	1:50:A:LYS:HE3	4	0.16
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	3	0.16
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	6	0.16
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	12	0.16
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	9	0.16
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	9	0.16
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	9	0.16
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	9	0.16
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	6	0.16
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	6	0.16
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	4	0.16
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	4	0.16
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	4	0.16
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	4	0.16
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	4	0.16
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	4	0.16
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	11	0.16
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	11	0.16
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	11	0.16
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	11	0.16
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	11	0.16
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	5	0.16
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	5	0.16
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	5	0.16
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	5	0.16
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	5	0.16
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	5	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	1	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	1	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	1	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	1	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	1	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	1	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	1	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	1	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	1	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	5	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	5	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	5	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	5	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	5	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	5	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	5	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	5	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	5	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	8	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	8	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	8	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	8	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	8	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	8	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	8	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	8	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	8	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	11	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	11	0.16
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	11	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	11	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	11	0.16
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	11	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	11	0.16
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	11	0.16
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	13	0.16
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD2	13	0.16
(1,1482)	1:41:A:ARG:HB3	1:41:A:ARG:HD3	13	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	2	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	2	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	5	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	5	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	8	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	8	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	13	0.16
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	13	0.16
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	9	0.16
(1,1378)	1:34:A:PRO:HA	1:38:A:LYS:HG2	12	0.16
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	7	0.16
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	8	0.16
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	12	0.16
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	4	0.16
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	10	0.16
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	5	0.16
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	6	0.16
(1,1256)	1:23:A:ALA:HB1	1:43:A:VAL:HG11	1	0.16
(1,1256)	1:23:A:ALA:HB1	1:43:A:VAL:HG12	1	0.16
(1,1256)	1:23:A:ALA:HB1	1:43:A:VAL:HG13	1	0.16
(1,1256)	1:23:A:ALA:HB2	1:43:A:VAL:HG11	1	0.16
(1,1256)	1:23:A:ALA:HB2	1:43:A:VAL:HG12	1	0.16
(1,1256)	1:23:A:ALA:HB2	1:43:A:VAL:HG13	1	0.16
(1,1256)	1:23:A:ALA:HB3	1:43:A:VAL:HG11	1	0.16
(1,1256)	1:23:A:ALA:HB3	1:43:A:VAL:HG12	1	0.16
(1,1256)	1:23:A:ALA:HB3	1:43:A:VAL:HG13	1	0.16
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	5	0.16
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	7	0.16
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	13	0.16
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	1	0.16
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	8	0.16
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	9	0.16
(1,1112)	1:17:A:ILE:HB	1:20:A:LEU:HB3	11	0.16
(1,1048)	1:11:A:LEU:HA	1:14:A:GLN:HB2	11	0.16
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	5	0.16
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	8	0.16
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	5	0.16
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	5	0.16
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	5	0.16
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	14	0.16
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG2	11	0.16
(1,995)	1:5:A:PRO:HB2	1:9:A:ARG:HG3	11	0.16
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	1	0.16
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	8	0.16
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	1	0.16
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	2	0.16
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	1	0.16
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	1	0.16
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	12	0.16
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	12	0.16
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	2	0.16
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	3	0.16
(1,851)	2:11:B:LEU:HD11	2:12:B:SER:H	3	0.16
(1,851)	2:11:B:LEU:HD12	2:12:B:SER:H	3	0.16
(1,851)	2:11:B:LEU:HD13	2:12:B:SER:H	3	0.16
(1,845)	2:11:B:LEU:HG	2:11:B:LEU:H	7	0.16
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	6	0.16
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	6	0.16
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	8	0.16
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	8	0.16
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	15	0.16
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	15	0.16
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	6	0.16
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	10	0.16
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	3	0.16
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	10	0.16
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	11	0.16
(1,747)	1:75:A:GLN:HG2	1:75:A:GLN:H	6	0.16
(1,747)	1:75:A:GLN:HG3	1:75:A:GLN:H	6	0.16
(1,741)	1:73:A:HIS:HB3	1:73:A:HIS:H	10	0.16
(1,739)	1:72:A:LYS:HB3	1:73:A:HIS:H	5	0.16
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	8	0.16
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	13	0.16
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	12	0.16
(1,726)	1:68:A:ALA:HB1	1:68:A:ALA:H	7	0.16
(1,726)	1:68:A:ALA:HB2	1:68:A:ALA:H	7	0.16
(1,726)	1:68:A:ALA:HB3	1:68:A:ALA:H	7	0.16
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	9	0.16
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	1	0.16
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	1	0.16
(1,724)	1:67:A:ALA:HB1	1:67:A:ALA:H	9	0.16
(1,724)	1:67:A:ALA:HB2	1:67:A:ALA:H	9	0.16
(1,724)	1:67:A:ALA:HB3	1:67:A:ALA:H	9	0.16
(1,701)	1:62:A:GLN:HG2	1:62:A:GLN:HE21	13	0.16
(1,701)	1:62:A:GLN:HG3	1:62:A:GLN:HE21	13	0.16
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	3	0.16
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	12	0.16
(1,681)	1:61:A:LYS:H	1:62:A:GLN:H	9	0.16
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	2	0.16
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	2	0.16
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	2	0.16
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	5	0.16
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	13	0.16
(1,613)	1:54:A:ASN:HB2	1:54:A:ASN:H	12	0.16
(1,613)	1:54:A:ASN:HB3	1:54:A:ASN:H	12	0.16
(1,602)	1:53:A:THR:H	1:54:A:ASN:H	6	0.16
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	4	0.16
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	12	0.16
(1,565)	1:50:A:LYS:HG2	1:50:A:LYS:H	4	0.16
(1,557)	1:49:A:CYS:H	1:50:A:LYS:HE2	14	0.16
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	11	0.16
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	3	0.16
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	3	0.16
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	15	0.16
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	15	0.16
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	11	0.16
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	2	0.16
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	5	0.16
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	8	0.16
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	10	0.16
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	12	0.16
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	13	0.16
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	15	0.16
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	15	0.16
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	10	0.16
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	14	0.16
(1,414)	1:36:A:CYS:HB2	1:36:A:CYS:H	1	0.16
(1,414)	1:36:A:CYS:HB2	1:36:A:CYS:H	3	0.16
(1,388)	1:33:A:LEU:HB3	1:35:A:SER:H	9	0.16
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	4	0.16
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	6	0.16
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	7	0.16
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	8	0.16
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	14	0.16
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	8	0.16
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	14	0.16
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	2	0.16
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	2	0.16
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	2	0.16
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	11	0.16
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	6	0.16
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	9	0.16
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	14	0.16
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	10	0.16
(1,224)	1:21:A:VAL:HG11	1:25:A:GLN:HE21	5	0.16
(1,224)	1:21:A:VAL:HG12	1:25:A:GLN:HE21	5	0.16
(1,224)	1:21:A:VAL:HG13	1:25:A:GLN:HE21	5	0.16
(1,224)	1:21:A:VAL:HG11	1:25:A:GLN:HE21	10	0.16
(1,224)	1:21:A:VAL:HG12	1:25:A:GLN:HE21	10	0.16
(1,224)	1:21:A:VAL:HG13	1:25:A:GLN:HE21	10	0.16
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	5	0.16
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	8	0.16
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	9	0.16
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	15	0.16
(1,162)	1:16:A:ALA:H	1:19:A:SER:H	14	0.16
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	3	0.16
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	3	0.16
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	3	0.16
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	9	0.16
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	9	0.16
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	9	0.16
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	12	0.16
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	12	0.16
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	12	0.16
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	1	0.16
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	4	0.16
(1,137)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	10	0.16
(1,137)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	10	0.16
(1,125)	1:13:A:ILE:HB	1:14:A:GLN:H	5	0.16
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	15	0.16
(1,122)	1:13:A:ILE:HG12	1:14:A:GLN:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:8:A:SER:H	1:11:A:LEU:HG	5	0.16
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	1	0.16
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	13	0.16
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	7	0.16
(1,18)	2:5:B:ALA:H	1:17:A:ILE:H	5	0.16
(1,18)	2:5:B:ALA:H	1:17:A:ILE:H	15	0.16
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	4	0.15
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	10	0.15
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	1	0.15
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	12	0.15
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	13	0.15
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	12	0.15
(2,54)	1:44:A:GLN:O	1:48:A:GLY:N	14	0.15
(1,1913)	1:78:A:LYS:HA	1:78:A:LYS:HG2	6	0.15
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	1	0.15
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	2	0.15
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	12	0.15
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	13	0.15
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	15	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	4	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	4	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	4	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	7	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	7	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	7	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	13	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	13	0.15
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	13	0.15
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	1	0.15
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	1	0.15
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	1	0.15
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	12	0.15
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	12	0.15
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	12	0.15
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB1	14	0.15
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB2	14	0.15
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB3	14	0.15
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD11	14	0.15
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD12	14	0.15
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD13	14	0.15
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD11	14	0.15
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD12	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD13	14	0.15
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	9	0.15
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	12	0.15
(1,1738)	1:59:A:ILE:HG21	1:60:A:CYS:H	8	0.15
(1,1738)	1:59:A:ILE:HG22	1:60:A:CYS:H	8	0.15
(1,1738)	1:59:A:ILE:HG23	1:60:A:CYS:H	8	0.15
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	11	0.15
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	12	0.15
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	15	0.15
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	5	0.15
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	11	0.15
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	13	0.15
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	1	0.15
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	1	0.15
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	1	0.15
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	12	0.15
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	5	0.15
(1,1658)	1:51:A:ARG:HD2	1:55:A:GLY:HA2	7	0.15
(1,1658)	1:51:A:ARG:HD2	1:55:A:GLY:HA3	7	0.15
(1,1658)	1:51:A:ARG:HD3	1:55:A:GLY:HA2	7	0.15
(1,1658)	1:51:A:ARG:HD3	1:55:A:GLY:HA3	7	0.15
(1,1644)	1:50:A:LYS:HB2	1:52:A:LYS:HG3	1	0.15
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	4	0.15
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	4	0.15
(1,1630)	1:50:A:LYS:HA	1:50:A:LYS:HG2	8	0.15
(1,1623)	1:49:A:CYS:HB2	1:57:A:CYS:HB3	14	0.15
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	1	0.15
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	1	0.15
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	4	0.15
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	4	0.15
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	4	0.15
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	4	0.15
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD21	3	0.15
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD22	3	0.15
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD23	3	0.15
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD21	3	0.15
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD22	3	0.15
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD23	3	0.15
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD21	3	0.15
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD22	3	0.15
