



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 9URO / pdb_00009uro
BMRB ID : 36756
Title : Response regulator RR468 binding with Mg²⁺
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Deposited on : 2025-04-30

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

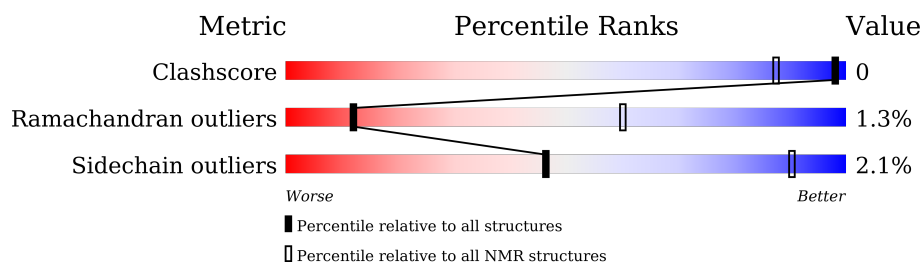
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 70%.

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	122	 62% 36% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:3-A:122 (120)	0.57	9

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 11 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1995 atoms, of which 1024 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Response regulator.

Mol	Chain	Residues	Atoms						Trace
1	A	122	Total	C	H	N	O	S	0
			1994	625	1024	157	183	5	

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

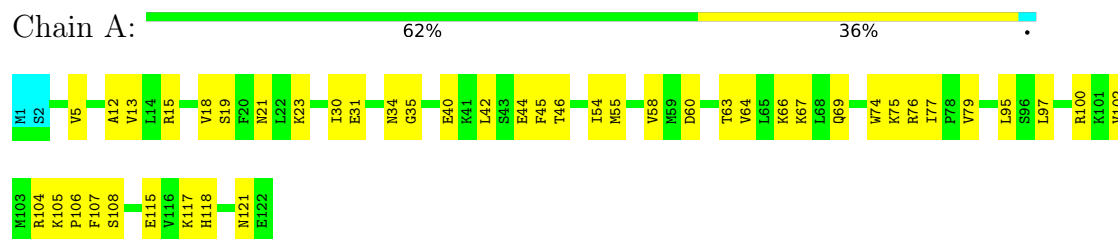
Mol	Chain	Residues	Atoms	
2	A	1	Total	Mg
			1	1