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD23	3	0.15
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	6	0.15
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	6	0.15
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	10	0.15
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	10	0.15
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	10	0.15
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	3	0.15
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	11	0.15
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	3	0.15
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	9	0.15
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	11	0.15
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	4	0.15
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	10	0.15
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	6	0.15
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	6	0.15
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD2	9	0.15
(1,1458)	1:40:A:LYS:HB3	1:40:A:LYS:HD3	9	0.15
(1,1441)	1:39:A:MET:HB2	1:40:A:LYS:HE3	6	0.15
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	14	0.15
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	1	0.15
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	2	0.15
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	13	0.15
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	1	0.15
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	11	0.15
(1,1295)	1:27:A:ARG:HB2	1:27:A:ARG:HD2	1	0.15
(1,1295)	1:27:A:ARG:HB2	1:27:A:ARG:HD3	1	0.15
(1,1253)	1:23:A:ALA:HA	1:40:A:LYS:HA	9	0.15
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	12	0.15
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	14	0.15
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	10	0.15
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	6	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	1	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	1	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	1	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	1	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	1	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	1	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	1	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	1	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	1	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	10	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	10	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	10	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	10	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	10	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	10	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	10	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	10	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	11	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	11	0.15
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	11	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	11	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	11	0.15
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	11	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	11	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	11	0.15
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	11	0.15
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	6	0.15
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	6	0.15
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	11	0.15
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	7	0.15
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	11	0.15
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD11	6	0.15
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD12	6	0.15
(1,1030)	1:10:A:ARG:HA	1:13:A:ILE:HD13	6	0.15
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD11	4	0.15
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD12	4	0.15
(1,1009)	1:7:A:ASP:HA	1:11:A:LEU:HD13	4	0.15
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	6	0.15
(1,975)	1:4:A:SER:HA	1:5:A:PRO:HD3	6	0.15
(1,972)	1:3:A:GLN:HB3	1:8:A:SER:HA	4	0.15
(1,972)	1:3:A:GLN:HB3	1:8:A:SER:HA	10	0.15
(1,962)	1:2:A:THR:HB	1:3:A:GLN:HA	10	0.15
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	5	0.15
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	1	0.15
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	13	0.15
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	15	0.15
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	2	0.15
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	2	0.15
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	5	0.15
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	3	0.15
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	7	0.15
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	13	0.15
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	13	0.15
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	13	0.15
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	1	0.15
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	3	0.15
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	4	0.15
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	8	0.15
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	9	0.15
(1,786)	1:86:A:ASN:H	1:90:A:LYS:H	15	0.15
(1,761)	1:77:A:ASN:HB3	1:77:A:ASN:H	9	0.15
(1,761)	1:77:A:ASN:HB3	1:77:A:ASN:H	14	0.15
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	7	0.15
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	1	0.15
(1,742)	1:73:A:HIS:HB2	1:73:A:HIS:H	5	0.15
(1,741)	1:73:A:HIS:HB3	1:73:A:HIS:H	2	0.15
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	4	0.15
(1,725)	1:67:A:ALA:H	1:68:A:ALA:H	12	0.15
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	8	0.15
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	10	0.15
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	1	0.15
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	5	0.15
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	8	0.15
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	13	0.15
(1,681)	1:61:A:LYS:H	1:62:A:GLN:H	7	0.15
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	8	0.15
(1,664)	1:59:A:ILE:HA	1:62:A:GLN:HE22	2	0.15
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	12	0.15
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	8	0.15
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	11	0.15
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	2	0.15
(1,626)	1:55:A:GLY:H	1:56:A:GLY:H	11	0.15
(1,602)	1:53:A:THR:H	1:54:A:ASN:H	1	0.15
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	7	0.15
(1,562)	1:50:A:LYS:HB2	1:50:A:LYS:H	13	0.15
(1,551)	1:49:A:CYS:HB3	1:49:A:CYS:H	1	0.15
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	9	0.15
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	15	0.15
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	10	0.15
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	1	0.15
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	11	0.15
(1,460)	1:39:A:MET:H	1:40:A:LYS:H	15	0.15
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	2	0.15
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:33:A:LEU:HG	1:33:A:LEU:H	2	0.15
(1,375)	1:32:A:SER:H	1:36:A:CYS:HB3	3	0.15
(1,369)	1:32:A:SER:HA	1:33:A:LEU:H	9	0.15
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	1	0.15
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	2	0.15
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	5	0.15
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	12	0.15
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	13	0.15
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	4	0.15
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	12	0.15
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	5	0.15
(1,335)	1:29:A:ALA:HB1	1:29:A:ALA:H	5	0.15
(1,335)	1:29:A:ALA:HB2	1:29:A:ALA:H	5	0.15
(1,335)	1:29:A:ALA:HB3	1:29:A:ALA:H	5	0.15
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	2	0.15
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	1	0.15
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	4	0.15
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	9	0.15
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	13	0.15
(1,308)	1:27:A:ARG:H	1:28:A:ASN:HD22	1	0.15
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	12	0.15
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	12	0.15
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	3	0.15
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	9	0.15
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	2	0.15
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	8	0.15
(1,242)	1:23:A:ALA:HB1	1:24:A:ALA:H	4	0.15
(1,242)	1:23:A:ALA:HB2	1:24:A:ALA:H	4	0.15
(1,242)	1:23:A:ALA:HB3	1:24:A:ALA:H	4	0.15
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	1	0.15
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	10	0.15
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	12	0.15
(1,164)	1:17:A:ILE:HG13	1:17:A:ILE:H	6	0.15
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	2	0.15
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	2	0.15
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	2	0.15
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	12	0.15
(1,129)	1:13:A:ILE:HG12	1:16:A:ALA:H	7	0.15
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	5	0.15
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	12	0.15
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	12	0.15
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:5:A:PRO:HA	1:9:A:ARG:H	1	0.15
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	2	0.15
(1,19)	2:9:B:LEU:HA	1:70:A:HIS:HA	6	0.15
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	2	0.14
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	7	0.14
(2,82)	1:81:A:VAL:O	1:85:A:LEU:N	12	0.14
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	5	0.14
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	11	0.14
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	10	0.14
(2,54)	1:44:A:GLN:O	1:48:A:GLY:N	6	0.14
(2,54)	1:44:A:GLN:O	1:48:A:GLY:N	13	0.14
(2,1)	1:5:A:PRO:O	1:9:A:ARG:H	7	0.14
(1,1988)	2:17:B:GLU:HA	2:18:B:GLN:HA	15	0.14
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	3	0.14
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	7	0.14
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	14	0.14
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	15	0.14
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD1	2	0.14
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD2	2	0.14
(1,1938)	1:81:A:VAL:HG11	1:84:A:CYS:HB3	11	0.14
(1,1938)	1:81:A:VAL:HG12	1:84:A:CYS:HB3	11	0.14
(1,1938)	1:81:A:VAL:HG13	1:84:A:CYS:HB3	11	0.14
(1,1888)	1:74:A:CYS:HB3	1:84:A:CYS:HB2	5	0.14
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	13	0.14
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	14	0.14
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	14	0.14
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	11	0.14
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	11	0.14
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	11	0.14
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	1	0.14
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	1	0.14
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	1	0.14
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	9	0.14
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	9	0.14
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	9	0.14
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE1	1	0.14
(1,1819)	1:65:A:ALA:HB1	1:69:A:TYR:HE2	1	0.14
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE1	1	0.14
(1,1819)	1:65:A:ALA:HB2	1:69:A:TYR:HE2	1	0.14
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE1	1	0.14
(1,1819)	1:65:A:ALA:HB3	1:69:A:TYR:HE2	1	0.14
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD1	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD2	13	0.14
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD1	13	0.14
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD2	13	0.14
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD1	13	0.14
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD2	13	0.14
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB1	7	0.14
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB2	7	0.14
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB3	7	0.14
(1,1780)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	9	0.14
(1,1780)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	9	0.14
(1,1780)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	9	0.14
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	13	0.14
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	14	0.14
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	7	0.14
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	6	0.14
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	2	0.14
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	14	0.14
(1,1692)	1:53:A:THR:HG21	1:61:A:LYS:HA	12	0.14
(1,1692)	1:53:A:THR:HG22	1:61:A:LYS:HA	12	0.14
(1,1692)	1:53:A:THR:HG23	1:61:A:LYS:HA	12	0.14
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	3	0.14
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	4	0.14
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	13	0.14
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	8	0.14
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	8	0.14
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	6	0.14
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	7	0.14
(1,1632)	1:50:A:LYS:HA	1:50:A:LYS:HG3	12	0.14
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	3	0.14
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	3	0.14
(1,1623)	1:49:A:CYS:HB2	1:57:A:CYS:HB3	1	0.14
(1,1623)	1:49:A:CYS:HB2	1:57:A:CYS:HB3	5	0.14
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	13	0.14
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD2	2	0.14
(1,1538)	1:43:A:VAL:HG11	1:47:A:LYS:HD3	2	0.14
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD2	2	0.14
(1,1538)	1:43:A:VAL:HG12	1:47:A:LYS:HD3	2	0.14
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD2	2	0.14
(1,1538)	1:43:A:VAL:HG13	1:47:A:LYS:HD3	2	0.14
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	14	0.14
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	14	0.14
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	14	0.14
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	14	0.14
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	14	0.14
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	4	0.14
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	4	0.14
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	4	0.14
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	4	0.14
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	4	0.14
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	4	0.14
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	4	0.14
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	4	0.14
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	4	0.14
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	12	0.14
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	12	0.14
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	12	0.14
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	12	0.14
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	12	0.14
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	12	0.14
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	12	0.14
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	12	0.14
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	12	0.14
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	9	0.14
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	13	0.14
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	4	0.14
(1,1413)	1:38:A:LYS:HE2	1:38:A:LYS:HB2	7	0.14
(1,1413)	1:38:A:LYS:HE3	1:38:A:LYS:HB2	7	0.14
(1,1413)	1:38:A:LYS:HE2	1:38:A:LYS:HB2	13	0.14
(1,1413)	1:38:A:LYS:HE3	1:38:A:LYS:HB2	13	0.14
(1,1413)	1:38:A:LYS:HE2	1:38:A:LYS:HB2	14	0.14
(1,1413)	1:38:A:LYS:HE3	1:38:A:LYS:HB2	14	0.14
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	2	0.14
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	10	0.14
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	13	0.14
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	5	0.14
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	8	0.14
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB2	10	0.14
(1,1379)	1:35:A:SER:HA	1:38:A:LYS:HB3	10	0.14
(1,1347)	1:33:A:LEU:HA	1:36:A:CYS:HA	6	0.14
(1,1321)	1:31:A:CYS:HB3	1:37:A:GLN:HG3	7	0.14
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	5	0.14
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	3	0.14
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	1	0.14
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	3	0.14
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	4	0.14
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	4	0.14
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	6	0.14
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	7	0.14
(1,1209)	1:21:A:VAL:HA	1:24:A:ALA:HB1	9	0.14
(1,1209)	1:21:A:VAL:HA	1:24:A:ALA:HB2	9	0.14
(1,1209)	1:21:A:VAL:HA	1:24:A:ALA:HB3	9	0.14
(1,1150)	1:19:A:SER:HA	1:22:A:HIS:HB3	7	0.14
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD11	13	0.14
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD12	13	0.14
(1,1102)	1:16:A:ALA:HB1	1:66:A:LEU:HD13	13	0.14
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD11	13	0.14
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD12	13	0.14
(1,1102)	1:16:A:ALA:HB2	1:66:A:LEU:HD13	13	0.14
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD11	13	0.14
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD12	13	0.14
(1,1102)	1:16:A:ALA:HB3	1:66:A:LEU:HD13	13	0.14