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: Response regulator

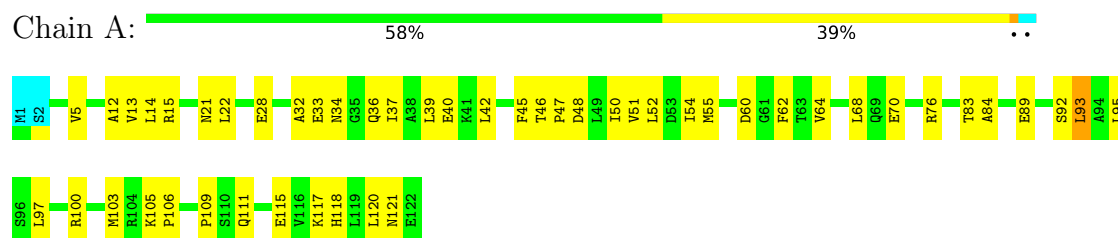


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

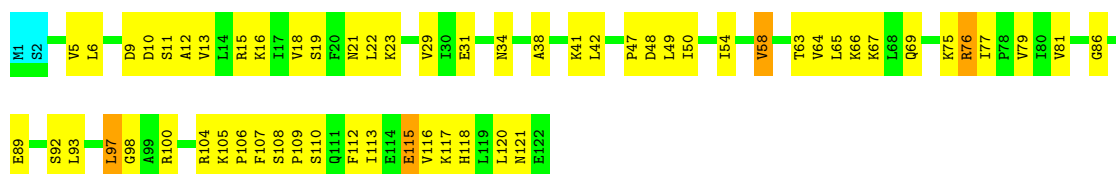
- Molecule 1: Response regulator



4.2.2 Score per residue for model 2

- Molecule 1: Response regulator

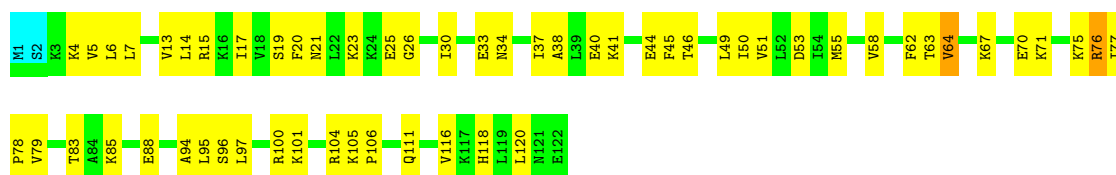




4.2.3 Score per residue for model 3

- Molecule 1: Response regulator

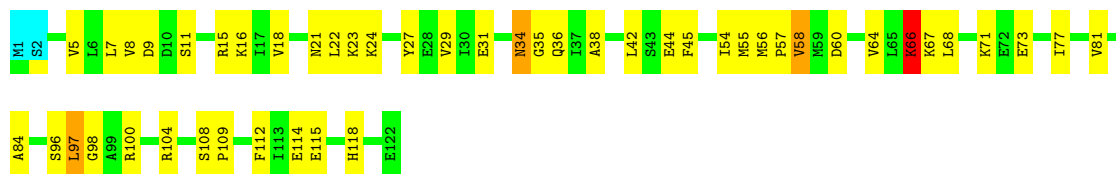
Chain A: 52% 45%



4.2.4 Score per residue for model 4

- Molecule 1: Response regulator

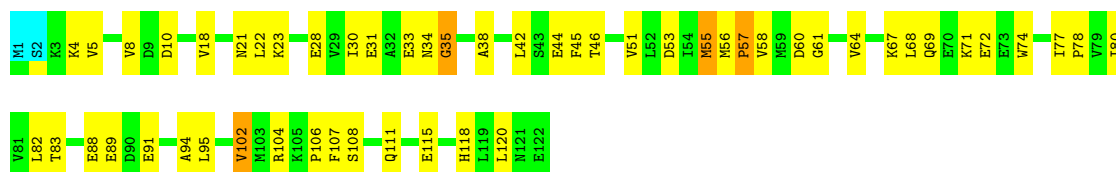
Chain A: 59% 36%



4.2.5 Score per residue for model 5

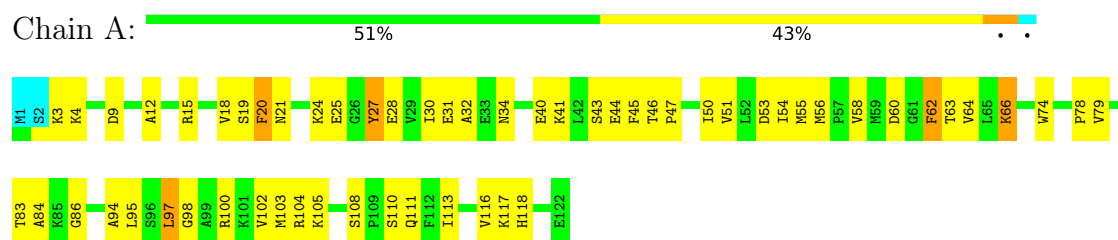
- Molecule 1: Response regulator

Chain A: 55% 40%



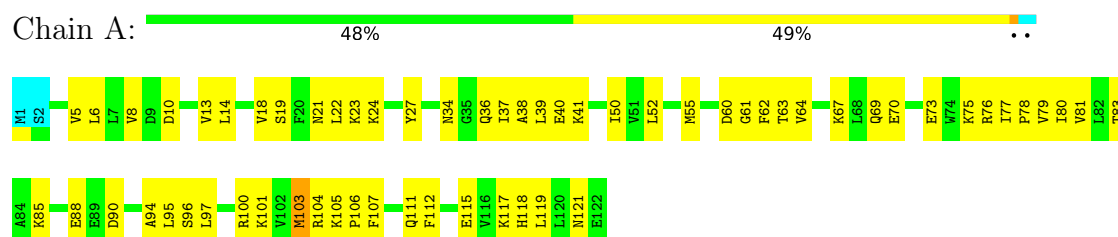
4.2.6 Score per residue for model 6

- Molecule 1: Response regulator



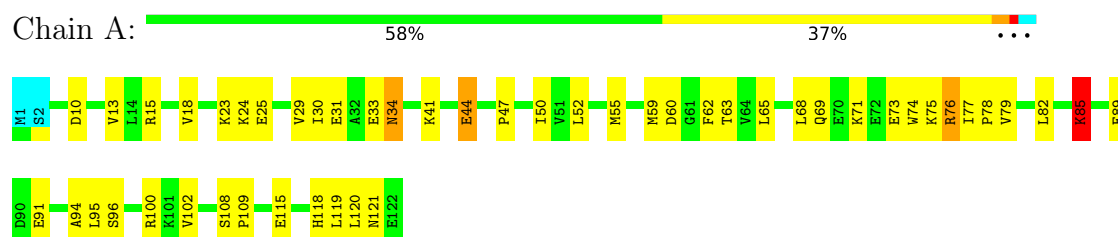
4.2.7 Score per residue for model 7

- Molecule 1: Response regulator



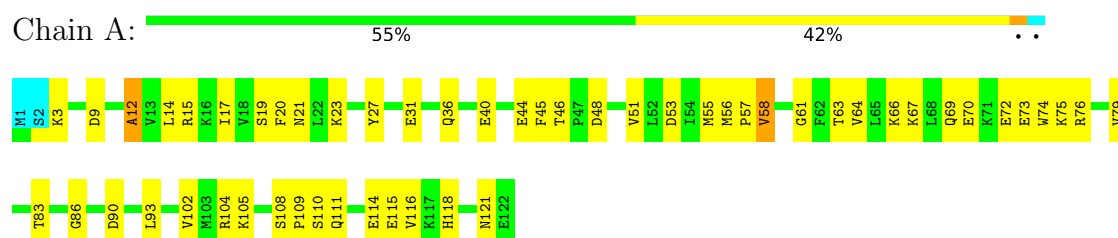
4.2.8 Score per residue for model 8

- Molecule 1: Response regulator



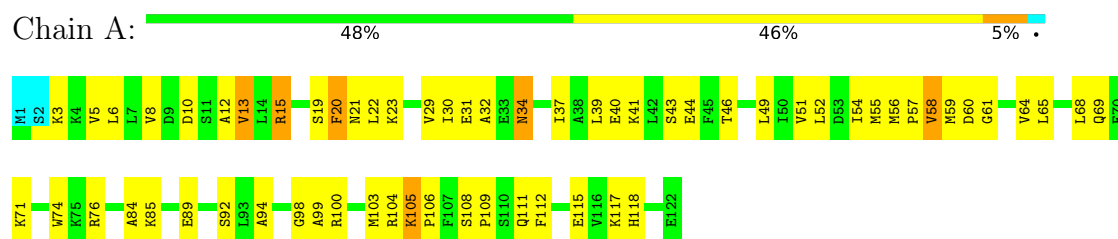
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Response regulator



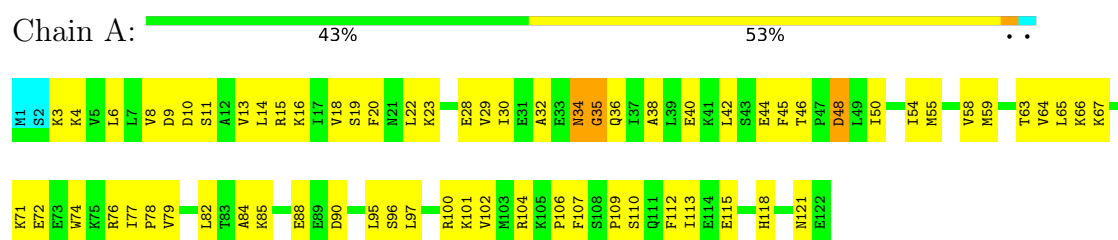
4.2.10 Score per residue for model 10

- Molecule 1: Response regulator



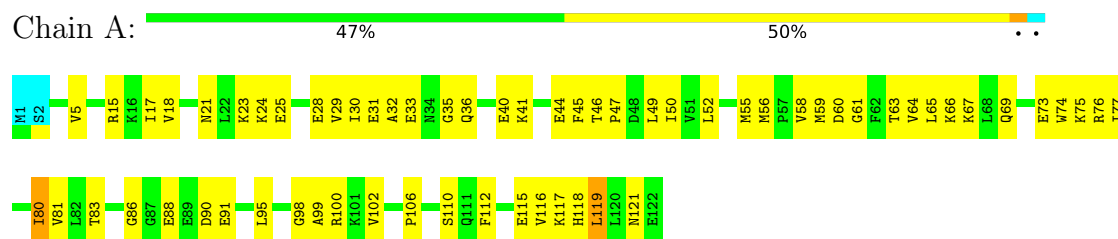
4.2.11 Score per residue for model 11

- Molecule 1: Response regulator



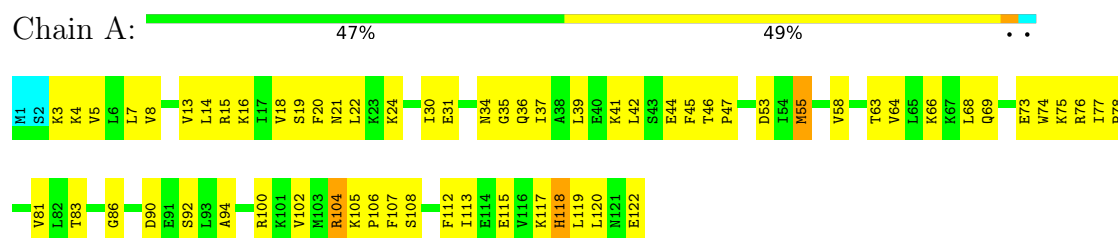
4.2.12 Score per residue for model 12

- Molecule 1: Response regulator



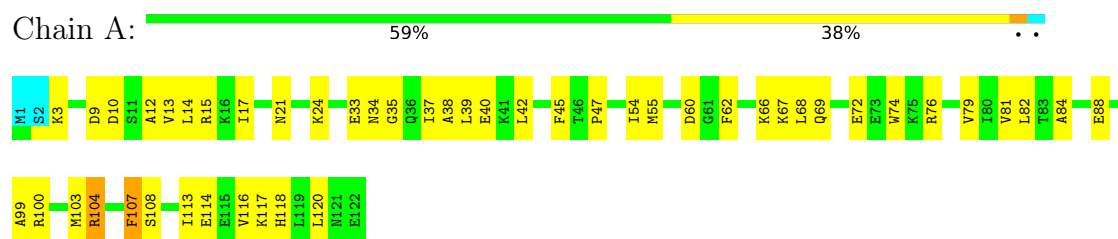
4.2.13 Score per residue for model 13

- Molecule 1: Response regulator



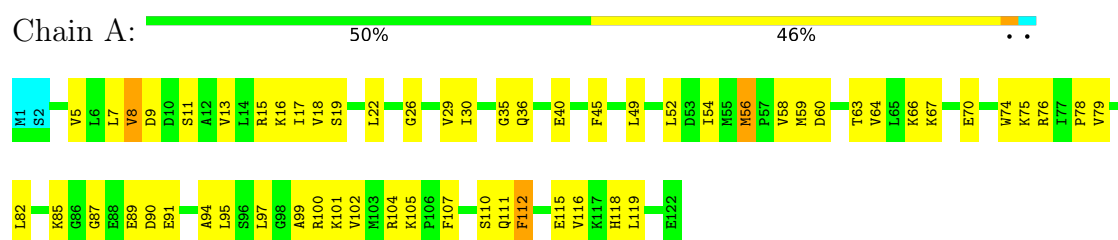
4.2.14 Score per residue for model 14

- Molecule 1: Response regulator



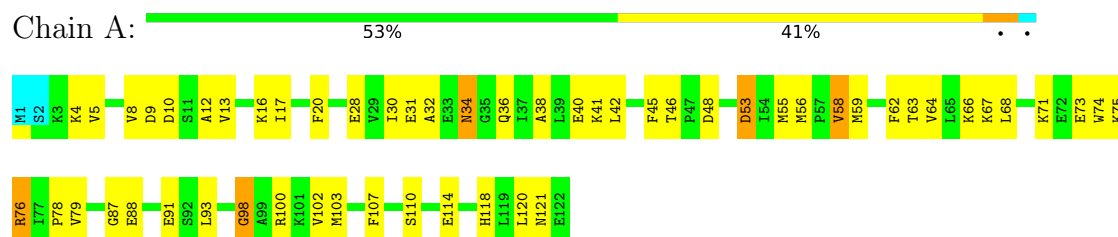
4.2.15 Score per residue for model 15

- Molecule 1: Response regulator



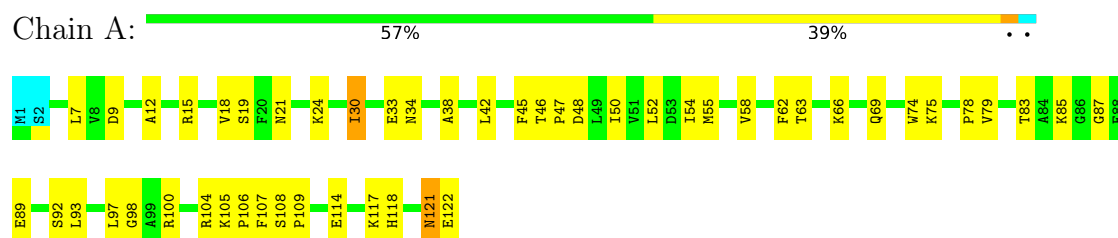
4.2.16 Score per residue for model 16

- Molecule 1: Response regulator



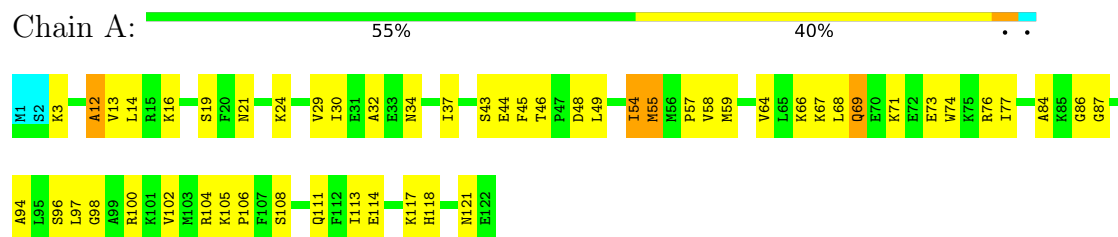
4.2.17 Score per residue for model 17

- Molecule 1: Response regulator



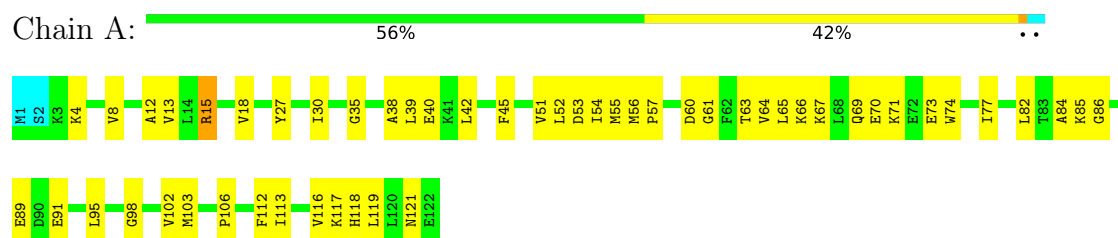
4.2.18 Score per residue for model 18

- Molecule 1: Response regulator



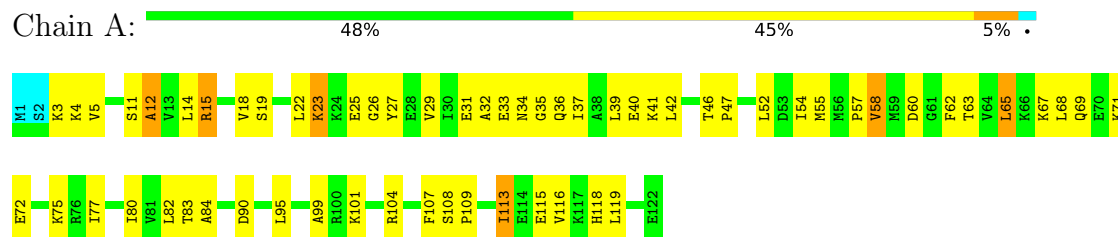
4.2.19 Score per residue for model 19

- Molecule 1: Response regulator



4.2.20 Score per residue for model 20

- Molecule 1: Response regulator



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1209
Number of shifts mapped to atoms	1209
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	70%

6 Model quality

6.1 Standard geometry

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

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	2.01±0.06	22±5/969 (2.3± 0.5%)	2.40±0.08	59±11/1300 (4.6± 0.8%)
All	All	2.01	440/19380 (2.3%)	2.40	1186/26000 (4.6%)