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	1	0.14
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	1	0.14
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	4	0.14
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	4	0.14
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	14	0.14
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	14	0.14
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG21	7	0.14
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG22	7	0.14
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG23	7	0.14
(1,1048)	1:11:A:LEU:HA	1:14:A:GLN:HB2	5	0.14
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	12	0.14
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	8	0.14
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	12	0.14
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD11	8	0.14
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD12	8	0.14
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD13	8	0.14
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD11	8	0.14
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD12	8	0.14
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD13	8	0.14
(1,996)	1:5:A:PRO:HB3	1:9:A:ARG:HB2	1	0.14
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	4	0.14
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	11	0.14
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	7	0.14
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	8	0.14
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	11	0.14
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	14	0.14
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	3	0.14
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	3	0.14
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	9	0.14
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	9	0.14
(1,835)	2:9:B:LEU:HA	2:11:B:LEU:H	11	0.14
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	14	0.14
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	14	0.14
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	5	0.14
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	9	0.14
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	15	0.14
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	12	0.14
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	15	0.14
(1,756)	1:75:A:GLN:HA	1:76:A:GLU:H	9	0.14
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	12	0.14
(1,746)	1:74:A:CYS:HA	1:75:A:GLN:HE21	12	0.14
(1,745)	1:74:A:CYS:HA	1:75:A:GLN:H	5	0.14
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	15	0.14
(1,694)	1:62:A:GLN:HG2	1:62:A:GLN:H	7	0.14
(1,694)	1:62:A:GLN:HG3	1:62:A:GLN:H	7	0.14
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	2	0.14
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	4	0.14
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	5	0.14
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	14	0.14
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	2	0.14
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	10	0.14
(1,673)	1:60:A:CYS:HB2	1:61:A:LYS:H	7	0.14
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	13	0.14
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	14	0.14
(1,664)	1:59:A:ILE:HA	1:62:A:GLN:HE22	13	0.14
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	8	0.14
(1,586)	1:52:A:LYS:HB2	1:53:A:THR:H	14	0.14
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	11	0.14
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	15	0.14
(1,578)	1:51:A:ARG:HB2	1:55:A:GLY:H	12	0.14
(1,578)	1:51:A:ARG:HB3	1:55:A:GLY:H	12	0.14
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	1	0.14
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	1	0.14
(1,538)	1:47:A:LYS:HB2	1:48:A:GLY:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:47:A:LYS:HB3	1:48:A:GLY:H	7	0.14
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	9	0.14
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	11	0.14
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	1	0.14
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	4	0.14
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	14	0.14
(1,441)	1:38:A:LYS:HB3	1:38:A:LYS:H	9	0.14
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	10	0.14
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	10	0.14
(1,429)	1:37:A:GLN:HG3	1:37:A:GLN:H	9	0.14
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	11	0.14
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	6	0.14
(1,393)	1:33:A:LEU:HB2	1:36:A:CYS:H	11	0.14
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	1	0.14
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	9	0.14
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	11	0.14
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	11	0.14
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	12	0.14
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	1	0.14
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	3	0.14
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	9	0.14
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	1	0.14
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	3	0.14
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	6	0.14
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	10	0.14
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	12	0.14
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	6	0.14
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	7	0.14
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	5	0.14
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	11	0.14
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	8	0.14
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	12	0.14
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	14	0.14
(1,242)	1:23:A:ALA:HB1	1:24:A:ALA:H	6	0.14
(1,242)	1:23:A:ALA:HB2	1:24:A:ALA:H	6	0.14
(1,242)	1:23:A:ALA:HB3	1:24:A:ALA:H	6	0.14
(1,242)	1:23:A:ALA:HB1	1:24:A:ALA:H	10	0.14
(1,242)	1:23:A:ALA:HB2	1:24:A:ALA:H	10	0.14
(1,242)	1:23:A:ALA:HB3	1:24:A:ALA:H	10	0.14
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	2	0.14
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	12	0.14
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	4	0.14
(1,157)	1:15:A:ARG:HG2	1:18:A:GLN:HE21	5	0.14
(1,157)	1:15:A:ARG:HG3	1:18:A:GLN:HE21	5	0.14
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	5	0.14
(1,125)	1:13:A:ILE:HB	1:14:A:GLN:H	7	0.14
(1,125)	1:13:A:ILE:HB	1:14:A:GLN:H	8	0.14
(1,125)	1:13:A:ILE:HB	1:14:A:GLN:H	11	0.14
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	6	0.14
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	7	0.14
(1,117)	1:13:A:ILE:HB	1:13:A:ILE:H	6	0.14
(1,63)	1:5:A:PRO:HD2	1:8:A:SER:H	12	0.14
(1,50)	1:3:A:GLN:HB3	1:4:A:SER:H	9	0.14
(1,48)	1:3:A:GLN:HA	1:4:A:SER:H	13	0.14
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	1	0.14
(1,18)	2:5:B:ALA:H	1:17:A:ILE:H	1	0.14
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	1	0.13
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	8	0.13
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	5	0.13
(2,36)	1:35:A:SER:O	1:39:A:MET:N	3	0.13
(2,2)	1:5:A:PRO:O	1:9:A:ARG:N	3	0.13
(1,1988)	2:17:B:GLU:HA	2:18:B:GLN:HA	6	0.13
(1,1988)	2:17:B:GLU:HA	2:18:B:GLN:HA	11	0.13
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD2	14	0.13
(1,1965)	1:90:A:LYS:HA	1:90:A:LYS:HD3	14	0.13
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	13	0.13
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD1	15	0.13
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD2	15	0.13
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE2	8	0.13
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE3	8	0.13
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	7	0.13
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	7	0.13
(1,1851)	1:69:A:TYR:HA	1:70:A:HIS:HA	5	0.13
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	8	0.13
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	8	0.13
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	8	0.13
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	10	0.13
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	10	0.13
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	10	0.13
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB1	15	0.13
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB2	15	0.13
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB3	15	0.13
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	14	0.13
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	1	0.13
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	4	0.13
(1,1684)	1:52:A:LYS:HG2	1:60:A:CYS:HB3	7	0.13
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	2	0.13
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	10	0.13
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	15	0.13
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB2	5	0.13
(1,1655)	1:51:A:ARG:HA	1:54:A:ASN:HB3	5	0.13
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	3	0.13
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	8	0.13
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	12	0.13
(1,1632)	1:50:A:LYS:HA	1:50:A:LYS:HG3	4	0.13
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD2	8	0.13
(1,1631)	1:50:A:LYS:HA	1:50:A:LYS:HD3	8	0.13
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD21	15	0.13
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD22	15	0.13
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD23	15	0.13
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD21	15	0.13
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD22	15	0.13
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD23	15	0.13
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD21	15	0.13
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD22	15	0.13
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD23	15	0.13
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	2	0.13
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	2	0.13
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	2	0.13
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	2	0.13
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	2	0.13
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	2	0.13
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	2	0.13
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	2	0.13
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	4	0.13
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	4	0.13
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	4	0.13
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	4	0.13
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	4	0.13
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	4	0.13
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	7	0.13
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	7	0.13
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	7	0.13
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	7	0.13
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	7	0.13
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD21	3	0.13
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD22	3	0.13
(1,1520)	1:42:A:VAL:HG11	1:63:A:LEU:HD23	3	0.13
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD21	3	0.13
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD22	3	0.13
(1,1520)	1:42:A:VAL:HG12	1:63:A:LEU:HD23	3	0.13
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD21	3	0.13
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD22	3	0.13
(1,1520)	1:42:A:VAL:HG13	1:63:A:LEU:HD23	3	0.13
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	8	0.13
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	3	0.13
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	1	0.13
(1,1471)	1:40:A:LYS:HA	1:42:A:VAL:HB	9	0.13
(1,1465)	1:40:A:LYS:HA	1:40:A:LYS:HG2	2	0.13
(1,1465)	1:40:A:LYS:HA	1:40:A:LYS:HG3	2	0.13
(1,1443)	1:39:A:MET:HB2	1:40:A:LYS:HB2	6	0.13
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	4	0.13
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	14	0.13
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	10	0.13
(1,1430)	1:38:A:LYS:HB3	1:41:A:ARG:HB2	9	0.13
(1,1422)	1:38:A:LYS:HG3	1:39:A:MET:HA	12	0.13
(1,1410)	1:38:A:LYS:HE2	1:38:A:LYS:HG2	3	0.13
(1,1410)	1:38:A:LYS:HE3	1:38:A:LYS:HG2	3	0.13
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	1	0.13
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	6	0.13
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	8	0.13
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	1	0.13
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	9	0.13
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	10	0.13
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	13	0.13
(1,1378)	1:34:A:PRO:HA	1:38:A:LYS:HG2	15	0.13
(1,1369)	1:34:A:PRO:HA	1:37:A:GLN:HG2	5	0.13
(1,1321)	1:31:A:CYS:HB3	1:37:A:GLN:HG3	6	0.13
(1,1321)	1:31:A:CYS:HB3	1:37:A:GLN:HG3	11	0.13
(1,1312)	1:30:A:ASN:HA	1:31:A:CYS:HB3	3	0.13
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	2	0.13
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	11	0.13
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	6	0.13
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	8	0.13
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	11	0.13
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	14	0.13
(1,1249)	1:23:A:ALA:HA	1:40:A:LYS:HE3	1	0.13
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	6	0.13
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	8	0.13
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	9	0.13
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	5	0.13
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	12	0.13
(1,1173)	1:20:A:LEU:HA	1:39:A:MET:HB3	12	0.13
(1,1173)	1:20:A:LEU:HA	1:39:A:MET:HB3	15	0.13
(1,1150)	1:19:A:SER:HA	1:22:A:HIS:HB3	10	0.13
(1,1150)	1:19:A:SER:HA	1:22:A:HIS:HB3	12	0.13
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD11	11	0.13
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD12	11	0.13
(1,1126)	1:17:A:ILE:HG12	1:66:A:LEU:HD13	11	0.13
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	11	0.13
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	3	0.13
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	3	0.13
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	12	0.13
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	12	0.13
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	13	0.13
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	13	0.13
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	15	0.13
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	3	0.13
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	4	0.13
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	5	0.13
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	10	0.13
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	15	0.13
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD11	5	0.13
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD12	5	0.13
(1,1034)	1:10:A:ARG:HG2	1:13:A:ILE:HD13	5	0.13
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD11	5	0.13
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD12	5	0.13
(1,1034)	1:10:A:ARG:HG3	1:13:A:ILE:HD13	5	0.13
(1,1031)	1:10:A:ARG:HA	1:13:A:ILE:HG12	9	0.13
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	1	0.13
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	5	0.13
(1,972)	1:3:A:GLN:HB3	1:8:A:SER:HA	8	0.13
(1,972)	1:3:A:GLN:HB3	1:8:A:SER:HA	12	0.13
(1,955)	2:24:B:PRO:HA	2:25:B:GLY:H	12	0.13
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	14	0.13
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	4	0.13
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	9	0.13
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	15	0.13
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	15	0.13
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	4	0.13
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	11	0.13
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	13	0.13
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	5	0.13
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	9	0.13
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	10	0.13
(1,845)	2:11:B:LEU:HG	2:11:B:LEU:H	5	0.13
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	5	0.13
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	5	0.13
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	13	0.13
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	13	0.13
(1,838)	2:10:B:MET:HG2	2:10:B:MET:H	5	0.13
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	1	0.13
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	1	0.13
(1,801)	2:4:B:GLN:HG2	2:4:B:GLN:HE21	10	0.13
(1,801)	2:4:B:GLN:HG3	2:4:B:GLN:HE21	10	0.13
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	2	0.13
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	11	0.13
(1,767)	1:78:A:LYS:HB3	1:78:A:LYS:H	8	0.13
(1,761)	1:77:A:ASN:HB3	1:77:A:ASN:H	10	0.13
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	5	0.13
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	8	0.13
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	4	0.13
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	6	0.13
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	5	0.13
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	6	0.13
(1,748)	1:75:A:GLN:HB2	1:75:A:GLN:H	14	0.13
(1,742)	1:73:A:HIS:HB2	1:73:A:HIS:H	13	0.13
(1,741)	1:73:A:HIS:HB3	1:73:A:HIS:H	11	0.13
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	2	0.13
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	15	0.13
(1,736)	1:72:A:LYS:HG2	1:72:A:LYS:H	4	0.13
(1,736)	1:72:A:LYS:HG3	1:72:A:LYS:H	4	0.13
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	10	0.13
(1,701)	1:62:A:GLN:HG2	1:62:A:GLN:HE21	11	0.13
(1,701)	1:62:A:GLN:HG3	1:62:A:GLN:HE21	11	0.13