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	2.1±1.0
All	All	0	43

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	85	LYS	CA-C	10.20	1.64	1.52	8	3
1	A	52	LEU	N-CA	8.90	1.56	1.46	17	4
1	A	8	VAL	CA-C	8.88	1.64	1.52	7	3
1	A	46	THR	CA-C	8.85	1.60	1.53	1	5
1	A	49	LEU	CA-C	8.81	1.62	1.52	12	1
1	A	103	MET	CA-C	8.78	1.63	1.52	6	2
1	A	106	PRO	N-CA	-8.63	1.36	1.47	11	2
1	A	13	VAL	CA-C	8.60	1.62	1.52	1	1
1	A	45	PHE	N-CA	-8.51	1.34	1.46	4	2
1	A	46	THR	CA-CB	8.41	1.59	1.52	16	2
1	A	80	ILE	N-CA	8.36	1.56	1.46	7	1
1	A	98	GLY	CA-C	8.30	1.63	1.51	18	1
1	A	89	GLU	CA-C	8.24	1.63	1.52	15	1
1	A	4	LYS	N-CA	-8.09	1.36	1.46	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	54	ILE	N-CA	8.02	1.55	1.46	6	4
1	A	99	ALA	CA-C	7.98	1.62	1.52	10	2
1	A	10	ASP	N-CA	7.92	1.56	1.46	16	3
1	A	78	PRO	CA-C	7.80	1.61	1.52	5	3
1	A	23	LYS	N-CA	7.78	1.55	1.46	3	2
1	A	107	PHE	N-CA	7.78	1.56	1.46	5	1
1	A	12	ALA	CA-C	7.73	1.63	1.52	19	3
1	A	113	ILE	CA-CB	7.72	1.64	1.54	18	1
1	A	39	LEU	C-N	7.67	1.43	1.33	13	1
1	A	86	GLY	C-N	-7.67	1.27	1.33	19	1
1	A	54	ILE	CA-C	7.65	1.63	1.52	14	1
1	A	116	VAL	N-CA	7.64	1.55	1.46	19	2
1	A	75	LYS	CA-C	7.62	1.62	1.52	3	2
1	A	100	ARG	N-CA	7.55	1.55	1.46	16	3
1	A	118	HIS	CG-ND1	7.53	1.46	1.38	9	2
1	A	106	PRO	CA-C	7.49	1.62	1.52	2	3
1	A	101	LYS	N-CA	7.46	1.54	1.46	15	1
1	A	52	LEU	CA-C	7.45	1.61	1.52	10	2
1	A	113	ILE	N-CA	7.39	1.55	1.46	11	1
1	A	79	VAL	CA-C	7.34	1.62	1.52	14	3
1	A	53	ASP	N-CA	-7.31	1.37	1.46	16	2
1	A	31	GLU	CA-C	-7.22	1.44	1.52	9	3
1	A	65	LEU	N-CA	7.15	1.54	1.46	10	3
1	A	71	LYS	CA-CB	7.14	1.63	1.53	5	1
1	A	104	ARG	CZ-NH2	-7.14	1.24	1.33	17	2
1	A	98	GLY	N-CA	7.11	1.55	1.45	19	2
1	A	118	HIS	CE1-NE2	7.01	1.39	1.32	8	5
1	A	40	GLU	CA-C	6.96	1.61	1.52	14	2
1	A	96	SER	N-CA	6.96	1.55	1.46	4	2
1	A	108	SER	CA-C	6.96	1.58	1.52	13	2
1	A	24	LYS	N-CA	6.94	1.55	1.46	14	1
1	A	47	PRO	CA-C	6.92	1.60	1.52	8	4
1	A	50	ILE	CA-C	-6.92	1.44	1.52	6	2
1	A	12	ALA	N-CA	-6.91	1.37	1.46	1	1
1	A	66	LYS	CA-C	6.85	1.61	1.52	4	3
1	A	41	LYS	N-CA	6.84	1.55	1.46	8	3
1	A	64	VAL	N-CA	6.83	1.54	1.46	11	2
1	A	49	LEU	N-CA	6.82	1.53	1.46	15	3
1	A	75	LYS	CA-CB	6.79	1.63	1.53	17	1
1	A	105	LYS	N-CA	6.77	1.54	1.45	9	4
1	A	34	ASN	CA-C	6.75	1.59	1.52	6	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	67	LYS	CA-CB	6.75	1.63	1.53	9	1
1	A	63	THR	N-CA	6.74	1.54	1.46	12	5
1	A	121	ASN	CA-C	6.72	1.60	1.53	11	4
1	A	64	VAL	CA-C	6.72	1.61	1.52	6	2
1	A	45	PHE	CA-C	6.69	1.61	1.52	6	2
1	A	60	ASP	CA-CB	-6.68	1.42	1.53	8	1
1	A	9	ASP	CA-C	6.67	1.60	1.52	6	3
1	A	25	GLU	CA-C	6.66	1.61	1.52	12	3
1	A	15	ARG	CZ-NH2	-6.66	1.24	1.33	9	2
1	A	96	SER	CA-C	6.66	1.61	1.52	7	2
1	A	5	VAL	C-O	-6.66	1.16	1.24	20	1
1	A	30	ILE	N-CA	6.65	1.53	1.46	3	2
1	A	63	THR	CA-C	6.63	1.61	1.52	6	2
1	A	60	ASP	C-N	6.63	1.41	1.33	8	1
1	A	76	ARG	CD-NE	6.63	1.55	1.46	2	2
1	A	36	GLN	CA-C	6.62	1.61	1.52	11	1
1	A	77	ILE	CA-C	6.61	1.59	1.52	20	4
1	A	85	LYS	C-O	-6.60	1.16	1.24	10	1
1	A	60	ASP	N-CA	-6.58	1.38	1.46	6	2
1	A	13	VAL	N-CA	6.57	1.54	1.46	16	1
1	A	30	ILE	C-O	6.55	1.30	1.24	11	4
1	A	112	PHE	N-CA	6.55	1.54	1.46	13	2
1	A	18	VAL	N-CA	6.53	1.54	1.46	7	3
1	A	83	THR	N-CA	6.52	1.54	1.45	7	1
1	A	100	ARG	CA-C	6.51	1.61	1.52	4	1
1	A	64	VAL	CA-CB	-6.51	1.46	1.54	19	2
1	A	46	THR	C-O	6.51	1.27	1.23	16	2
1	A	71	LYS	C-N	-6.51	1.25	1.33	16	2
1	A	102	VAL	CA-CB	6.49	1.63	1.54	11	1
1	A	40	GLU	N-CA	6.48	1.54	1.46	19	3
1	A	88	GLU	N-CA	6.47	1.54	1.46	11	1
1	A	100	ARG	CD-NE	6.44	1.55	1.46	15	2
1	A	101	LYS	CA-CB	6.44	1.64	1.53	11	1
1	A	92	SER	N-CA	6.44	1.54	1.46	17	1
1	A	114	GLU	N-CA	6.44	1.54	1.46	4	1
1	A	102	VAL	N-CA	6.43	1.53	1.46	5	1
1	A	20	PHE	N-CA	6.42	1.54	1.46	13	3
1	A	80	ILE	CA-C	6.41	1.60	1.52	20	1
1	A	31	GLU	N-CA	6.41	1.53	1.46	16	2
1	A	82	LEU	C-O	6.40	1.31	1.23	11	2
1	A	74	TRP	N-CA	6.39	1.54	1.46	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	68	LEU	N-CA	-6.38	1.38	1.46	18	1
1	A	120	LEU	CA-C	6.37	1.61	1.52	8	3
1	A	83	THR	CA-C	6.37	1.60	1.52	12	2
1	A	8	VAL	CA-CB	6.36	1.62	1.54	19	2
1	A	86	GLY	CA-C	6.35	1.59	1.51	9	2
1	A	83	THR	CA-CB	6.34	1.64	1.53	5	1
1	A	48	ASP	N-CA	6.33	1.54	1.46	18	2
1	A	29	VAL	N-CA	6.33	1.53	1.46	15	2
1	A	69	GLN	CA-C	6.32	1.61	1.52	19	1
1	A	34	ASN	C-O	-6.30	1.16	1.23	14	1
1	A	5	VAL	N-CA	6.29	1.53	1.46	2	4
1	A	13	VAL	CA-CB	6.29	1.62	1.54	18	1
1	A	42	LEU	CA-C	6.28	1.61	1.52	13	1
1	A	82	LEU	CA-C	6.28	1.60	1.52	20	2
1	A	17	ILE	CA-CB	6.26	1.61	1.54	3	1
1	A	38	ALA	CA-C	6.26	1.60	1.52	7	1
1	A	50	ILE	CA-CB	6.24	1.62	1.54	17	2
1	A	58	VAL	N-CA	6.22	1.54	1.46	2	3
1	A	112	PHE	CA-C	6.22	1.60	1.52	2	1
1	A	22	LEU	CA-C	6.20	1.61	1.52	1	1
1	A	80	ILE	CA-CB	6.19	1.62	1.54	20	1
1	A	75	LYS	N-CA	6.14	1.53	1.46	9	3
1	A	95	LEU	CB-CG	6.14	1.65	1.53	3	1
1	A	18	VAL	CA-C	6.12	1.60	1.52	20	1
1	A	4	LYS	CA-CB	6.10	1.62	1.53	6	1
1	A	50	ILE	C-O	6.09	1.30	1.24	2	1
1	A	119	LEU	CA-C	6.07	1.60	1.52	19	2
1	A	24	LYS	CA-C	6.03	1.60	1.52	17	1
1	A	71	LYS	N-CA	6.02	1.53	1.46	20	3
1	A	30	ILE	CA-CB	6.01	1.61	1.54	8	2
1	A	21	ASN	CA-C	6.01	1.60	1.52	14	1
1	A	23	LYS	CA-C	6.00	1.60	1.52	3	2
1	A	58	VAL	C-O	-5.99	1.17	1.24	9	1
1	A	118	HIS	ND1-CE1	5.97	1.38	1.32	4	2
1	A	103	MET	N-CA	5.97	1.53	1.45	16	3
1	A	41	LYS	CA-C	5.97	1.61	1.52	20	1
1	A	15	ARG	N-CA	5.95	1.53	1.46	3	3
1	A	84	ALA	CA-C	5.95	1.60	1.52	14	3
1	A	36	GLN	CA-CB	5.95	1.62	1.53	9	1
1	A	118	HIS	N-CA	5.94	1.53	1.46	20	1
1	A	104	ARG	N-CA	5.94	1.53	1.46	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	73	GLU	N-CA	5.93	1.53	1.46	12	1
1	A	34	ASN	N-CA	-5.93	1.39	1.46	6	2
1	A	18	VAL	CA-CB	5.93	1.60	1.54	15	1
1	A	79	VAL	N-CA	5.90	1.53	1.46	17	2
1	A	6	LEU	CA-CB	5.90	1.60	1.52	7	2
1	A	7	LEU	CA-C	5.89	1.60	1.52	13	1
1	A	91	GLU	CA-C	-5.89	1.45	1.52	12	1
1	A	104	ARG	CA-C	-5.88	1.45	1.52	4	1
1	A	15	ARG	C-N	5.88	1.41	1.34	1	1
1	A	5	VAL	CA-CB	5.88	1.61	1.54	3	1
1	A	95	LEU	CA-C	-5.86	1.45	1.52	8	1
1	A	6	LEU	CA-C	-5.86	1.45	1.52	2	1
1	A	50	ILE	N-CA	5.86	1.53	1.46	2	1
1	A	70	GLU	N-CA	5.86	1.53	1.46	19	2
1	A	16	LYS	CA-CB	5.85	1.62	1.53	11	1
1	A	68	LEU	C-O	5.85	1.30	1.24	16	1
1	A	67	LYS	CA-C	5.83	1.60	1.52	20	2
1	A	36	GLN	N-CA	-5.79	1.39	1.46	16	2
1	A	74	TRP	NE1-CE2	5.79	1.43	1.37	6	1
1	A	108	SER	C-N	5.79	1.41	1.33	18	1
1	A	55	MET	N-CA	5.75	1.53	1.46	5	1
1	A	105	LYS	CA-C	5.75	1.60	1.52	6	2
1	A	113	ILE	CA-C	-5.75	1.45	1.52	19	2
1	A	73	GLU	C-O	5.75	1.31	1.24	19	1
1	A	111	GLN	CA-C	5.73	1.60	1.52	9	2
1	A	10	ASP	CA-C	5.71	1.60	1.52	5	2
1	A	10	ASP	C-N	-5.71	1.26	1.33	7	1
1	A	97	LEU	N-CA	5.71	1.53	1.46	17	2
1	A	90	ASP	N-CA	5.70	1.53	1.46	11	1
1	A	23	LYS	CA-CB	5.69	1.62	1.53	10	1
1	A	30	ILE	C-N	5.69	1.41	1.33	15	1
1	A	19	SER	N-CA	5.68	1.52	1.46	9	1
1	A	44	GLU	N-CA	5.67	1.53	1.46	8	3
1	A	111	GLN	C-N	5.67	1.41	1.34	6	1
1	A	14	LEU	CA-CB	5.67	1.62	1.53	7	1
1	A	35	GLY	N-CA	5.66	1.53	1.45	12	1
1	A	32	ALA	CA-C	5.65	1.59	1.52	12	1
1	A	38	ALA	CA-CB	5.65	1.62	1.53	3	1
1	A	66	LYS	N-CA	5.64	1.53	1.46	14	4
1	A	77	ILE	CA-CB	5.64	1.61	1.54	19	1
1	A	107	PHE	CA-C	5.64	1.60	1.52	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	16	LYS	N-CA	5.63	1.53	1.46	13	1
1	A	25	GLU	N-CA	5.62	1.53	1.46	20	1
1	A	118	HIS	CB-CG	5.62	1.58	1.50	3	1
1	A	55	MET	CA-C	5.62	1.60	1.52	14	1
1	A	59	MET	N-CA	5.60	1.53	1.46	11	2
1	A	4	LYS	CA-C	5.59	1.59	1.52	11	3
1	A	31	GLU	C-N	5.59	1.41	1.33	12	1
1	A	52	LEU	CA-CB	5.59	1.62	1.53	15	1
1	A	64	VAL	C-O	-5.58	1.17	1.24	15	1
1	A	73	GLU	CA-CB	5.57	1.62	1.53	13	2
1	A	67	LYS	N-CA	5.56	1.53	1.46	11	1
1	A	56	MET	C-N	5.55	1.40	1.33	15	1
1	A	76	ARG	CA-C	5.54	1.60	1.52	14	1
1	A	60	ASP	CA-C	5.52	1.59	1.52	7	2
1	A	116	VAL	CA-C	5.52	1.59	1.52	3	1
1	A	64	VAL	C-N	-5.52	1.26	1.33	13	1
1	A	101	LYS	CA-C	5.50	1.59	1.52	15	1
1	A	67	LYS	C-O	-5.50	1.17	1.24	18	2
1	A	28	GLU	CA-C	-5.49	1.47	1.53	6	2
1	A	53	ASP	CA-C	5.49	1.59	1.52	5	2
1	A	85	LYS	N-CA	5.48	1.53	1.46	11	1
1	A	22	LEU	N-CA	5.48	1.52	1.46	4	1
1	A	26	GLY	N-CA	5.47	1.53	1.45	20	1
1	A	105	LYS	CA-CB	5.47	1.61	1.53	2	1
1	A	57	PRO	CA-C	5.46	1.58	1.52	4	1
1	A	102	VAL	CA-C	-5.46	1.45	1.52	15	1
1	A	7	LEU	CA-CB	5.45	1.59	1.53	3	2
1	A	3	LYS	CA-C	5.45	1.60	1.53	13	1
1	A	6	LEU	N-CA	5.44	1.52	1.46	11	1
1	A	68	LEU	C-N	5.44	1.41	1.33	13	2
1	A	109	PRO	N-CA	-5.44	1.40	1.47	17	1
1	A	94	ALA	CA-C	5.42	1.59	1.52	6	2
1	A	97	LEU	CA-C	5.42	1.60	1.52	3	1
1	A	19	SER	C-O	-5.41	1.17	1.24	9	2
1	A	25	GLU	C-O	5.40	1.30	1.24	12	1
1	A	91	GLU	N-CA	5.40	1.52	1.46	19	1
1	A	10	ASP	C-O	-5.39	1.17	1.24	10	1
1	A	27	TYR	N-CA	5.38	1.52	1.46	4	1
1	A	115	GLU	CA-C	5.38	1.59	1.52	11	1
1	A	55	MET	CA-CB	5.37	1.62	1.53	13	1
1	A	108	SER	CA-CB	5.36	1.61	1.53	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	115	GLU	N-CA	5.36	1.52	1.46	2	1
1	A	74	TRP	CA-C	5.36	1.59	1.52	11	2
1	A	29	VAL	CA-CB	5.35	1.61	1.54	18	1
1	A	69	GLN	N-CA	5.35	1.53	1.46	18	1
1	A	39	LEU	N-CA	5.35	1.53	1.46	10	1
1	A	72	GLU	N-CA	5.34	1.52	1.46	14	1
1	A	19	SER	CA-C	-5.34	1.46	1.52	18	1
1	A	17	ILE	N-CA	5.31	1.52	1.46	16	2
1	A	15	ARG	NE-CZ	-5.31	1.27	1.33	6	1
1	A	117	LYS	C-O	-5.30	1.18	1.24	13	1
1	A	22	LEU	CA-CB	5.30	1.61	1.53	4	1
1	A	63	THR	CB-OG1	-5.30	1.35	1.43	13	1
1	A	76	ARG	CZ-NH2	-5.29	1.26	1.33	7	2
1	A	110	SER	CB-OG	5.29	1.52	1.42	9	1
1	A	78	PRO	C-O	-5.29	1.17	1.23	11	1
1	A	10	ASP	CA-CB	5.28	1.61	1.53	2	1
1	A	22	LEU	C-O	5.28	1.30	1.24	2	1
1	A	41	LYS	CA-CB	5.28	1.62	1.53	20	1
1	A	37	ILE	N-CA	5.27	1.52	1.46	7	2
1	A	56	MET	CA-C	5.27	1.58	1.52	15	2
1	A	79	VAL	CA-CB	5.25	1.60	1.53	6	1
1	A	42	LEU	N-CA	5.25	1.52	1.46	2	1
1	A	30	ILE	CA-C	5.25	1.58	1.52	19	1
1	A	46	THR	C-N	5.24	1.40	1.33	1	2
1	A	33	GLU	C-N	-5.24	1.26	1.33	3	1
1	A	14	LEU	N-CA	5.24	1.52	1.45	3	1
1	A	94	ALA	N-CA	-5.22	1.40	1.46	10	1
1	A	23	LYS	C-O	5.22	1.30	1.24	7	1