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	1	0.13
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	12	0.13
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	13	0.13
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	11	0.13
(1,673)	1:60:A:CYS:HB2	1:61:A:LYS:H	9	0.13
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	11	0.13
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	12	0.13
(1,658)	1:59:A:ILE:H	1:60:A:CYS:HA	14	0.13
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	5	0.13
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	11	0.13
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	13	0.13
(1,628)	1:55:A:GLY:H	1:57:A:CYS:H	6	0.13
(1,622)	1:54:A:ASN:HA	1:56:A:GLY:H	1	0.13
(1,602)	1:53:A:THR:H	1:54:A:ASN:H	14	0.13
(1,591)	1:52:A:LYS:HD2	1:53:A:THR:H	6	0.13
(1,591)	1:52:A:LYS:HD3	1:53:A:THR:H	6	0.13
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	6	0.13
(1,578)	1:51:A:ARG:HB2	1:55:A:GLY:H	11	0.13
(1,578)	1:51:A:ARG:HB3	1:55:A:GLY:H	11	0.13
(1,570)	1:51:A:ARG:HB2	1:51:A:ARG:H	4	0.13
(1,570)	1:51:A:ARG:HB3	1:51:A:ARG:H	4	0.13
(1,544)	1:47:A:LYS:HA	1:49:A:CYS:H	8	0.13
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	13	0.13
(1,527)	1:45:A:HIS:H	1:49:A:CYS:H	9	0.13
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	3	0.13
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	10	0.13
(1,486)	1:41:A:ARG:H	1:42:A:VAL:H	11	0.13
(1,420)	1:36:A:CYS:HB2	1:37:A:GLN:H	9	0.13
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	2	0.13
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	4	0.13
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	5	0.13
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	6	0.13
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	14	0.13
(1,417)	1:36:A:CYS:H	1:37:A:GLN:H	3	0.13
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	1	0.13
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	5	0.13
(1,377)	1:33:A:LEU:HB2	1:33:A:LEU:H	11	0.13
(1,371)	1:32:A:SER:H	1:33:A:LEU:HG	3	0.13
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	10	0.13
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	15	0.13
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	4	0.13
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	11	0.13
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	7	0.13
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	9	0.13
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	11	0.13
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	13	0.13
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	2	0.13
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	3	0.13
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	12	0.13
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	14	0.13
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	11	0.13
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	11	0.13
(1,293)	1:26:A:CYS:HA	1:28:A:ASN:H	9	0.13
(1,286)	1:26:A:CYS:HB3	1:26:A:CYS:H	5	0.13
(1,285)	1:25:A:GLN:H	1:27:A:ARG:H	5	0.13
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	11	0.13
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	15	0.13
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	1	0.13
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	7	0.13
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	12	0.13
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	15	0.13
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	9	0.13
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	3	0.13
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	5	0.13
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	9	0.13
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	2	0.13
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	5	0.13
(1,227)	1:22:A:HIS:HB3	1:22:A:HIS:H	8	0.13
(1,227)	1:22:A:HIS:HB3	1:22:A:HIS:H	10	0.13
(1,227)	1:22:A:HIS:HB3	1:22:A:HIS:H	14	0.13
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	1	0.13
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	6	0.13
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	12	0.13
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	6	0.13
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	10	0.13
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	14	0.13
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	13	0.13
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	11	0.13
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	11	0.13
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	11	0.13
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	3	0.13
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	9	0.13
(1,88)	1:10:A:ARG:HB2	1:10:A:ARG:H	14	0.13
(1,88)	1:10:A:ARG:HB3	1:10:A:ARG:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	7	0.13
(1,51)	1:3:A:GLN:HA	1:7:A:ASP:H	10	0.13
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	9	0.13
(1,18)	2:5:B:ALA:H	1:17:A:ILE:H	14	0.13
(1,11)	1:62:A:GLN:HE22	2:13:B:PRO:HA	14	0.13
(2,87)	2:18:B:GLN:O	2:22:B:GLU:H	14	0.12
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	6	0.12
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	6	0.12
(2,56)	1:50:A:LYS:O	1:54:A:ASN:N	14	0.12
(2,52)	1:43:A:VAL:O	1:47:A:LYS:N	11	0.12
(2,52)	1:43:A:VAL:O	1:47:A:LYS:N	13	0.12
(2,36)	1:35:A:SER:O	1:39:A:MET:N	4	0.12
(1,1988)	2:17:B:GLU:HA	2:18:B:GLN:HA	2	0.12
(1,1987)	2:17:B:GLU:HA	2:17:B:GLU:HG2	6	0.12
(1,1987)	2:17:B:GLU:HA	2:17:B:GLU:HG3	6	0.12
(1,1968)	1:90:A:LYS:HE2	1:90:A:LYS:HB3	11	0.12
(1,1968)	1:90:A:LYS:HE3	1:90:A:LYS:HB3	11	0.12
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	2	0.12
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD1	7	0.12
(1,1943)	1:83:A:PHE:HB2	1:83:A:PHE:HD2	7	0.12
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE2	14	0.12
(1,1918)	1:78:A:LYS:HG2	1:78:A:LYS:HE3	14	0.12
(1,1916)	1:78:A:LYS:HB2	1:78:A:LYS:HD2	5	0.12
(1,1916)	1:78:A:LYS:HB2	1:78:A:LYS:HD3	5	0.12
(1,1894)	1:76:A:GLU:HA	1:77:A:ASN:HB2	5	0.12
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD2	3	0.12
(1,1874)	1:72:A:LYS:HB2	1:72:A:LYS:HD3	3	0.12
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG21	8	0.12
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG22	8	0.12
(1,1866)	1:71:A:ALA:HB1	1:87:A:ILE:HG23	8	0.12
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG21	8	0.12
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG22	8	0.12
(1,1866)	1:71:A:ALA:HB2	1:87:A:ILE:HG23	8	0.12
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG21	8	0.12
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG22	8	0.12
(1,1866)	1:71:A:ALA:HB3	1:87:A:ILE:HG23	8	0.12
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB1	3	0.12
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB2	3	0.12
(1,1847)	1:68:A:ALA:HA	1:71:A:ALA:HB3	3	0.12
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	3	0.12
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	3	0.12
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	4	0.12
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	4	0.12
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	4	0.12
(1,1792)	1:63:A:LEU:HD11	1:66:A:LEU:HD21	7	0.12
(1,1792)	1:63:A:LEU:HD11	1:66:A:LEU:HD22	7	0.12
(1,1792)	1:63:A:LEU:HD11	1:66:A:LEU:HD23	7	0.12
(1,1792)	1:63:A:LEU:HD12	1:66:A:LEU:HD21	7	0.12
(1,1792)	1:63:A:LEU:HD12	1:66:A:LEU:HD22	7	0.12
(1,1792)	1:63:A:LEU:HD12	1:66:A:LEU:HD23	7	0.12
(1,1792)	1:63:A:LEU:HD13	1:66:A:LEU:HD21	7	0.12
(1,1792)	1:63:A:LEU:HD13	1:66:A:LEU:HD22	7	0.12
(1,1792)	1:63:A:LEU:HD13	1:66:A:LEU:HD23	7	0.12
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	11	0.12
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	11	0.12
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	11	0.12
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	13	0.12
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	13	0.12
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	13	0.12
(1,1780)	1:63:A:LEU:HD11	1:63:A:LEU:HB2	14	0.12
(1,1780)	1:63:A:LEU:HD12	1:63:A:LEU:HB2	14	0.12
(1,1780)	1:63:A:LEU:HD13	1:63:A:LEU:HB2	14	0.12
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	7	0.12
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	8	0.12
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	11	0.12
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	4	0.12
(1,1743)	1:60:A:CYS:HB3	1:61:A:LYS:HB2	15	0.12
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	5	0.12
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	10	0.12
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	14	0.12
(1,1722)	1:58:A:PRO:HB2	1:61:A:LYS:HB3	2	0.12
(1,1719)	1:58:A:PRO:HG3	1:59:A:ILE:HA	6	0.12
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	13	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	3	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	3	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	3	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	4	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	4	0.12
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	4	0.12
(1,1667)	1:52:A:LYS:HB3	1:52:A:LYS:HD3	11	0.12
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	4	0.12
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	7	0.12
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1662)	1:52:A:LYS:HA	1:52:A:LYS:HD3	9	0.12
(1,1632)	1:50:A:LYS:HA	1:50:A:LYS:HG3	6	0.12
(1,1632)	1:50:A:LYS:HA	1:50:A:LYS:HG3	14	0.12
(1,1623)	1:49:A:CYS:HB2	1:57:A:CYS:HB3	15	0.12
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	10	0.12
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	11	0.12
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	15	0.12
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE2	14	0.12
(1,1599)	1:47:A:LYS:HA	1:52:A:LYS:HE3	14	0.12
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	8	0.12
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	8	0.12
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	8	0.12
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	8	0.12
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD21	2	0.12
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD22	2	0.12
(1,1586)	1:46:A:THR:HG21	1:63:A:LEU:HD23	2	0.12
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD21	2	0.12
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD22	2	0.12
(1,1586)	1:46:A:THR:HG22	1:63:A:LEU:HD23	2	0.12
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD21	2	0.12
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD22	2	0.12
(1,1586)	1:46:A:THR:HG23	1:63:A:LEU:HD23	2	0.12
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	8	0.12
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	3	0.12
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	3	0.12
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	3	0.12
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	3	0.12
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	3	0.12
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	3	0.12
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	1	0.12
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	1	0.12
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	1	0.12
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	11	0.12
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	11	0.12
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	11	0.12
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	13	0.12
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	13	0.12
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	13	0.12
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	5	0.12
(1,1503)	1:42:A:VAL:HA	1:45:A:HIS:HB3	14	0.12
(1,1494)	1:41:A:ARG:HA	1:45:A:HIS:HA	6	0.12
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	11	0.12
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD2	1	0.12
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD3	1	0.12
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	3	0.12
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	3	0.12
(1,1463)	1:40:A:LYS:HG2	1:40:A:LYS:HE2	9	0.12
(1,1463)	1:40:A:LYS:HG3	1:40:A:LYS:HE2	9	0.12
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	8	0.12
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	3	0.12
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	4	0.12
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	7	0.12
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	15	0.12
(1,1377)	1:34:A:PRO:HA	1:38:A:LYS:HG3	11	0.12
(1,1312)	1:30:A:ASN:HA	1:31:A:CYS:HB3	6	0.12
(1,1312)	1:30:A:ASN:HA	1:31:A:CYS:HB3	9	0.12
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	15	0.12
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	2	0.12
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	12	0.12
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	13	0.12
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	15	0.12
(1,1298)	1:27:A:ARG:HA	1:28:A:ASN:HB3	1	0.12
(1,1298)	1:27:A:ARG:HA	1:28:A:ASN:HB3	4	0.12
(1,1295)	1:27:A:ARG:HB2	1:27:A:ARG:HD2	10	0.12
(1,1295)	1:27:A:ARG:HB2	1:27:A:ARG:HD3	10	0.12
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	13	0.12
(1,1249)	1:23:A:ALA:HA	1:40:A:LYS:HE3	11	0.12
(1,1234)	1:23:A:ALA:HA	1:26:A:CYS:HA	14	0.12
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	2	0.12
(1,1230)	1:22:A:HIS:HB2	1:26:A:CYS:HB3	11	0.12
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	11	0.12
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	13	0.12
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	15	0.12
(1,1173)	1:20:A:LEU:HA	1:39:A:MET:HB3	7	0.12
(1,1173)	1:20:A:LEU:HA	1:39:A:MET:HB3	14	0.12
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD11	11	0.12
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD12	11	0.12
(1,1158)	1:20:A:LEU:HA	1:20:A:LEU:HD13	11	0.12
(1,1110)	1:17:A:ILE:HB	1:18:A:GLN:HB2	7	0.12
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	1	0.12
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	10	0.12
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	15	0.12
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	10	0.12
(1,1084)	1:14:A:GLN:HA	1:17:A:ILE:HD11	13	0.12
(1,1084)	1:14:A:GLN:HA	1:17:A:ILE:HD12	13	0.12
(1,1084)	1:14:A:GLN:HA	1:17:A:ILE:HD13	13	0.12
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	11	0.12
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	11	0.12
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	11	0.12
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	11	0.12
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	11	0.12
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	11	0.12
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	11	0.12
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	11	0.12
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	11	0.12
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG21	8	0.12
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG22	8	0.12
(1,1064)	1:13:A:ILE:HA	1:13:A:ILE:HG23	8	0.12
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	1	0.12
(1,1015)	1:8:A:SER:HA	1:12:A:SER:HB2	9	0.12
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB2	12	0.12
(1,999)	1:6:A:GLY:HA2	1:7:A:ASP:HB3	12	0.12
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB2	12	0.12
(1,999)	1:6:A:GLY:HA3	1:7:A:ASP:HB3	12	0.12
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	2	0.12
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	7	0.12
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	15	0.12
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	6	0.12
(1,974)	1:4:A:SER:HA	1:5:A:PRO:HD2	14	0.12
(1,945)	2:22:B:GLU:HB2	2:23:B:ASP:H	2	0.12
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	2	0.12
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	6	0.12
(1,924)	2:20:B:PHE:HB2	2:20:B:PHE:H	7	0.12
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	3	0.12
(1,923)	2:20:B:PHE:HB3	2:20:B:PHE:H	12	0.12
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	8	0.12
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	8	0.12
(1,900)	2:18:B:GLN:HG2	2:18:B:GLN:HE21	14	0.12
(1,900)	2:18:B:GLN:HG3	2:18:B:GLN:HE21	14	0.12
(1,883)	2:16:B:ILE:HG12	2:17:B:GLU:H	13	0.12
(1,872)	2:15:B:ASP:HA	2:17:B:GLU:H	7	0.12
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	1	0.12
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	1	0.12
(1,841)	2:10:B:MET:HB2	2:11:B:LEU:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	2:10:B:MET:HB3	2:11:B:LEU:H	4	0.12
(1,821)	2:8:B:ASP:HA	2:9:B:LEU:H	4	0.12
(1,767)	1:78:A:LYS:HB3	1:78:A:LYS:H	1	0.12
(1,761)	1:77:A:ASN:HB3	1:77:A:ASN:H	1	0.12
(1,761)	1:77:A:ASN:HB3	1:77:A:ASN:H	6	0.12
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	7	0.12
(1,759)	1:76:A:GLU:HB3	1:76:A:GLU:H	13	0.12
(1,744)	1:74:A:CYS:HB3	1:74:A:CYS:H	3	0.12
(1,743)	1:73:A:HIS:H	1:74:A:CYS:H	6	0.12
(1,741)	1:73:A:HIS:HB3	1:73:A:HIS:H	8	0.12
(1,741)	1:73:A:HIS:HB3	1:73:A:HIS:H	15	0.12
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	11	0.12
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	2	0.12
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	11	0.12
(1,704)	1:62:A:GLN:H	1:63:A:LEU:H	6	0.12
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	6	0.12
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	11	0.12
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	9	0.12
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	7	0.12
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	10	0.12
(1,658)	1:59:A:ILE:H	1:60:A:CYS:HA	10	0.12
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	4	0.12
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	7	0.12
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	10	0.12
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	6	0.12
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	11	0.12
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	1	0.12
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	1	0.12
(1,620)	1:54:A:ASN:HB2	1:55:A:GLY:H	15	0.12
(1,620)	1:54:A:ASN:HB3	1:55:A:GLY:H	15	0.12
(1,603)	1:53:A:THR:H	1:54:A:ASN:HA	6	0.12
(1,571)	1:51:A:ARG:HG2	1:51:A:ARG:H	9	0.12
(1,571)	1:51:A:ARG:HG3	1:51:A:ARG:H	9	0.12
(1,571)	1:51:A:ARG:HG2	1:51:A:ARG:H	10	0.12
(1,571)	1:51:A:ARG:HG3	1:51:A:ARG:H	10	0.12
(1,562)	1:50:A:LYS:HB2	1:50:A:LYS:H	10	0.12
(1,546)	1:48:A:GLY:H	1:49:A:CYS:H	2	0.12
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	12	0.12
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	1	0.12
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	4	0.12
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	8	0.12
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:38:A:LYS:HB3	1:38:A:LYS:H	7	0.12
(1,431)	1:37:A:GLN:HB2	1:37:A:GLN:HE21	10	0.12
(1,431)	1:37:A:GLN:HB3	1:37:A:GLN:HE21	10	0.12
(1,430)	1:37:A:GLN:HG2	1:37:A:GLN:HE21	2	0.12
(1,430)	1:37:A:GLN:HG3	1:37:A:GLN:HE21	2	0.12
(1,429)	1:37:A:GLN:HG3	1:37:A:GLN:H	1	0.12
(1,429)	1:37:A:GLN:HG3	1:37:A:GLN:H	11	0.12
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	7	0.12
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	8	0.12
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	10	0.12
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	12	0.12
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	13	0.12
(1,419)	1:36:A:CYS:HB3	1:37:A:GLN:H	15	0.12
(1,411)	1:35:A:SER:HB2	1:35:A:SER:H	14	0.12
(1,411)	1:35:A:SER:HB3	1:35:A:SER:H	14	0.12
(1,377)	1:33:A:LEU:HB2	1:33:A:LEU:H	9	0.12
(1,375)	1:32:A:SER:H	1:36:A:CYS:HB3	1	0.12
(1,364)	1:32:A:SER:HB3	1:32:A:SER:H	4	0.12
(1,364)	1:32:A:SER:HB3	1:32:A:SER:H	5	0.12
(1,364)	1:32:A:SER:HB3	1:32:A:SER:H	14	0.12
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	9	0.12
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	7	0.12
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	10	0.12
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	12	0.12
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	4	0.12
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	8	0.12
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	14	0.12
(1,319)	1:28:A:ASN:HB2	1:28:A:ASN:HD21	15	0.12
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	5	0.12
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	8	0.12
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	10	0.12
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	15	0.12
(1,297)	1:27:A:ARG:HD2	1:27:A:ARG:H	7	0.12
(1,297)	1:27:A:ARG:HD3	1:27:A:ARG:H	7	0.12
(1,286)	1:26:A:CYS:HB3	1:26:A:CYS:H	1	0.12
(1,286)	1:26:A:CYS:HB3	1:26:A:CYS:H	2	0.12
(1,286)	1:26:A:CYS:HB3	1:26:A:CYS:H	12	0.12
(1,286)	1:26:A:CYS:HB3	1:26:A:CYS:H	15	0.12
(1,285)	1:25:A:GLN:H	1:27:A:ARG:H	4	0.12
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	10	0.12
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	14	0.12
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	11	0.12
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	15	0.12
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	6	0.12
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	2	0.12
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	7	0.12
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	8	0.12
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	12	0.12
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	14	0.12
(1,249)	1:23:A:ALA:HA	1:27:A:ARG:H	7	0.12
(1,242)	1:23:A:ALA:HB1	1:24:A:ALA:H	14	0.12
(1,242)	1:23:A:ALA:HB2	1:24:A:ALA:H	14	0.12
(1,242)	1:23:A:ALA:HB3	1:24:A:ALA:H	14	0.12
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	3	0.12
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	9	0.12
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	9	0.12
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	15	0.12
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	4	0.12
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	4	0.12
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	4	0.12
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	14	0.12
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	14	0.12
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	14	0.12
(1,125)	1:13:A:ILE:HB	1:14:A:GLN:H	6	0.12
(1,118)	1:13:A:ILE:HG13	1:13:A:ILE:H	8	0.12
(1,112)	1:12:A:SER:HB2	1:12:A:SER:H	8	0.12
(1,111)	1:12:A:SER:HB3	1:12:A:SER:H	8	0.12
(1,79)	1:8:A:SER:HB2	1:8:A:SER:H	12	0.12
(1,79)	1:8:A:SER:HB3	1:8:A:SER:H	12	0.12
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	8	0.12
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	10	0.12
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	7	0.12
(1,16)	1:69:A:TYR:HA	2:10:B:MET:HB2	6	0.12
(2,61)	1:59:A:ILE:O	1:63:A:LEU:H	7	0.11
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	3	0.11
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	4	0.11
(2,59)	1:58:A:PRO:O	1:62:A:GLN:H	10	0.11
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	3	0.11
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	8	0.11
(2,54)	1:44:A:GLN:O	1:48:A:GLY:N	10	0.11
(2,36)	1:35:A:SER:O	1:39:A:MET:N	5	0.11
(2,36)	1:35:A:SER:O	1:39:A:MET:N	7	0.11
(2,36)	1:35:A:SER:O	1:39:A:MET:N	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,10)	1:9:A:ARG:O	1:13:A:ILE:N	10	0.11
(1,1962)	1:89:A:GLN:HB3	1:90:A:LYS:HA	1	0.11
(1,1953)	1:85:A:LEU:HD11	1:85:A:LEU:HB3	10	0.11
(1,1953)	1:85:A:LEU:HD12	1:85:A:LEU:HB3	10	0.11
(1,1953)	1:85:A:LEU:HD13	1:85:A:LEU:HB3	10	0.11
(1,1916)	1:78:A:LYS:HB2	1:78:A:LYS:HD2	3	0.11
(1,1916)	1:78:A:LYS:HB2	1:78:A:LYS:HD3	3	0.11
(1,1913)	1:78:A:LYS:HA	1:78:A:LYS:HG2	11	0.11
(1,1884)	1:74:A:CYS:HB3	1:76:A:GLU:HB3	5	0.11
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	13	0.11
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	13	0.11
(1,1855)	1:69:A:TYR:HB3	1:72:A:LYS:HB2	1	0.11
(1,1852)	1:69:A:TYR:HA	1:72:A:LYS:HA	6	0.11
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	5	0.11
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	5	0.11
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	5	0.11
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD1	4	0.11
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD2	4	0.11
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD1	4	0.11
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD2	4	0.11
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD1	4	0.11
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD2	4	0.11
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB1	2	0.11
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB2	2	0.11
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB3	2	0.11
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD11	13	0.11
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD12	13	0.11
(1,1777)	1:63:A:LEU:HB2	1:63:A:LEU:HD13	13	0.11
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD11	13	0.11
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD12	13	0.11
(1,1777)	1:63:A:LEU:HB3	1:63:A:LEU:HD13	13	0.11
(1,1762)	1:61:A:LYS:HA	1:64:A:ILE:HB	4	0.11
(1,1745)	1:60:A:CYS:HA	1:63:A:LEU:HB3	3	0.11
(1,1732)	1:59:A:ILE:HA	1:59:A:ILE:HG13	8	0.11
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	12	0.11
(1,1690)	1:53:A:THR:HA	1:60:A:CYS:HB3	12	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	9	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	9	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	9	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	11	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	11	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG21	12	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG22	12	0.11
(1,1687)	1:53:A:THR:HA	1:53:A:THR:HG23	12	0.11
(1,1684)	1:52:A:LYS:HG2	1:60:A:CYS:HB3	9	0.11
(1,1684)	1:52:A:LYS:HG2	1:60:A:CYS:HB3	15	0.11
(1,1679)	1:52:A:LYS:HA	1:60:A:CYS:HB2	9	0.11
(1,1658)	1:51:A:ARG:HD2	1:55:A:GLY:HA2	1	0.11
(1,1658)	1:51:A:ARG:HD2	1:55:A:GLY:HA3	1	0.11
(1,1658)	1:51:A:ARG:HD3	1:55:A:GLY:HA2	1	0.11
(1,1658)	1:51:A:ARG:HD3	1:55:A:GLY:HA3	1	0.11
(1,1656)	1:51:A:ARG:HD2	1:54:A:ASN:HB2	11	0.11
(1,1656)	1:51:A:ARG:HD2	1:54:A:ASN:HB3	11	0.11
(1,1656)	1:51:A:ARG:HD3	1:54:A:ASN:HB2	11	0.11
(1,1656)	1:51:A:ARG:HD3	1:54:A:ASN:HB3	11	0.11
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	3	0.11
(1,1642)	1:50:A:LYS:HA	1:52:A:LYS:HG3	4	0.11
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	6	0.11
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	14	0.11
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	4	0.11
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	3	0.11
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	7	0.11
(1,1598)	1:47:A:LYS:HA	1:52:A:LYS:HD2	6	0.11
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	5	0.11
(1,1593)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	5	0.11
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	5	0.11
(1,1593)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	5	0.11
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD2	5	0.11
(1,1553)	1:44:A:GLN:HA	1:47:A:LYS:HD3	5	0.11
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG2	10	0.11
(1,1528)	1:43:A:VAL:HG11	1:44:A:GLN:HG3	10	0.11
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG2	10	0.11
(1,1528)	1:43:A:VAL:HG12	1:44:A:GLN:HG3	10	0.11
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG2	10	0.11
(1,1528)	1:43:A:VAL:HG13	1:44:A:GLN:HG3	10	0.11
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	4	0.11
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	4	0.11
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	4	0.11
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	8	0.11
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	8	0.11
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	8	0.11
(1,1527)	1:43:A:VAL:HG11	1:44:A:GLN:HA	12	0.11
(1,1527)	1:43:A:VAL:HG12	1:44:A:GLN:HA	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1527)	1:43:A:VAL:HG13	1:44:A:GLN:HA	12	0.11
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	2	0.11
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	2	0.11
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	2	0.11
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	11	0.11
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	11	0.11
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	11	0.11
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	7	0.11
(1,1500)	1:42:A:VAL:HA	1:45:A:HIS:HB2	14	0.11
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	8	0.11
(1,1471)	1:40:A:LYS:HA	1:42:A:VAL:HB	7	0.11
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	1	0.11
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	2	0.11
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	5	0.11
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	13	0.11
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	11	0.11
(1,1430)	1:38:A:LYS:HB3	1:41:A:ARG:HB2	15	0.11
(1,1426)	1:38:A:LYS:HA	1:41:A:ARG:HB2	12	0.11
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	5	0.11
(1,1407)	1:38:A:LYS:HA	1:38:A:LYS:HG2	11	0.11
(1,1405)	1:37:A:GLN:HA	1:41:A:ARG:HB2	6	0.11
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	11	0.11
(1,1312)	1:30:A:ASN:HA	1:31:A:CYS:HB3	5	0.11
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	6	0.11
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	7	0.11
(1,1303)	1:28:A:ASN:HB3	1:31:A:CYS:HB2	12	0.11
(1,1302)	1:28:A:ASN:HB3	1:31:A:CYS:HB3	9	0.11
(1,1292)	1:26:A:CYS:HB3	1:40:A:LYS:HE2	5	0.11
(1,1284)	1:25:A:GLN:HB2	1:80:A:PRO:HG3	2	0.11
(1,1281)	1:25:A:GLN:HG3	1:80:A:PRO:HD3	7	0.11
(1,1279)	1:25:A:GLN:HA	1:80:A:PRO:HB3	3	0.11
(1,1254)	1:23:A:ALA:HB1	1:40:A:LYS:HA	1	0.11
(1,1254)	1:23:A:ALA:HB2	1:40:A:LYS:HA	1	0.11
(1,1254)	1:23:A:ALA:HB3	1:40:A:LYS:HA	1	0.11
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	8	0.11
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	9	0.11
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB1	14	0.11
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB2	14	0.11
(1,1196)	1:20:A:LEU:HD21	1:67:A:ALA:HB3	14	0.11
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB1	14	0.11
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB2	14	0.11
(1,1196)	1:20:A:LEU:HD22	1:67:A:ALA:HB3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB1	14	0.11
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB2	14	0.11
(1,1196)	1:20:A:LEU:HD23	1:67:A:ALA:HB3	14	0.11
(1,1173)	1:20:A:LEU:HA	1:39:A:MET:HB3	4	0.11
(1,1150)	1:19:A:SER:HA	1:22:A:HIS:HB3	15	0.11
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	7	0.11
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	14	0.11
(1,1091)	1:15:A:ARG:HA	1:16:A:ALA:HA	2	0.11
(1,1091)	1:15:A:ARG:HA	1:16:A:ALA:HA	9	0.11
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG2	5	0.11
(1,1090)	1:15:A:ARG:HA	1:15:A:ARG:HG3	5	0.11
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB1	7	0.11
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB2	7	0.11
(1,1068)	1:13:A:ILE:HG21	1:16:A:ALA:HB3	7	0.11
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB1	7	0.11
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB2	7	0.11
(1,1068)	1:13:A:ILE:HG22	1:16:A:ALA:HB3	7	0.11
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB1	7	0.11
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB2	7	0.11
(1,1068)	1:13:A:ILE:HG23	1:16:A:ALA:HB3	7	0.11
(1,1062)	1:13:A:ILE:HA	1:13:A:ILE:HG13	2	0.11
(1,1062)	1:13:A:ILE:HA	1:13:A:ILE:HG13	10	0.11
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	3	0.11
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	9	0.11
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	1	0.11
(1,1043)	1:11:A:LEU:HB2	1:12:A:SER:HA	13	0.11
(1,1032)	1:10:A:ARG:HA	1:13:A:ILE:HB	6	0.11
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD11	15	0.11
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD12	15	0.11
(1,1029)	1:10:A:ARG:HB2	1:11:A:LEU:HD13	15	0.11
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD11	15	0.11
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD12	15	0.11
(1,1029)	1:10:A:ARG:HB3	1:11:A:LEU:HD13	15	0.11
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	8	0.11
(1,998)	1:5:A:PRO:HB2	1:9:A:ARG:HB2	1	0.11
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	10	0.11
(1,980)	1:4:A:SER:HA	1:7:A:ASP:HB3	13	0.11
(1,972)	1:3:A:GLN:HB3	1:8:A:SER:HA	3	0.11
(1,948)	2:22:B:GLU:H	2:22:B:GLU:HB2	14	0.11
(1,942)	2:22:B:GLU:HA	2:23:B:ASP:H	6	0.11
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	7	0.11
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,905)	2:18:B:GLN:HA	2:19:B:TRP:HE1	10	0.11
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	4	0.11
(1,861)	2:13:B:PRO:HB2	2:14:B:ASP:H	12	0.11
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	4	0.11
(1,858)	2:12:B:SER:HB2	2:14:B:ASP:H	9	0.11
(1,850)	2:11:B:LEU:HB2	2:12:B:SER:H	6	0.11
(1,850)	2:11:B:LEU:HB3	2:12:B:SER:H	6	0.11
(1,845)	2:11:B:LEU:HG	2:11:B:LEU:H	3	0.11
(1,838)	2:10:B:MET:HG2	2:10:B:MET:H	6	0.11
(1,821)	2:8:B:ASP:HA	2:9:B:LEU:H	13	0.11
(1,788)	1:89:A:GLN:HA	1:90:A:LYS:H	12	0.11
(1,767)	1:78:A:LYS:HB3	1:78:A:LYS:H	9	0.11
(1,760)	1:76:A:GLU:HA	1:77:A:ASN:H	11	0.11
(1,759)	1:76:A:GLU:HB3	1:76:A:GLU:H	7	0.11
(1,744)	1:74:A:CYS:HB3	1:74:A:CYS:H	6	0.11
(1,741)	1:73:A:HIS:HB3	1:73:A:HIS:H	4	0.11
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	7	0.11
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	13	0.11
(1,740)	1:72:A:LYS:HB2	1:73:A:HIS:H	14	0.11
(1,730)	1:70:A:HIS:HB3	1:70:A:HIS:H	7	0.11
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	15	0.11
(1,704)	1:62:A:GLN:H	1:63:A:LEU:H	8	0.11
(1,704)	1:62:A:GLN:H	1:63:A:LEU:H	12	0.11
(1,704)	1:62:A:GLN:H	1:63:A:LEU:H	13	0.11
(1,685)	1:61:A:LYS:HB2	1:62:A:GLN:H	7	0.11
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	7	0.11
(1,679)	1:61:A:LYS:HB2	1:61:A:LYS:H	7	0.11
(1,679)	1:61:A:LYS:HB2	1:61:A:LYS:H	9	0.11
(1,667)	1:60:A:CYS:HB3	1:60:A:CYS:H	14	0.11
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	9	0.11
(1,653)	1:59:A:ILE:HB	1:60:A:CYS:H	7	0.11
(1,650)	1:59:A:ILE:HG12	1:59:A:ILE:H	9	0.11
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	6	0.11
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	14	0.11
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	15	0.11
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	2	0.11
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	12	0.11
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	13	0.11
(1,633)	1:56:A:GLY:H	1:57:A:CYS:HB3	5	0.11
(1,600)	1:53:A:THR:HG21	1:53:A:THR:H	7	0.11
(1,600)	1:53:A:THR:HG22	1:53:A:THR:H	7	0.11
(1,600)	1:53:A:THR:HG23	1:53:A:THR:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:52:A:LYS:HA	1:53:A:THR:H	3	0.11
(1,590)	1:52:A:LYS:HA	1:53:A:THR:H	9	0.11
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	1	0.11
(1,578)	1:51:A:ARG:HB2	1:55:A:GLY:H	13	0.11
(1,578)	1:51:A:ARG:HB3	1:55:A:GLY:H	13	0.11
(1,577)	1:51:A:ARG:HA	1:54:A:ASN:HD21	11	0.11
(1,565)	1:50:A:LYS:HG2	1:50:A:LYS:H	12	0.11
(1,546)	1:48:A:GLY:H	1:49:A:CYS:H	1	0.11
(1,546)	1:48:A:GLY:H	1:49:A:CYS:H	12	0.11
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	7	0.11
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	11	0.11
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	2	0.11
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	3	0.11
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	5	0.11
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	6	0.11
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	10	0.11
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	12	0.11
(1,523)	1:45:A:HIS:H	1:46:A:THR:H	15	0.11
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	7	0.11
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	12	0.11
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	13	0.11
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	14	0.11
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	15	0.11
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	7	0.11
(1,499)	1:42:A:VAL:HB	1:42:A:VAL:H	9	0.11
(1,483)	1:41:A:ARG:HB2	1:41:A:ARG:H	1	0.11