1	A	21	ASN	N-CA	-5.21	1.40	1.46	4	1
1	A	57	PRO	N-CA	5.18	1.53	1.47	20	1
1	A	54	ILE	CA-CB	5.17	1.59	1.54	6	2
1	A	121	ASN	N-CA	5.17	1.52	1.46	2	2
1	A	92	SER	CA-C	5.16	1.59	1.52	2	1
1	A	33	GLU	CA-C	5.14	1.60	1.52	8	1
1	A	81	VAL	C-O	-5.13	1.18	1.24	14	1
1	A	117	LYS	N-CA	5.12	1.52	1.46	14	1
1	A	28	GLU	CA-CB	5.12	1.59	1.52	16	1
1	A	66	LYS	C-O	-5.11	1.18	1.24	11	1
1	A	102	VAL	C-N	-5.11	1.27	1.33	18	1
1	A	4	LYS	C-N	5.10	1.39	1.33	3	1
1	A	46	THR	N-CA	5.10	1.52	1.45	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	75	LYS	C-N	5.10	1.40	1.33	15	1
1	A	106	PRO	N-CD	-5.07	1.40	1.47	10	1
1	A	99	ALA	CA-CB	5.06	1.61	1.53	14	1
1	A	51	VAL	CA-C	5.06	1.59	1.52	6	1
1	A	47	PRO	CA-CB	5.04	1.60	1.53	12	1
1	A	58	VAL	CA-C	5.03	1.59	1.52	10	1
1	A	17	ILE	C-N	5.02	1.40	1.33	9	1
1	A	112	PHE	C-O	-5.02	1.18	1.24	12	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	46	THR	O-C-N	-15.33	114.48	121.53	16	3
1	A	77	ILE	CA-C-O	-13.03	111.46	119.15	11	2
1	A	107	PHE	CA-CB-CG	12.25	126.05	113.80	2	3
1	A	76	ARG	NE-CZ-NH2	12.02	130.01	119.20	12	6
1	A	69	GLN	OE1-CD-NE2	-11.63	110.97	122.60	19	9
1	A	34	ASN	CA-CB-CG	10.85	123.45	112.60	8	6
1	A	64	VAL	CA-C-O	-10.57	110.42	121.41	13	2
1	A	106	PRO	N-CA-CB	10.43	110.22	103.23	5	5
1	A	5	VAL	O-C-N	-10.22	113.12	123.03	7	3
1	A	21	ASN	CA-CB-CG	10.07	122.67	112.60	18	7
1	A	15	ARG	CD-NE-CZ	9.85	138.19	124.40	6	4
1	A	105	LYS	CA-C-N	9.66	131.05	120.13	7	3
1	A	105	LYS	C-N-CA	9.66	131.05	120.13	7	3
1	A	34	ASN	OD1-CG-ND2	-9.55	113.05	122.60	1	6
1	A	56	MET	N-CA-C	9.54	116.72	108.13	12	2
1	A	100	ARG	NE-CZ-NH2	9.36	127.62	119.20	11	2
1	A	95	LEU	N-CA-C	9.30	121.42	111.28	3	3
1	A	90	ASP	CA-CB-CG	9.29	121.89	112.60	20	4
1	A	65	LEU	CA-C-N	9.23	132.83	120.65	19	1
1	A	65	LEU	C-N-CA	9.23	132.83	120.65	19	1
1	A	60	ASP	CB-CA-C	9.18	122.46	109.71	14	3
1	A	15	ARG	NE-CZ-NH1	9.15	130.66	121.50	9	6
1	A	106	PRO	CA-C-N	9.07	132.44	120.28	1	4
1	A	106	PRO	C-N-CA	9.07	132.44	120.28	1	4
1	A	16	LYS	CA-C-N	9.04	132.14	120.56	16	2
1	A	16	LYS	C-N-CA	9.04	132.14	120.56	16	2
1	A	45	PHE	CA-C-N	9.04	132.59	122.83	1	3
1	A	45	PHE	C-N-CA	9.04	132.59	122.83	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	100	ARG	NH1-CZ-NH2	-8.95	107.67	119.30	7	5
1	A	109	PRO	N-CA-CB	8.81	112.50	103.25	11	3
1	A	76	ARG	NH1-CZ-NH2	-8.77	107.90	119.30	14	3
1	A	44	GLU	O-C-N	8.58	131.35	122.09	6	1
1	A	116	VAL	CA-C-N	8.57	132.13	120.38	15	2
1	A	116	VAL	C-N-CA	8.57	132.13	120.38	15	2
1	A	102	VAL	CA-C-O	8.53	129.72	120.43	12	2
1	A	77	ILE	CA-C-N	8.50	128.52	119.76	13	3
1	A	77	ILE	C-N-CA	8.50	128.52	119.76	13	3
1	A	10	ASP	CA-CB-CG	8.48	121.08	112.60	2	4
1	A	84	ALA	N-CA-C	8.48	121.36	111.02	19	2
1	A	50	ILE	O-C-N	-8.43	114.08	123.10	1	2
1	A	15	ARG	NH1-CZ-NH2	-8.39	108.40	119.30	9	4
1	A	53	ASP	CA-C-N	8.25	132.20	120.98	19	3
1	A	53	ASP	C-N-CA	8.25	132.20	120.98	19	3
1	A	11	SER	CA-C-O	8.21	129.91	120.80	20	3
1	A	104	ARG	NE-CZ-NH2	-8.16	111.85	119.20	20	2
1	A	118	HIS	CB-CG-CD2	-8.13	120.63	131.20	10	9
1	A	13	VAL	O-C-N	-8.13	113.69	121.90	10	2
1	A	47	PRO	N-CA-CB	8.06	110.36	103.35	1	2
1	A	115	GLU	CA-C-N	8.02	131.28	120.77	1	7
1	A	115	GLU	C-N-CA	8.02	131.28	120.77	1	7
1	A	23	LYS	O-C-N	8.01	130.32	122.07	3	2
1	A	100	ARG	NE-CZ-NH1	8.00	129.50	121.50	7	3
1	A	29	VAL	CA-C-N	7.96	132.65	121.66	8	3
1	A	29	VAL	C-N-CA	7.96	132.65	121.66	8	3
1	A	48	ASP	CA-CB-CG	-7.95	104.65	112.60	17	3
1	A	22	LEU	N-CA-C	-7.94	102.61	111.82	11	2
1	A	72	GLU	CA-C-N	7.94	132.38	120.31	11	1
1	A	72	GLU	C-N-CA	7.94	132.38	120.31	11	1
1	A	46	THR	CA-C-N	7.92	129.30	120.66	16	4
1	A	46	THR	C-N-CA	7.92	129.30	120.66	16	4
1	A	21	ASN	OD1-CG-ND2	-7.92	114.68	122.60	9	8
1	A	75	LYS	CA-C-N	7.92	131.68	120.28	20	4
1	A	75	LYS	C-N-CA	7.92	131.68	120.28	20	4
1	A	63	THR	CA-CB-OG1	-7.87	97.79	109.60	9	3
1	A	117	LYS	CA-C-N	7.83	131.12	120.54	19	2
1	A	117	LYS	C-N-CA	7.83	131.12	120.54	19	2
1	A	34	ASN	CA-C-N	7.80	129.89	120.14	18	7
1	A	34	ASN	C-N-CA	7.80	129.89	120.14	18	7
1	A	112	PHE	N-CA-C	7.75	119.36	111.07	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	117	LYS	N-CA-C	7.73	119.34	111.07	17	5
1	A	15	ARG	NE-CZ-NH2	-7.72	112.25	119.20	2	5
1	A	51	VAL	CA-C-O	-7.70	113.37	120.22	1	1
1	A	20	PHE	CA-CB-CG	7.70	121.50	113.80	10	2
1	A	51	VAL	CB-CA-C	7.69	119.18	110.41	1	1
1	A	108	SER	CA-C-N	7.68	126.96	118.97	4	6
1	A	108	SER	C-N-CA	7.68	126.96	118.97	4	6
1	A	114	GLU	CA-C-N	7.68	131.20	120.29	14	3
1	A	114	GLU	C-N-CA	7.68	131.20	120.29	14	3
1	A	118	HIS	CA-C-O	-7.68	112.68	120.90	19	3
1	A	83	THR	CA-C-N	7.68	130.42	120.44	13	5
1	A	83	THR	C-N-CA	7.68	130.42	120.44	13	5
1	A	98	GLY	O-C-N	-7.64	113.40	122.33	16	3
1	A	41	LYS	N-CA-C	7.60	119.64	111.36	13	2
1	A	60	ASP	CA-CB-CG	7.58	120.19	112.60	15	3
1	A	18	VAL	CG1-CB-CG2	-7.58	94.12	110.80	5	2
1	A	120	LEU	N-CA-C	7.54	121.37	112.93	14	2