(1,483)	1:41:A:ARG:HB2	1:41:A:ARG:H	4	0.11
(1,483)	1:41:A:ARG:HB2	1:41:A:ARG:H	6	0.11
(1,483)	1:41:A:ARG:HB2	1:41:A:ARG:H	7	0.11
(1,441)	1:38:A:LYS:HB3	1:38:A:LYS:H	1	0.11
(1,441)	1:38:A:LYS:HB3	1:38:A:LYS:H	4	0.11
(1,429)	1:37:A:GLN:HG3	1:37:A:GLN:H	3	0.11
(1,429)	1:37:A:GLN:HG3	1:37:A:GLN:H	12	0.11
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	7	0.11
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	13	0.11
(1,393)	1:33:A:LEU:HB2	1:36:A:CYS:H	9	0.11
(1,359)	1:31:A:CYS:HB2	1:32:A:SER:H	3	0.11
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	1	0.11
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	5	0.11
(1,347)	1:30:A:ASN:HA	1:30:A:ASN:HD21	1	0.11
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	8	0.11
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	14	0.11
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	15	0.11
(1,340)	1:29:A:ALA:HB1	1:30:A:ASN:HD21	3	0.11
(1,340)	1:29:A:ALA:HB2	1:30:A:ASN:HD21	3	0.11
(1,340)	1:29:A:ALA:HB3	1:30:A:ASN:HD21	3	0.11
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	6	0.11
(1,315)	1:28:A:ASN:HB3	1:28:A:ASN:HD22	7	0.11
(1,285)	1:25:A:GLN:H	1:27:A:ARG:H	6	0.11
(1,283)	1:25:A:GLN:HE21	1:26:A:CYS:HA	1	0.11
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	1	0.11
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	4	0.11
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	5	0.11
(1,282)	1:25:A:GLN:HE22	1:26:A:CYS:HA	13	0.11
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	2	0.11
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	3	0.11
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	1	0.11
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	3	0.11
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	7	0.11
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	3	0.11
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	12	0.11
(1,257)	1:24:A:ALA:H	1:25:A:GLN:HG2	4	0.11
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	1	0.11
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	6	0.11
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	10	0.11
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	11	0.11
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	13	0.11
(1,255)	1:24:A:ALA:H	1:25:A:GLN:H	15	0.11
(1,239)	1:23:A:ALA:HB1	1:23:A:ALA:H	6	0.11
(1,239)	1:23:A:ALA:HB2	1:23:A:ALA:H	6	0.11
(1,239)	1:23:A:ALA:HB3	1:23:A:ALA:H	6	0.11
(1,239)	1:23:A:ALA:HB1	1:23:A:ALA:H	7	0.11
(1,239)	1:23:A:ALA:HB2	1:23:A:ALA:H	7	0.11
(1,239)	1:23:A:ALA:HB3	1:23:A:ALA:H	7	0.11
(1,227)	1:22:A:HIS:HB3	1:22:A:HIS:H	4	0.11
(1,227)	1:22:A:HIS:HB3	1:22:A:HIS:H	13	0.11
(1,227)	1:22:A:HIS:HB3	1:22:A:HIS:H	15	0.11
(1,224)	1:21:A:VAL:HG11	1:25:A:GLN:HE21	3	0.11
(1,224)	1:21:A:VAL:HG12	1:25:A:GLN:HE21	3	0.11
(1,224)	1:21:A:VAL:HG13	1:25:A:GLN:HE21	3	0.11
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	4	0.11
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	5	0.11
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	11	0.11
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	15	0.11
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	2	0.11
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	3	0.11
(1,165)	1:17:A:ILE:HG12	1:17:A:ILE:H	14	0.11
(1,161)	1:16:A:ALA:HB1	1:17:A:ILE:H	13	0.11
(1,161)	1:16:A:ALA:HB2	1:17:A:ILE:H	13	0.11
(1,161)	1:16:A:ALA:HB3	1:17:A:ILE:H	13	0.11
(1,146)	1:15:A:ARG:HB2	1:15:A:ARG:H	11	0.11
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	10	0.11
(1,126)	1:13:A:ILE:HD11	1:14:A:GLN:H	10	0.11
(1,126)	1:13:A:ILE:HD12	1:14:A:GLN:H	10	0.11
(1,126)	1:13:A:ILE:HD13	1:14:A:GLN:H	10	0.11
(1,124)	1:13:A:ILE:HG13	1:14:A:GLN:H	10	0.11
(1,117)	1:13:A:ILE:HB	1:13:A:ILE:H	15	0.11
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	4	0.11
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	12	0.11
(1,64)	1:5:A:PRO:HA	1:9:A:ARG:H	6	0.11
(1,54)	1:4:A:SER:HA	1:6:A:GLY:H	14	0.11
(1,51)	1:3:A:GLN:HA	1:7:A:ASP:H	4	0.11
(1,51)	1:3:A:GLN:HA	1:7:A:ASP:H	5	0.11
(1,47)	1:3:A:GLN:H	1:4:A:SER:HA	14	0.11
(1,40)	2:19:B:TRP:H	1:59:A:ILE:HG12	14	0.11
(1,12)	1:62:A:GLN:HE22	2:11:B:LEU:HG	13	0.11
(2,61)	1:59:A:ILE:O	1:63:A:LEU:H	9	0.1
(2,55)	1:50:A:LYS:O	1:54:A:ASN:H	1	0.1
(2,54)	1:44:A:GLN:O	1:48:A:GLY:N	12	0.1
(2,52)	1:43:A:VAL:O	1:47:A:LYS:N	9	0.1
(2,10)	1:9:A:ARG:O	1:13:A:ILE:N	12	0.1
(1,1979)	2:10:B:MET:HG2	2:10:B:MET:HA	8	0.1
(1,1979)	2:10:B:MET:HG3	2:10:B:MET:HA	8	0.1
(1,1968)	1:90:A:LYS:HE2	1:90:A:LYS:HB3	12	0.1
(1,1968)	1:90:A:LYS:HE3	1:90:A:LYS:HB3	12	0.1
(1,1968)	1:90:A:LYS:HE2	1:90:A:LYS:HB3	13	0.1
(1,1968)	1:90:A:LYS:HE3	1:90:A:LYS:HB3	13	0.1
(1,1939)	1:82:A:PRO:HD2	1:83:A:PHE:HA	2	0.1
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD2	7	0.1
(1,1873)	1:72:A:LYS:HB3	1:72:A:LYS:HD3	7	0.1
(1,1855)	1:69:A:TYR:HB3	1:72:A:LYS:HB2	12	0.1
(1,1822)	1:66:A:LEU:HD21	1:66:A:LEU:HA	8	0.1
(1,1822)	1:66:A:LEU:HD22	1:66:A:LEU:HA	8	0.1
(1,1822)	1:66:A:LEU:HD23	1:66:A:LEU:HA	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1821)	1:66:A:LEU:HD11	1:66:A:LEU:HB2	11	0.1
(1,1821)	1:66:A:LEU:HD12	1:66:A:LEU:HB2	11	0.1
(1,1821)	1:66:A:LEU:HD13	1:66:A:LEU:HB2	11	0.1
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD1	1	0.1
(1,1818)	1:65:A:ALA:HB1	1:69:A:TYR:HD2	1	0.1
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD1	1	0.1
(1,1818)	1:65:A:ALA:HB2	1:69:A:TYR:HD2	1	0.1
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD1	1	0.1
(1,1818)	1:65:A:ALA:HB3	1:69:A:TYR:HD2	1	0.1
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB1	10	0.1
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB2	10	0.1
(1,1809)	1:64:A:ILE:HA	1:67:A:ALA:HB3	10	0.1
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	5	0.1
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	5	0.1
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	5	0.1
(1,1781)	1:63:A:LEU:HD21	1:63:A:LEU:HB3	10	0.1
(1,1781)	1:63:A:LEU:HD22	1:63:A:LEU:HB3	10	0.1
(1,1781)	1:63:A:LEU:HD23	1:63:A:LEU:HB3	10	0.1
(1,1770)	1:62:A:GLN:HG2	1:62:A:GLN:HA	11	0.1
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD11	6	0.1
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD12	6	0.1
(1,1731)	1:59:A:ILE:HB	1:59:A:ILE:HD13	6	0.1
(1,1728)	1:58:A:PRO:HB2	1:62:A:GLN:HG2	1	0.1
(1,1681)	1:52:A:LYS:HD3	1:60:A:CYS:HB2	9	0.1
(1,1681)	1:52:A:LYS:HD3	1:60:A:CYS:HB2	15	0.1
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	5	0.1
(1,1654)	1:51:A:ARG:HA	1:52:A:LYS:HG3	8	0.1
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE2	2	0.1
(1,1646)	1:50:A:LYS:HD2	1:52:A:LYS:HE3	2	0.1
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE2	2	0.1
(1,1646)	1:50:A:LYS:HD3	1:52:A:LYS:HE3	2	0.1
(1,1638)	1:50:A:LYS:HA	1:51:A:ARG:HA	5	0.1
(1,1630)	1:50:A:LYS:HA	1:50:A:LYS:HG2	7	0.1
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	5	0.1
(1,1617)	1:49:A:CYS:HB2	1:52:A:LYS:HG2	14	0.1
(1,1601)	1:47:A:LYS:HA	1:52:A:LYS:HD3	2	0.1
(1,1556)	1:45:A:HIS:HA	1:46:A:THR:HB	1	0.1
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	9	0.1
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	9	0.1
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	9	0.1
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG11	15	0.1
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG12	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	1:43:A:VAL:HA	1:43:A:VAL:HG13	15	0.1
(1,1483)	1:41:A:ARG:HB3	1:42:A:VAL:HB	2	0.1
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD2	7	0.1
(1,1481)	1:41:A:ARG:HB2	1:41:A:ARG:HD3	7	0.1
(1,1471)	1:40:A:LYS:HA	1:42:A:VAL:HB	6	0.1
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	3	0.1
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	7	0.1
(1,1435)	1:39:A:MET:HA	1:39:A:MET:HG2	15	0.1
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	2	0.1
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	6	0.1
(1,1433)	1:38:A:LYS:HG3	1:42:A:VAL:HB	13	0.1
(1,1430)	1:38:A:LYS:HB3	1:41:A:ARG:HB2	5	0.1
(1,1426)	1:38:A:LYS:HA	1:41:A:ARG:HB2	1	0.1
(1,1426)	1:38:A:LYS:HA	1:41:A:ARG:HB2	3	0.1
(1,1426)	1:38:A:LYS:HA	1:41:A:ARG:HB2	6	0.1
(1,1411)	1:38:A:LYS:HE2	1:38:A:LYS:HB3	1	0.1
(1,1411)	1:38:A:LYS:HE3	1:38:A:LYS:HB3	1	0.1
(1,1393)	1:36:A:CYS:HB3	1:40:A:LYS:HE3	9	0.1
(1,1377)	1:34:A:PRO:HA	1:38:A:LYS:HG3	2	0.1
(1,1369)	1:34:A:PRO:HA	1:37:A:GLN:HG2	2	0.1
(1,1312)	1:30:A:ASN:HA	1:31:A:CYS:HB3	12	0.1
(1,1298)	1:27:A:ARG:HA	1:28:A:ASN:HB3	9	0.1
(1,1298)	1:27:A:ARG:HA	1:28:A:ASN:HB3	13	0.1
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	1	0.1
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	2	0.1
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	3	0.1
(1,1228)	1:22:A:HIS:HA	1:26:A:CYS:HB3	14	0.1
(1,1150)	1:19:A:SER:HA	1:22:A:HIS:HB3	14	0.1
(1,1110)	1:17:A:ILE:HB	1:18:A:GLN:HB2	5	0.1
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	3	0.1
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	5	0.1
(1,1105)	1:17:A:ILE:HG12	1:17:A:ILE:HA	8	0.1
(1,1091)	1:15:A:ARG:HA	1:16:A:ALA:HA	6	0.1
(1,1091)	1:15:A:ARG:HA	1:16:A:ALA:HA	13	0.1
(1,1047)	1:11:A:LEU:HA	1:14:A:GLN:HB3	6	0.1
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG2	14	0.1
(1,1023)	1:10:A:ARG:HA	1:10:A:ARG:HG3	14	0.1
(1,1021)	1:9:A:ARG:HB3	1:12:A:SER:HB3	8	0.1
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	4	0.1
(1,1008)	1:7:A:ASP:HA	1:11:A:LEU:HG	12	0.1
(1,962)	1:2:A:THR:HB	1:3:A:GLN:HA	8	0.1
(1,962)	1:2:A:THR:HB	1:3:A:GLN:HA	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,945)	2:22:B:GLU:HB2	2:23:B:ASP:H	5	0.1
(1,936)	2:21:B:THR:H	2:22:B:GLU:HA	15	0.1
(1,845)	2:11:B:LEU:HG	2:11:B:LEU:H	2	0.1
(1,821)	2:8:B:ASP:HA	2:9:B:LEU:H	1	0.1
(1,821)	2:8:B:ASP:HA	2:9:B:LEU:H	11	0.1
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	5	0.1
(1,757)	1:75:A:GLN:HE21	1:88:A:LYS:HA	10	0.1
(1,744)	1:74:A:CYS:HB3	1:74:A:CYS:H	11	0.1
(1,727)	1:68:A:ALA:H	1:69:A:TYR:H	2	0.1
(1,726)	1:68:A:ALA:HB1	1:68:A:ALA:H	15	0.1
(1,726)	1:68:A:ALA:HB2	1:68:A:ALA:H	15	0.1
(1,726)	1:68:A:ALA:HB3	1:68:A:ALA:H	15	0.1
(1,704)	1:62:A:GLN:H	1:63:A:LEU:H	4	0.1
(1,693)	1:62:A:GLN:HB2	1:62:A:GLN:H	13	0.1
(1,693)	1:62:A:GLN:HB3	1:62:A:GLN:H	13	0.1
(1,684)	1:61:A:LYS:HB3	1:62:A:GLN:H	14	0.1
(1,666)	1:60:A:CYS:HB2	1:60:A:CYS:H	5	0.1
(1,640)	1:58:A:PRO:HA	1:59:A:ILE:H	2	0.1
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	1	0.1
(1,638)	1:57:A:CYS:H	1:61:A:LYS:HA	10	0.1
(1,590)	1:52:A:LYS:HA	1:53:A:THR:H	7	0.1
(1,579)	1:51:A:ARG:HA	1:55:A:GLY:H	14	0.1
(1,578)	1:51:A:ARG:HB2	1:55:A:GLY:H	9	0.1
(1,578)	1:51:A:ARG:HB3	1:55:A:GLY:H	9	0.1
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	2	0.1
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	3	0.1
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	9	0.1
(1,531)	1:46:A:THR:H	1:47:A:LYS:H	15	0.1
(1,507)	1:43:A:VAL:HB	1:43:A:VAL:H	10	0.1
(1,483)	1:41:A:ARG:HB2	1:41:A:ARG:H	10	0.1
(1,429)	1:37:A:GLN:HG3	1:37:A:GLN:H	6	0.1
(1,404)	1:34:A:PRO:HB2	1:35:A:SER:H	12	0.1
(1,349)	1:30:A:ASN:HB2	1:30:A:ASN:HD21	10	0.1
(1,345)	1:30:A:ASN:HB3	1:30:A:ASN:H	4	0.1
(1,286)	1:26:A:CYS:HB3	1:26:A:CYS:H	11	0.1
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	8	0.1
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	10	0.1
(1,279)	1:25:A:GLN:H	1:26:A:CYS:H	14	0.1
(1,269)	1:25:A:GLN:HB2	1:25:A:GLN:H	12	0.1
(1,268)	1:25:A:GLN:HB3	1:25:A:GLN:H	1	0.1
(1,257)	1:24:A:ALA:H	1:25:A:GLN:HG2	11	0.1
(1,242)	1:23:A:ALA:HB1	1:24:A:ALA:H	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:23:A:ALA:HB2	1:24:A:ALA:H	15	0.1
(1,242)	1:23:A:ALA:HB3	1:24:A:ALA:H	15	0.1
(1,239)	1:23:A:ALA:HB1	1:23:A:ALA:H	12	0.1
(1,239)	1:23:A:ALA:HB2	1:23:A:ALA:H	12	0.1
(1,239)	1:23:A:ALA:HB3	1:23:A:ALA:H	12	0.1
(1,228)	1:22:A:HIS:HB2	1:22:A:HIS:H	1	0.1
(1,228)	1:22:A:HIS:HB2	1:22:A:HIS:H	3	0.1
(1,228)	1:22:A:HIS:HB2	1:22:A:HIS:H	9	0.1
(1,228)	1:22:A:HIS:HB2	1:22:A:HIS:H	14	0.1
(1,213)	1:21:A:VAL:HB	1:21:A:VAL:H	13	0.1
(1,189)	1:18:A:GLN:HB2	1:19:A:SER:H	7	0.1
(1,188)	1:18:A:GLN:HB3	1:19:A:SER:H	6	0.1
(1,167)	1:17:A:ILE:HB	1:17:A:ILE:H	2	0.1
(1,165)	1:17:A:ILE:HG12	1:17:A:ILE:H	7	0.1
(1,146)	1:15:A:ARG:HB2	1:15:A:ARG:H	1	0.1
(1,146)	1:15:A:ARG:HB2	1:15:A:ARG:H	5	0.1
(1,146)	1:15:A:ARG:HB2	1:15:A:ARG:H	8	0.1
(1,142)	1:14:A:GLN:HA	1:17:A:ILE:H	13	0.1
(1,133)	1:14:A:GLN:HG2	1:14:A:GLN:H	11	0.1
(1,133)	1:14:A:GLN:HG3	1:14:A:GLN:H	11	0.1
(1,71)	1:7:A:ASP:H	1:8:A:SER:H	3	0.1
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD1	5	0.1
(1,23)	2:11:B:LEU:H	1:69:A:TYR:HD2	5	0.1
(1,20)	2:9:B:LEU:HA	1:72:A:LYS:HB3	8	0.1
(1,15)	1:69:A:TYR:HA	2:10:B:MET:HB3	13	0.1
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD11	3	0.1
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD12	3	0.1
(1,14)	1:62:A:GLN:HE21	2:11:B:LEU:HD13	3	0.1
(1,12)	1:62:A:GLN:HE22	2:11:B:LEU:HG	5	0.1

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

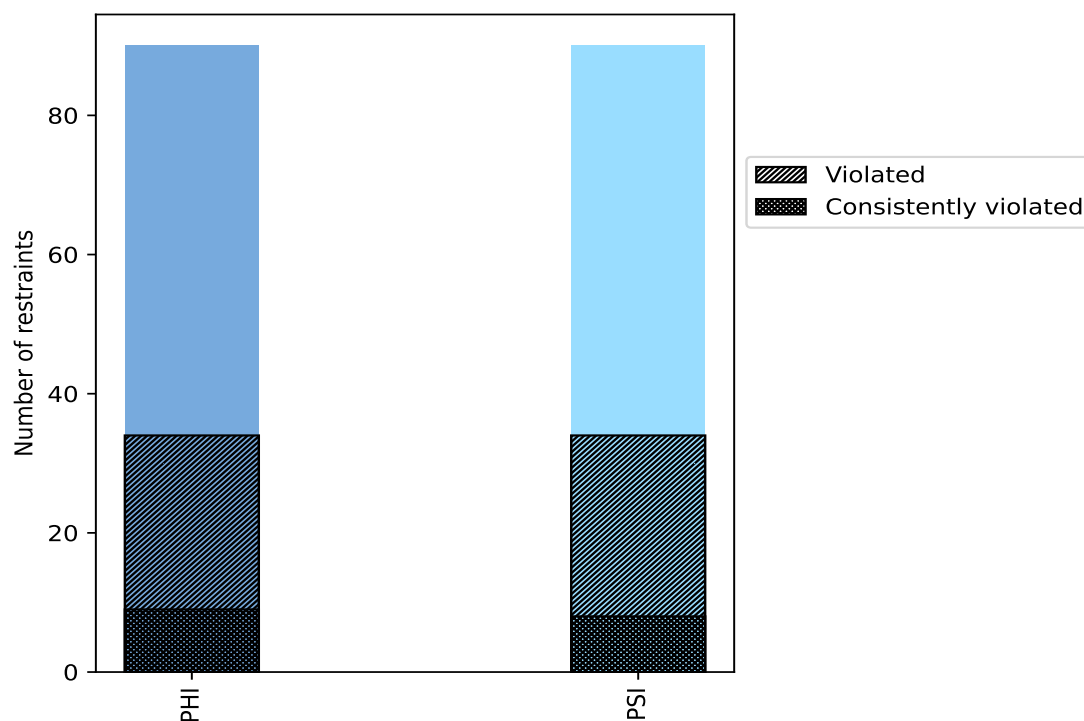
10.1 Summary of dihedral-angle violations [i](#)

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	90	50.0	34	37.8	18.9	9	10.0	5.0
PSI	90	50.0	34	37.8	18.9	8	8.9	4.4
Total	180	100.0	68	37.8	37.8	17	9.4	9.4

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](#)



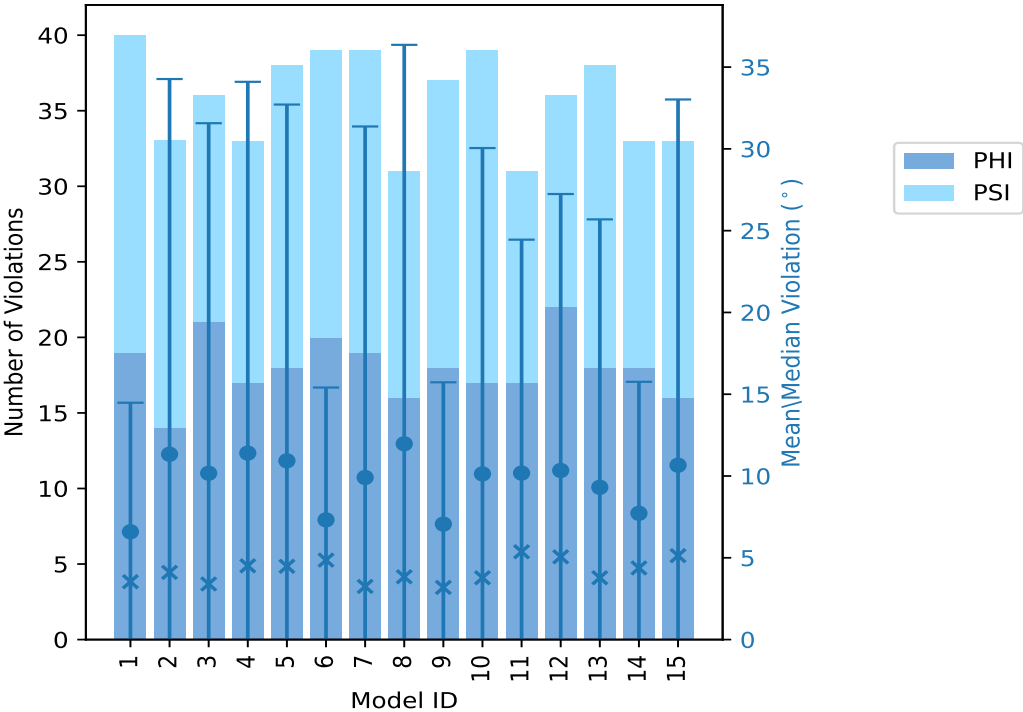
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	19	21	40	6.59	40.56	7.89	3.54
2	14	19	33	11.33	131.29	22.94	4.11
3	21	15	36	10.17	126.55	21.4	3.4
4	17	16	33	11.4	129.74	22.7	4.51
5	18	20	38	10.93	133.71	21.78	4.48
6	20	19	39	7.32	42.48	8.09	4.86
7	19	20	39	9.91	131.01	21.46	3.25
8	16	15	31	11.97	136.54	24.39	3.84
9	18	19	37	7.06	41.47	8.67	3.19
10	17	22	39	10.13	121.77	19.92	3.78
11	17	14	31	10.18	73.81	14.27	5.37
12	22	14	36	10.34	97.21	16.9	5.06
13	18	20	38	9.31	96.0	16.38	3.78
14	18	15	33	7.72	39.4	8.04	4.38
15	16	17	33	10.66	130.48	22.36	5.13

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

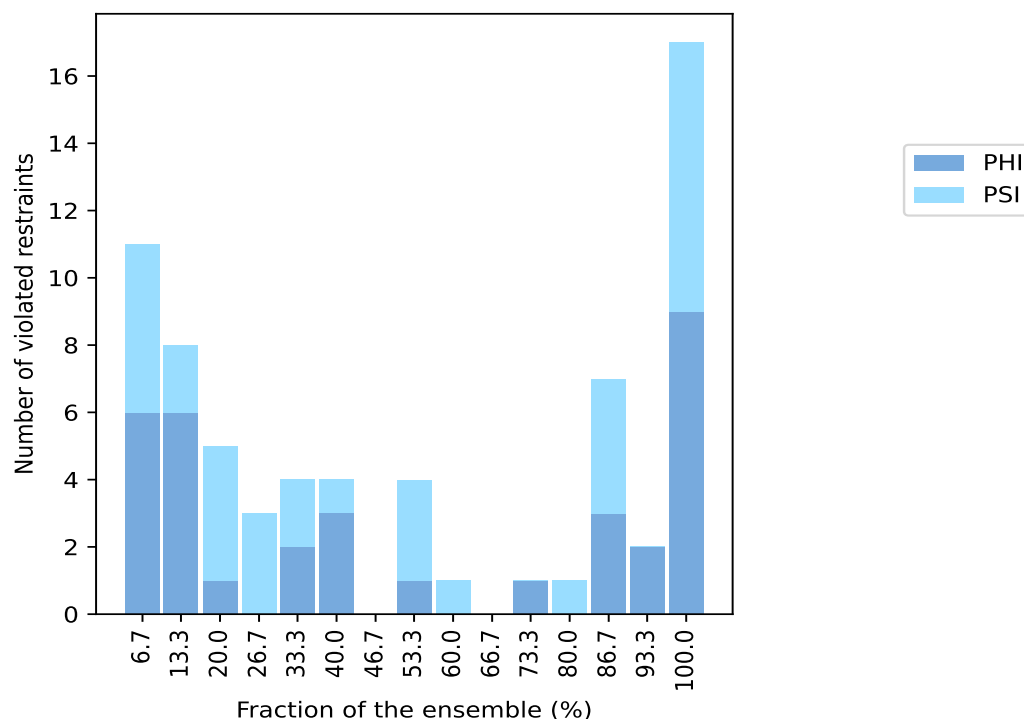
10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
6	5	11	1	6.7
6	2	8	2	13.3
1	4	5	3	20.0
0	3	3	4	26.7
2	2	4	5	33.3
3	1	4	6	40.0
0	0	0	7	46.7
1	3	4	8	53.3
0	1	1	9	60.0
0	0	0	10	66.7
1	0	1	11	73.3
0	1	1	12	80.0
3	4	7	13	86.7
2	0	2	14	93.3
9	8	17	15	100.0

¹ Number of models with violations

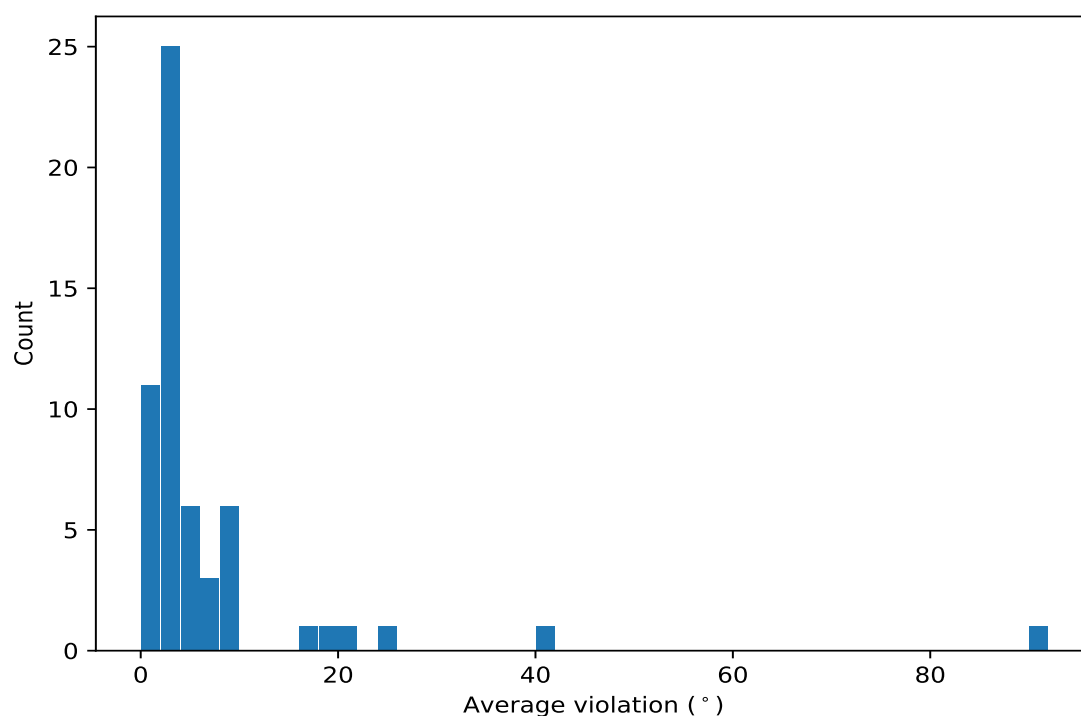
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	15	90.53	49.97	121.77
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	15	41.74	2.38	42.51
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	15	25.34	1.83	25.99
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	15	20.07	2.53	20.15
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	15	18.66	4.59	17.35
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	15	16.61	1.16	16.88
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	15	9.72	2.95	10.58
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	15	9.64	0.78	9.72
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	15	8.96	0.72	9.07
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	15	8.67	1.04	8.7
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	15	8.5	2.31	7.41
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	15	8.04	2.54	8.78
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	15	6.92	0.64	7.2
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	15	4.74	0.81	4.85
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	15	4.6	1.63	5.15
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	15	3.52	1.55	3.73
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	15	2.21	0.45	2.43
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	14	4.73	1.9	5.4
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	14	2.32	0.56	2.24
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	13	4.72	0.55	4.51
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	13	3.88	0.96	3.79

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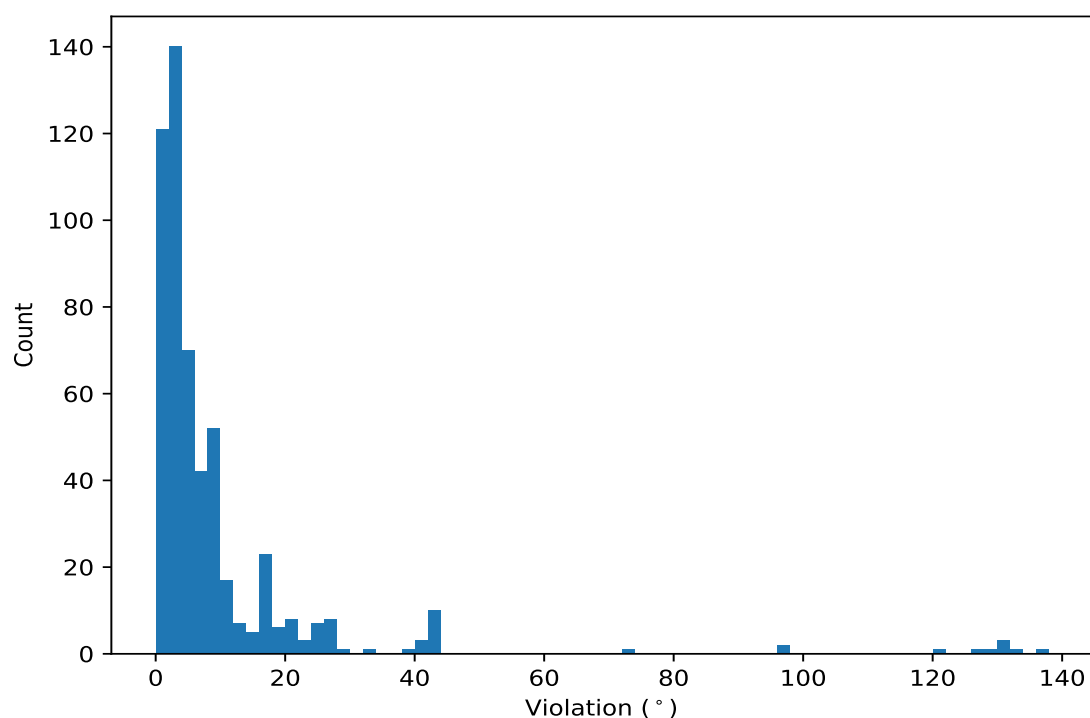
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	13	3.56	1.41	2.99
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	13	3.22	3.46	2.45
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	13	2.84	0.84	3.24
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	13	2.69	0.88	2.77
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	13	1.85	0.54	1.68
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	12	2.01	0.65	1.77
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	11	3.96	1.8	3.16
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	9	2.59	1.1	2.45
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	8	2.76	1.15	3.01
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	8	2.71	1.34	2.57
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	8	2.45	0.72	2.21
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	8	1.47	0.2	1.5
(1,83)	1:45:A:HIS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	6	2.44	0.7	2.66
(1,129)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	6	1.96	0.52	2.01
(1,90)	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1:50:A:LYS:N	6	1.66	0.42	1.6
(1,75)	1:41:A:ARG:C	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	6	1.43	0.4	1.31
(1,163)	2:16:B:ILE:C	2:17:B:GLU:N	2:17:B:GLU:CA	2:17:B:GLU:C	5	2.77	1.45	2.48
(1,175)	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	2:17:B:GLU:N	5	2.43	0.96	2.91
(1,148)	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	1:86:A:ASN:N	5	2.22	0.81	2.16
(1,133)	1:73:A:HIS:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	5	1.55	0.23	1.54
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:ASP:N	4	7.17	1.73	7.43
(1,152)	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	1:89:A:GLN:N	4	2.56	1.26	2.09
(1,172)	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	2:14:B:ASP:N	4	1.49	0.51	1.28
(1,168)	2:7:B:ASP:N	2:7:B:ASP:CA	2:7:B:ASP:C	2:8:B:ASP:N	3	5.47	5.6	1.84
(1,170)	2:9:B:LEU:N	2:9:B:LEU:CA	2:9:B:LEU:C	2:10:B:MET:N	3	3.03	1.08	3.5
(1,167)	2:22:B:GLU:C	2:23:B:ASP:N	2:23:B:ASP:CA	2:23:B:ASP:C	3	2.01	0.99	1.43
(1,150)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:ILE:N	3	1.71	0.14	1.7
(1,132)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:CYS:N	3	1.42	0.04	1.44
(1,1)	1:4:A:SER:C	1:5:A:PRO:N	1:5:A:PRO:CA	1:5:A:PRO:C	2	7.54	4.24	7.54
(1,156)	2:7:B:ASP:C	2:8:B:ASP:N	2:8:B:ASP:CA	2:8:B:ASP:C	2	4.23	1.87	4.23
(1,106)	1:60:A:CYS:N	1:60:A:CYS:CA	1:60:A:CYS:C	1:61:A:LYS:N	2	3.65	2.53	3.65
(1,151)	1:87:A:ILE:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	2	2.55	0.02	2.55
(1,162)	2:15:B:ASP:C	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	2	2.42	1.36	2.42
(1,2)	1:5:A:PRO:N	1:5:A:PRO:CA	1:5:A:PRO:C	1:6:A:GLY:N	2	2.27	1.24	2.27
(1,107)	1:60:A:CYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	2	1.6	0.17	1.6
(1,159)	2:12:B:SER:C	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	2	1.56	0.17	1.56

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 (°)
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	8	136.54
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	5	133.71
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	2	131.29
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	7	131.01
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	15	130.48
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	4	129.74
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	3	126.55
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	10	121.77
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	12	97.21
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	13	96.0
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	11	73.81
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	2	43.48
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	5	43.41
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	3	43.28
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	12	43.26
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	4	42.91
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	13	42.84
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	7	42.74
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	11	42.51
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	6	42.48
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	10	42.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	8	41.92
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	9	41.47
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	1	40.56
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	14	39.4
(1,102)	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1:59:A:ILE:N	15	33.83
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	7	28.4
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	9	27.06
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	6	26.78
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	8	26.71
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	2	26.61
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	5	26.5
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	13	26.39
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	15	26.11
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	10	26.02
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	12	25.99
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	4	25.93
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	3	25.82
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	7	25.27
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	14	25.26
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	1	24.95
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	9	24.05
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	1	23.77
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	10	23.42
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	11	22.2
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	12	21.54
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	4	21.46
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	9	21.11
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	8	20.77
(1,56)	1:32:A:SER:N	1:32:A:SER:CA	1:32:A:SER:C	1:33:A:LEU:N	11	20.64
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	4	20.59
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	3	20.44
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	6	20.15
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	6	19.74
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	5	19.59
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	2	19.38
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	5	18.83
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	14	18.48
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	10	18.19
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	2	17.93
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	8	17.85
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	7	17.55
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	15	17.46
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	5	17.38
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	11	17.35
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	8	17.3
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	10	17.24
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	2	17.15
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	13	16.99
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	6	16.97
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	15	16.95
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	13	16.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	14	16.88
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	7	16.8
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	3	16.77
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	12	16.71
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	12	16.68
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1	16.6
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	4	16.38
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	13	16.36
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	14	16.33
(1,146)	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1:85:A:LEU:N	3	16.25
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1	15.86
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	14	15.72
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	9	15.1
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	10	14.71
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	9	14.47
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	12	13.93
(1,57)	1:32:A:SER:C	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	11	13.5
(1,168)	2:7:B:ASP:N	2:7:B:ASP:CA	2:7:B:ASP:C	2:8:B:ASP:N	5	13.38
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	7	12.98
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	14	12.91
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	11	12.64
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	10	12.51
(1,1)	1:4:A:SER:C	1:5:A:PRO:N	1:5:A:PRO:CA	1:5:A:PRO:C	13	11.78
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	1	11.75
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	9	11.6
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	13	11.56
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	6	11.46
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	4	11.3
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	9	10.94
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	7	10.64
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	8	10.58
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	15	10.47
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	5	10.42
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	11	10.36
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	8	10.28
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	12	10.18
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	8	10.17
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	12	10.02
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	15	10.0
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	12	9.95
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	4	9.86
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	2	9.84
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	5	9.81
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	3	9.8
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	14	9.8
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	2	9.76
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	2	9.75
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	3	9.72
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	5	9.72
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	6	9.66
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	1	9.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	7	9.58
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	10	9.57
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	10	9.54
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	2	9.47
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	4	9.45
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	3	9.43
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	4	9.39
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	4	9.33
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	13	9.32
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	5	9.28
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	13	9.24
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	14	9.17
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	2	9.16
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	10	9.13
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	12	9.1
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	15	9.07
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:ASP:N	1	9.07
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	11	9.03
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	6	8.96
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	13	8.86
(1,3)	1:5:A:PRO:C	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1	8.82
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	3	8.78
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	6	8.78
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	8	8.75
(1,157)	2:8:B:ASP:C	2:9:B:LEU:N	2:9:B:LEU:CA	2:9:B:LEU:C	6	8.73
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	5	8.73
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	9	8.73
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1	8.71
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	12	8.7
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	11	8.66
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	15	8.66
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	5	8.59
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	7	8.59
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	11	8.52
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	8	8.51
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:ASP:N	6	8.51
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	13	8.39
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	12	8.35
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	10	8.33
(1,103)	1:58:A:PRO:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	15	8.02
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	14	7.92
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	11	7.85
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	6	7.84
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	2	7.78
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	1	7.76
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	12	7.72
(1,97)	1:52:A:LYS:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	6	7.67
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	3	7.67
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	12	7.66
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	4	7.54
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	12	7.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	14	7.51
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	2	7.48
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	9	7.41
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	1	7.41
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	5	7.37
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	10	7.35
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	15	7.33
(1,46)	1:27:A:ARG:N	1:27:A:ARG:CA	1:27:A:ARG:C	1:28:A:ASN:N	9	7.3
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	13	7.2
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	12	7.19
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	3	7.14
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	8	6.98
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	11	6.76
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	11	6.76
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	14	6.73
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	6	6.66
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	4	6.64
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	6	6.58
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	6	6.57
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	7	6.56
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	4	6.43
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	6	6.39
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:ASP:N	9	6.35
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	15	6.34
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	9	6.28
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	8	6.27
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	15	6.23
(1,106)	1:60:A:CYS:N	1:60:A:CYS:CA	1:60:A:CYS:C	1:61:A:LYS:N	15	6.18
(1,156)	2:7:B:ASP:C	2:8:B:ASP:N	2:8:B:ASP:CA	2:8:B:ASP:C	6	6.1
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	1	6.1
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	9	6.0
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	1	5.93
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	7	5.93
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	10	5.86
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	11	5.85
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	15	5.83
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	13	5.82
(1,47)	1:27:A:ARG:C	1:28:A:ASN:N	1:28:A:ASN:CA	1:28:A:ASN:C	3	5.82
(1,96)	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1:53:A:THR:N	1	5.81
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	14	5.79
(1,147)	1:84:A:CYS:C	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	10	5.75
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	2	5.71
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	9	5.64
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	5	5.62
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	3	5.57
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	7	5.55
(1,163)	2:16:B:ILE:C	2:17:B:GLU:N	2:17:B:GLU:CA	2:17:B:GLU:C	6	5.54
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	12	5.46
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	7	5.39
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	14	5.38
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	11	5.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	5	5.33
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1	5.32
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	11	5.32
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	8	5.29
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	13	5.16
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	3	5.15
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	4	5.15
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	15	5.14
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	15	5.13
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	14	5.12
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	8	5.12
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	2	5.08
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	13	5.03
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	13	5.03
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	11	5.02
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	7	5.01
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	2	4.87
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	6	4.86
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	4	4.85
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	5	4.8
(1,4)	1:6:A:GLY:N	1:6:A:GLY:CA	1:6:A:GLY:C	1:7:A:ASP:N	14	4.74
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	5	4.72
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	10	4.68
(1,152)	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	1:89:A:GLN:N	12	4.66
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	5	4.59
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	12	4.57
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	10	4.57
(1,155)	2:6:B:MET:C	2:7:B:ASP:N	2:7:B:ASP:CA	2:7:B:ASP:C	6	4.51
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	4	4.51
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	9	4.49
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	11	4.43
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	15	4.42
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	12	4.4
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	7	4.38
(1,144)	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	1:84:A:CYS:N	14	4.38
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	5	4.37
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	7	4.37
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	15	4.37
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	7	4.36
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	13	4.32
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	9	4.31
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	15	4.29
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	1	4.25
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	10	4.14
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	1	4.13
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	2	4.11