1	A	66	LYS	O-C-N	-7.46	114.39	122.07	13	5
1	A	33	GLU	CA-C-N	7.45	133.64	121.86	14	1
1	A	33	GLU	C-N-CA	7.45	133.64	121.86	14	1
1	A	12	ALA	N-CA-C	7.44	120.45	111.82	20	3
1	A	74	TRP	CA-C-N	7.44	130.25	120.28	16	3
1	A	74	TRP	C-N-CA	7.44	130.25	120.28	16	3
1	A	100	ARG	CD-NE-CZ	7.41	134.78	124.40	8	3
1	A	15	ARG	CA-C-N	7.39	130.49	120.44	11	3
1	A	15	ARG	C-N-CA	7.39	130.49	120.44	11	3
1	A	36	GLN	OE1-CD-NE2	-7.39	115.21	122.60	20	5
1	A	67	LYS	N-CA-C	7.38	119.41	111.36	5	1
1	A	60	ASP	CA-C-N	7.37	128.16	119.98	19	4
1	A	60	ASP	C-N-CA	7.37	128.16	119.98	19	4
1	A	65	LEU	CA-C-O	-7.35	113.04	120.90	10	2
1	A	18	VAL	CA-C-O	-7.33	113.32	120.95	17	2
1	A	87	GLY	CA-C-N	7.33	129.96	120.44	16	3
1	A	87	GLY	C-N-CA	7.33	129.96	120.44	16	3
1	A	74	TRP	N-CA-C	7.32	119.33	111.36	8	2
1	A	13	VAL	N-CA-C	7.30	117.83	110.23	16	7
1	A	100	ARG	N-CA-CB	-7.30	99.38	110.12	18	1
1	A	23	LYS	N-CA-C	-7.30	103.40	111.36	11	2
1	A	28	GLU	CA-C-O	-7.27	113.20	121.19	12	1
1	A	38	ALA	N-CA-C	7.26	119.28	111.36	2	2
1	A	117	LYS	O-C-N	7.26	129.55	122.07	12	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	GLU	CA-C-O	7.25	128.41	119.78	17	2
1	A	95	LEU	CA-C-O	-7.24	112.88	120.55	5	2
1	A	18	VAL	O-C-N	7.23	129.17	121.94	2	2
1	A	45	PHE	O-C-N	-7.22	114.75	122.19	1	1
1	A	18	VAL	CA-CB-CG1	7.22	122.67	110.40	19	2
1	A	16	LYS	CA-C-O	-7.21	112.90	120.55	13	1
1	A	111	GLN	OE1-CD-NE2	-7.18	115.42	122.60	15	5
1	A	90	ASP	O-C-N	7.18	129.73	122.12	7	1
1	A	104	ARG	NE-CZ-NH1	7.17	128.67	121.50	9	5
1	A	19	SER	CA-C-N	7.14	130.18	120.54	11	7
1	A	19	SER	C-N-CA	7.14	130.18	120.54	11	7
1	A	66	LYS	CA-C-N	7.12	129.82	120.28	13	4
1	A	66	LYS	C-N-CA	7.12	129.82	120.28	13	4
1	A	100	ARG	N-CA-C	7.12	119.04	111.28	1	1
1	A	99	ALA	N-CA-C	7.09	120.24	110.24	15	3
1	A	98	GLY	N-CA-C	7.05	125.37	115.43	17	1
1	A	121	ASN	CB-CG-ND2	-7.04	105.84	116.40	19	1
1	A	9	ASP	CA-CB-CG	7.03	119.63	112.60	9	2
1	A	82	LEU	CA-C-O	-7.03	112.68	120.69	19	1
1	A	76	ARG	CA-C-N	6.99	127.62	122.59	7	1
1	A	76	ARG	C-N-CA	6.99	127.62	122.59	7	1
1	A	44	GLU	N-CA-C	6.98	118.68	111.14	6	2
1	A	89	GLU	CA-C-O	-6.98	113.67	121.00	17	4
1	A	112	PHE	CA-C-N	6.96	129.58	120.60	7	2
1	A	112	PHE	C-N-CA	6.96	129.58	120.60	7	2
1	A	83	THR	O-C-N	-6.94	115.29	123.41	9	1
1	A	56	MET	CA-C-N	6.93	126.89	120.03	9	7
1	A	56	MET	C-N-CA	6.93	126.89	120.03	9	7
1	A	37	ILE	N-CA-C	6.93	117.43	110.23	10	3
1	A	18	VAL	CB-CA-C	6.92	120.74	111.88	15	3
1	A	62	PHE	CA-CB-CG	-6.91	106.89	113.80	7	6
1	A	112	PHE	CA-C-O	-6.90	113.59	120.70	10	3
1	A	71	LYS	CA-C-N	6.88	130.76	120.31	3	1
1	A	71	LYS	C-N-CA	6.88	130.76	120.31	3	1
1	A	69	GLN	CA-C-N	6.87	129.49	120.28	5	2
1	A	69	GLN	C-N-CA	6.87	129.49	120.28	5	2
1	A	76	ARG	NE-CZ-NH1	6.84	128.34	121.50	1	4
1	A	94	ALA	CA-C-N	6.83	129.32	120.44	7	3
1	A	94	ALA	C-N-CA	6.83	129.32	120.44	7	3
1	A	38	ALA	CA-C-N	6.83	130.11	120.28	5	1
1	A	38	ALA	C-N-CA	6.83	130.11	120.28	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	105	LYS	CA-C-O	-6.82	112.88	120.25	10	1
1	A	54	ILE	N-CA-C	6.82	116.92	110.30	15	1
1	A	107	PHE	N-CA-C	6.81	118.59	111.03	7	1
1	A	116	VAL	N-CA-C	-6.80	104.02	110.42	14	2
1	A	89	GLU	O-C-N	6.80	129.10	122.03	17	3
1	A	104	ARG	N-CA-C	6.79	120.34	110.28	6	2
1	A	107	PHE	CA-C-N	6.78	132.36	122.66	14	2
1	A	107	PHE	C-N-CA	6.78	132.36	122.66	14	2
1	A	41	LYS	CA-C-N	6.78	129.65	120.44	6	4
1	A	41	LYS	C-N-CA	6.78	129.65	120.44	6	4
1	A	48	ASP	CA-C-O	6.76	127.23	119.18	18	2
1	A	95	LEU	CA-C-N	6.75	129.32	120.28	7	2
1	A	95	LEU	C-N-CA	6.75	129.32	120.28	7	2
1	A	72	GLU	N-CA-C	6.74	121.10	112.34	9	2
1	A	92	SER	O-C-N	6.73	129.00	122.07	10	1
1	A	78	PRO	N-CA-CB	6.72	109.19	103.35	15	5
1	A	106	PRO	O-C-N	6.71	130.14	123.03	13	2
1	A	57	PRO	N-CA-CB	6.70	109.97	102.67	18	3
1	A	30	ILE	CA-CB-CG2	6.70	121.89	110.50	17	1
1	A	39	LEU	N-CA-C	6.67	118.64	111.36	19	2
1	A	65	LEU	CD1-CG-CD2	-6.67	96.13	110.80	11	1
1	A	89	GLU	N-CA-C	6.67	118.34	111.14	1	1
1	A	110	SER	CA-C-N	6.67	129.11	120.44	16	4
1	A	110	SER	C-N-CA	6.67	129.11	120.44	16	4
1	A	83	THR	CA-CB-CG2	6.66	121.83	110.50	20	3
1	A	54	ILE	CA-C-N	6.66	134.25	121.54	18	5
1	A	54	ILE	C-N-CA	6.66	134.25	121.54	18	5
1	A	104	ARG	CA-C-O	-6.64	114.51	121.55	9	1
1	A	113	ILE	N-CA-C	-6.64	103.86	110.30	11	2
1	A	118	HIS	ND1-CE1-NE2	6.64	115.04	108.40	13	4
1	A	88	GLU	CA-C-N	6.64	129.07	120.44	5	1
1	A	88	GLU	C-N-CA	6.64	129.07	120.44	5	1
1	A	40	GLU	CA-C-N	6.64	129.84	120.28	3	1
1	A	40	GLU	C-N-CA	6.64	129.84	120.28	3	1
1	A	40	GLU	N-CA-C	6.63	118.50	111.28	19	6
1	A	57	PRO	O-C-N	-6.63	114.91	123.00	9	1
1	A	118	HIS	ND1-CG-CD2	6.62	112.72	106.10	16	4
1	A	8	VAL	CA-C-O	-6.62	113.63	121.64	15	3
1	A	39	LEU	O-C-N	6.62	128.89	122.07	7	2
1	A	56	MET	N-CA-CB	-6.62	105.05	111.27	12	1
1	A	86	GLY	O-C-N	-6.62	114.95	122.56	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	SER	CA-C-O	-6.60	113.90	120.70	6	1