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	5	4.1
(1,170)	2:9:B:LEU:N	2:9:B:LEU:CA	2:9:B:LEU:C	2:10:B:MET:N	6	4.05
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	10	4.03
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	14	4.0
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	4	3.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	6	3.91
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	14	3.89
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	3	3.87
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	7	3.87
(1,94)	1:51:A:ARG:N	1:51:A:ARG:CA	1:51:A:ARG:C	1:52:A:LYS:N	3	3.86
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	8	3.84
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	13	3.84
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	12	3.83
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	11	3.81
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	11	3.79
(1,162)	2:15:B:ASP:C	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	10	3.78
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	2	3.75
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	9	3.73
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	13	3.73
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	14	3.7
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2	3.61
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1	3.61
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	13	3.61
(1,175)	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	2:17:B:GLU:N	6	3.59
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	15	3.59
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	1	3.56
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	10	3.53
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	1	3.51
(1,2)	1:5:A:PRO:N	1:5:A:PRO:CA	1:5:A:PRO:C	1:6:A:GLY:N	13	3.51
(1,170)	2:9:B:LEU:N	2:9:B:LEU:CA	2:9:B:LEU:C	2:10:B:MET:N	5	3.5
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	2	3.47
(1,167)	2:22:B:GLU:C	2:23:B:ASP:N	2:23:B:ASP:CA	2:23:B:ASP:C	11	3.41
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	1	3.4
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	3	3.4
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	3	3.39
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	10	3.38
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	10	3.31
(1,1)	1:4:A:SER:C	1:5:A:PRO:N	1:5:A:PRO:CA	1:5:A:PRO:C	12	3.3
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	5	3.26
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	7	3.25
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	1	3.25
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	4	3.24
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	8	3.23
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	9	3.19
(1,148)	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	1:86:A:ASN:N	14	3.19
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	4	3.16
(1,89)	1:48:A:GLY:C	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1	3.14
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	15	3.13
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	2	3.13
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	5	3.11
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	2	3.1
(1,83)	1:45:A:HIS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	14	3.1
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	10	3.09
(1,83)	1:45:A:HIS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	6	3.09
(1,175)	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	2:17:B:GLU:N	5	3.08
(1,148)	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	1:86:A:ASN:N	7	3.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	13	3.08
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	14	3.04
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	3	3.0
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	5	2.99
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	13	2.99
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	2	2.99
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	5	2.95
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	8	2.95
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	14	2.95
(1,175)	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	2:17:B:GLU:N	13	2.91
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	8	2.91
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	3	2.9
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	5	2.88
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	3	2.88
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	7	2.86
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	5	2.86
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	5	2.86
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	11	2.85
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	7	2.85
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	3	2.83
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	14	2.82
(1,83)	1:45:A:HIS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	10	2.82
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	8	2.78
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	9	2.77
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	8	2.75
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	3	2.74
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	10	2.73
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	11	2.71
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	13	2.7
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	2	2.68
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	9	2.65
(1,163)	2:16:B:ILE:C	2:17:B:GLU:N	2:17:B:GLU:CA	2:17:B:GLU:C	5	2.64
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	6	2.63
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	12	2.62
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	8	2.6
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	5	2.59
(1,129)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	14	2.58
(1,151)	1:87:A:ILE:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	15	2.57
(1,153)	1:88:A:LYS:C	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	12	2.53
(1,151)	1:87:A:ILE:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	3	2.53
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	4	2.53
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	2	2.53
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	13	2.52
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	3	2.51
(1,129)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	3	2.5
(1,83)	1:45:A:HIS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	5	2.5
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	9	2.49
(1,104)	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	1:60:A:CYS:N	4	2.49
(1,163)	2:16:B:ILE:C	2:17:B:GLU:N	2:17:B:GLU:CA	2:17:B:GLU:C	13	2.48
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	6	2.48
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	8	2.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	14	2.45
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	12	2.45
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	15	2.45
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	7	2.45
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	11	2.45
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	4	2.43
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	5	2.43
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	4	2.42
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	8	2.41
(1,180)	2:23:B:ASP:N	2:23:B:ASP:CA	2:23:B:ASP:C	2:24:B:PRO:N	1	2.38
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	10	2.37
(1,156)	2:7:B:ASP:C	2:8:B:ASP:N	2:8:B:ASP:CA	2:8:B:ASP:C	11	2.36
(1,152)	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	1:89:A:GLN:N	9	2.36
(1,172)	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	2:14:B:ASP:N	14	2.35
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	15	2.29
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	8	2.28
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	7	2.27
(1,90)	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1:50:A:LYS:N	10	2.27
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	7	2.26
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	6	2.23
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	12	2.23
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	1	2.22
(1,129)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	1	2.22
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	15	2.19
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	10	2.17
(1,148)	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	1:86:A:ASN:N	10	2.16
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	9	2.15
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	6	2.15
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	14	2.13
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	6	2.13
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	12	2.12
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	13	2.1
(1,90)	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1:50:A:LYS:N	5	2.1
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	1	2.06
(1,75)	1:41:A:ARG:C	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	9	2.05
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	1	2.01
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	10	2.0
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	11	1.98
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	6	1.98
(1,83)	1:45:A:HIS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	4	1.95
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	4	1.93
(1,133)	1:73:A:HIS:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	5	1.91
(1,150)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:ILE:N	10	1.89
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	8	1.88
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	13	1.87
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	1	1.87
(1,75)	1:41:A:ARG:C	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	12	1.87
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	14	1.86
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	11	1.86
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	14	1.85
(1,168)	2:7:B:ASP:N	2:7:B:ASP:CA	2:7:B:ASP:C	2:8:B:ASP:N	6	1.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	3	1.84
(1,166)	2:20:B:PHE:C	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	14	1.83
(1,152)	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	1:89:A:GLN:N	8	1.83
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	10	1.8
(1,129)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	7	1.8
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	4	1.76
(1,107)	1:60:A:CYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	1	1.76
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	1	1.75
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	9	1.75
(1,159)	2:12:B:SER:C	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	7	1.73
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	10	1.73
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	7	1.71
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	13	1.71
(1,163)	2:16:B:ILE:C	2:17:B:GLU:N	2:17:B:GLU:CA	2:17:B:GLU:C	8	1.71
(1,150)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:ILE:N	1	1.7
(1,90)	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1:50:A:LYS:N	4	1.7
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	9	1.69
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	4	1.68
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	9	1.68
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	6	1.67
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	12	1.67
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	5	1.67
(1,160)	2:13:B:PRO:C	2:14:B:ASP:N	2:14:B:ASP:CA	2:14:B:ASP:C	12	1.66
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	10	1.66
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	5	1.66
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	7	1.66
(1,154)	1:89:A:GLN:N	1:89:A:GLN:CA	1:89:A:GLN:C	1:90:A:LYS:N	12	1.65
(1,126)	1:70:A:HIS:N	1:70:A:HIS:CA	1:70:A:HIS:C	1:71:A:ALA:N	6	1.61
(1,101)	1:57:A:CYS:C	1:58:A:PRO:N	1:58:A:PRO:CA	1:58:A:PRO:C	9	1.61
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	6	1.6
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	8	1.59
(1,133)	1:73:A:HIS:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	13	1.59
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	15	1.58
(1,129)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	6	1.55
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	15	1.55
(1,170)	2:9:B:LEU:N	2:9:B:LEU:CA	2:9:B:LEU:C	2:10:B:MET:N	13	1.54
(1,150)	1:86:A:ASN:N	1:86:A:ASN:CA	1:86:A:ASN:C	1:87:A:ILE:N	7	1.54
(1,133)	1:73:A:HIS:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	12	1.54
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	7	1.54
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	7	1.53
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	4	1.53
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	6	1.52
(1,133)	1:73:A:HIS:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	14	1.5
(1,90)	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1:50:A:LYS:N	3	1.5
(1,163)	2:16:B:ILE:C	2:17:B:GLU:N	2:17:B:GLU:CA	2:17:B:GLU:C	10	1.49
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	1	1.49
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	2	1.49
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	1	1.49
(1,132)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:CYS:N	10	1.46
(1,75)	1:41:A:ARG:C	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	15	1.45
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	13	1.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,132)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:CYS:N	11	1.44
(1,167)	2:22:B:GLU:C	2:23:B:ASP:N	2:23:B:ASP:CA	2:23:B:ASP:C	9	1.43
(1,107)	1:60:A:CYS:C	1:61:A:LYS:N	1:61:A:LYS:CA	1:61:A:LYS:C	3	1.43
(1,174)	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	2:16:B:ILE:N	10	1.41
(1,87)	1:47:A:LYS:C	1:48:A:GLY:N	1:48:A:GLY:CA	1:48:A:GLY:C	9	1.41
(1,152)	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	1:89:A:GLN:N	4	1.4
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	8	1.4
(1,159)	2:12:B:SER:C	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	6	1.39
(1,110)	1:62:A:GLN:N	1:62:A:GLN:CA	1:62:A:GLN:C	1:63:A:LEU:N	9	1.39
(1,175)	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	2:17:B:GLU:N	1	1.38
(1,41)	1:24:A:ALA:C	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	12	1.38
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	12	1.37
(1,137)	1:75:A:GLN:C	1:76:A:GLU:N	1:76:A:GLU:CA	1:76:A:GLU:C	12	1.37
(1,132)	1:73:A:HIS:N	1:73:A:HIS:CA	1:73:A:HIS:C	1:74:A:CYS:N	9	1.37
(1,148)	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	1:86:A:ASN:N	9	1.34
(1,95)	1:51:A:ARG:C	1:52:A:LYS:N	1:52:A:LYS:CA	1:52:A:LYS:C	15	1.34
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	9	1.33
(1,148)	1:85:A:LEU:N	1:85:A:LEU:CA	1:85:A:LEU:C	1:86:A:ASN:N	2	1.31
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	2	1.31
(1,172)	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	2:14:B:ASP:N	6	1.29
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	1	1.28
(1,172)	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	2:14:B:ASP:N	13	1.27
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	8	1.27
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	4	1.27
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	3	1.26
(1,90)	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1:50:A:LYS:N	13	1.26
(1,140)	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	1:78:A:LYS:N	2	1.25
(1,74)	1:41:A:ARG:N	1:41:A:ARG:CA	1:41:A:ARG:C	1:42:A:VAL:N	9	1.24
(1,143)	1:82:A:PRO:C	1:83:A:PHE:N	1:83:A:PHE:CA	1:83:A:PHE:C	2	1.21
(1,175)	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	2:17:B:GLU:N	3	1.2
(1,168)	2:7:B:ASP:N	2:7:B:ASP:CA	2:7:B:ASP:C	2:8:B:ASP:N	7	1.2
(1,167)	2:22:B:GLU:C	2:23:B:ASP:N	2:23:B:ASP:CA	2:23:B:ASP:C	13	1.2
(1,133)	1:73:A:HIS:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	3	1.2
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	4	1.18
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	11	1.18
(1,161)	2:14:B:ASP:C	2:15:B:ASP:N	2:15:B:ASP:CA	2:15:B:ASP:C	13	1.18
(1,111)	1:62:A:GLN:C	1:63:A:LEU:N	1:63:A:LEU:CA	1:63:A:LEU:C	7	1.18
(1,145)	1:83:A:PHE:C	1:84:A:CYS:N	1:84:A:CYS:CA	1:84:A:CYS:C	7	1.17
(1,75)	1:41:A:ARG:C	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	7	1.17
(1,83)	1:45:A:HIS:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1	1.15
(1,58)	1:33:A:LEU:N	1:33:A:LEU:CA	1:33:A:LEU:C	1:34:A:PRO:N	15	1.14
(1,42)	1:25:A:GLN:N	1:25:A:GLN:CA	1:25:A:GLN:C	1:26:A:CYS:N	7	1.14
(1,129)	1:71:A:ALA:C	1:72:A:LYS:N	1:72:A:LYS:CA	1:72:A:LYS:C	9	1.13
(1,106)	1:60:A:CYS:N	1:60:A:CYS:CA	1:60:A:CYS:C	1:61:A:LYS:N	10	1.12
(1,139)	1:76:A:GLU:C	1:77:A:ASN:N	1:77:A:ASN:CA	1:77:A:ASN:C	3	1.11
(1,90)	1:49:A:CYS:N	1:49:A:CYS:CA	1:49:A:CYS:C	1:50:A:LYS:N	7	1.11
(1,179)	2:21:B:THR:N	2:21:B:THR:CA	2:21:B:THR:C	2:22:B:GLU:N	15	1.1
(1,134)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	2	1.09
(1,162)	2:15:B:ASP:C	2:16:B:ILE:N	2:16:B:ILE:CA	2:16:B:ILE:C	3	1.06
(1,172)	2:13:B:PRO:N	2:13:B:PRO:CA	2:13:B:PRO:C	2:14:B:ASP:N	1	1.05
(1,118)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:ALA:N	2	1.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,75)	1:41:A:ARG:C	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	2	1.03
(1,2)	1:5:A:PRO:N	1:5:A:PRO:CA	1:5:A:PRO:C	1:6:A:GLY:N	1	1.03
(1,136)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:GLU:N	15	1.02
(1,142)	1:82:A:PRO:N	1:82:A:PRO:CA	1:82:A:PRO:C	1:83:A:PHE:N	3	1.01
(1,75)	1:41:A:ARG:C	1:42:A:VAL:N	1:42:A:VAL:CA	1:42:A:VAL:C	11	1.01