1	A	12	ALA	CA-C-N	6.60	129.00	120.56	9	3
1	A	12	ALA	C-N-CA	6.60	129.00	120.56	9	3
1	A	71	LYS	O-C-N	-6.59	115.55	123.13	10	1
1	A	36	GLN	CA-C-O	-6.59	113.90	120.82	15	1
1	A	22	LEU	CA-C-O	-6.58	113.45	120.42	5	1
1	A	100	ARG	CA-C-N	6.57	133.50	121.94	14	2
1	A	100	ARG	C-N-CA	6.57	133.50	121.94	14	2
1	A	22	LEU	CA-C-N	6.57	129.37	120.44	7	5
1	A	22	LEU	C-N-CA	6.57	129.37	120.44	7	5
1	A	27	TYR	O-C-N	-6.56	114.42	122.82	19	1
1	A	45	PHE	CA-CB-CG	6.56	120.36	113.80	16	4
1	A	45	PHE	CA-C-O	-6.55	111.69	119.35	12	2
1	A	63	THR	O-C-N	-6.55	114.69	122.15	8	1
1	A	21	ASN	N-CA-C	6.54	118.07	111.07	3	5
1	A	38	ALA	O-C-N	-6.52	115.35	122.07	19	4
1	A	118	HIS	N-CA-C	-6.52	104.10	111.14	10	1
1	A	27	TYR	N-CA-C	6.51	118.71	110.24	6	1
1	A	79	VAL	N-CA-C	6.50	117.62	107.28	6	4
1	A	51	VAL	CA-CB-CG2	6.50	121.44	110.40	10	2
1	A	46	THR	CA-CB-OG1	-6.49	99.87	109.60	10	1
1	A	52	LEU	O-C-N	-6.49	115.64	123.29	12	3
1	A	3	LYS	CA-C-O	6.48	128.93	121.47	14	2
1	A	5	VAL	N-CA-C	6.48	118.13	107.24	4	2
1	A	121	ASN	CA-CB-CG	-6.48	106.12	112.60	12	5
1	A	112	PHE	O-C-N	6.47	129.08	122.09	10	1
1	A	81	VAL	CA-C-N	6.46	130.00	120.95	2	2
1	A	81	VAL	C-N-CA	6.46	130.00	120.95	2	2
1	A	29	VAL	CA-C-O	6.46	127.81	120.90	20	2
1	A	17	ILE	CB-CA-C	6.45	120.47	112.02	16	2
1	A	67	LYS	CA-C-O	-6.45	114.05	120.82	15	3
1	A	35	GLY	CA-C-O	-6.45	114.11	120.75	11	5
1	A	3	LYS	CA-C-N	6.44	132.08	123.00	18	3
1	A	3	LYS	C-N-CA	6.44	132.08	123.00	18	3
1	A	70	GLU	N-CA-CB	-6.40	100.66	110.20	3	1
1	A	54	ILE	CA-C-O	-6.39	113.72	121.13	11	2
1	A	64	VAL	CA-C-N	6.39	128.74	120.44	9	2
1	A	64	VAL	C-N-CA	6.39	128.74	120.44	9	2
1	A	43	SER	CA-C-N	6.38	128.74	120.44	18	2
1	A	43	SER	C-N-CA	6.38	128.74	120.44	18	2
1	A	94	ALA	O-C-N	6.37	128.88	122.12	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	GLU	CA-CB-CG	6.37	126.85	114.10	20	1
1	A	82	LEU	CA-C-N	6.36	132.55	122.62	14	1
1	A	82	LEU	C-N-CA	6.36	132.55	122.62	14	1
1	A	77	ILE	CA-CB-CG1	6.36	121.20	110.40	2	2
1	A	106	PRO	CB-CA-C	6.35	118.48	111.56	18	2
1	A	38	ALA	CA-C-O	-6.34	113.83	120.55	17	2
1	A	109	PRO	N-CD-CG	6.34	112.71	103.20	9	1
1	A	90	ASP	CA-C-O	6.32	127.21	120.70	20	1
1	A	64	VAL	N-CA-C	6.30	117.08	110.72	3	4
1	A	95	LEU	O-C-N	6.29	128.79	122.12	6	4
1	A	63	THR	CA-CB-CG2	6.28	121.18	110.50	9	2
1	A	20	PHE	CA-C-N	6.28	128.60	120.44	3	1
1	A	20	PHE	C-N-CA	6.28	128.60	120.44	3	1
1	A	64	VAL	N-CA-CB	6.27	117.21	110.62	10	1
1	A	96	SER	CA-C-O	6.27	127.09	119.38	3	2
1	A	46	THR	CA-CB-CG2	6.26	121.14	110.50	1	1
1	A	21	ASN	CA-C-O	-6.26	113.91	120.55	9	1
1	A	54	ILE	CA-CB-CG1	6.26	121.04	110.40	2	1
1	A	73	GLU	N-CA-C	6.25	118.61	111.11	18	3
1	A	119	LEU	O-C-N	-6.25	115.50	122.12	7	1
1	A	58	VAL	CA-C-O	-6.25	112.97	120.78	20	2
1	A	44	GLU	CA-C-O	-6.25	114.27	120.70	6	2
1	A	24	LYS	CA-C-O	6.24	127.29	119.12	7	3
1	A	79	VAL	CA-C-O	-6.24	112.56	120.86	11	3
1	A	35	GLY	N-CA-C	6.23	120.18	112.64	19	3
1	A	60	ASP	N-CA-CB	-6.23	100.42	109.83	4	1
1	A	63	THR	CB-CA-C	6.23	120.66	110.88	6	1
1	A	23	LYS	CB-CA-C	6.22	120.74	110.90	7	1
1	A	118	HIS	O-C-N	6.21	128.72	122.08	18	2
1	A	93	LEU	CA-C-O	-6.20	114.49	121.00	16	2
1	A	42	LEU	N-CA-C	-6.20	104.52	111.28	17	2
1	A	66	LYS	N-CA-CB	6.20	119.00	110.01	13	1
1	A	119	LEU	N-CA-C	6.20	118.84	111.71	15	2
1	A	23	LYS	N-CA-CB	6.19	119.22	110.12	4	1
1	A	97	LEU	CD1-CG-CD2	6.19	124.41	110.80	4	1
1	A	102	VAL	CA-CB-CG2	6.19	120.92	110.40	15	1
1	A	34	ASN	CB-CG-ND2	6.18	125.67	116.40	13	1
1	A	12	ALA	CA-C-O	-6.17	112.38	119.60	14	1
1	A	98	GLY	CA-C-O	-6.17	112.00	119.03	4	2
1	A	111	GLN	O-C-N	-6.17	115.72	122.07	15	2
1	A	57	PRO	CA-C-N	6.17	133.07	121.97	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	PRO	C-N-CA	6.17	133.07	121.97	20	2
1	A	17	ILE	CA-C-N	6.16	128.40	120.70	12	1
1	A	17	ILE	C-N-CA	6.16	128.40	120.70	12	1
1	A	3	LYS	CA-CB-CG	-6.15	101.79	114.10	20	1
1	A	20	PHE	N-CA-C	-6.15	104.65	111.36	13	2
1	A	51	VAL	O-C-N	-6.14	116.69	123.20	19	3
1	A	86	GLY	CA-C-N	6.12	126.49	120.98	12	2
1	A	86	GLY	C-N-CA	6.12	126.49	120.98	12	2
1	A	91	GLU	CB-CA-C	6.12	120.38	110.96	15	1
1	A	50	ILE	N-CA-C	6.11	116.72	108.17	2	2
1	A	87	GLY	CA-C-O	-6.10	116.09	121.58	18	1
1	A	16	LYS	O-C-N	6.10	128.58	122.12	2	2
1	A	88	GLU	CA-C-O	6.10	127.03	120.20	3	1
1	A	39	LEU	CA-C-N	6.10	128.45	120.28	14	1
1	A	39	LEU	C-N-CA	6.10	128.45	120.28	14	1
1	A	35	GLY	CA-C-N	6.08	128.34	120.44	15	1
1	A	35	GLY	C-N-CA	6.08	128.34	120.44	15	1
1	A	53	ASP	CB-CA-C	6.08	119.74	109.84	6	1
1	A	33	GLU	CB-CG-CD	-6.07	102.29	112.60	5	2
1	A	83	THR	OG1-CB-CG2	-6.04	97.22	109.30	7	2
1	A	24	LYS	CB-CA-C	6.04	120.36	110.88	17	1
1	A	74	TRP	CE2-CD2-CE3	-6.04	112.76	118.80	17	2
1	A	110	SER	N-CA-C	6.03	121.26	111.37	11	2
1	A	32	ALA	CA-C-N	6.02	130.23	120.60	11	4
1	A	32	ALA	C-N-CA	6.02	130.23	120.60	11	4
1	A	47	PRO	CA-C-N	6.01	130.90	120.68	6	2
1	A	47	PRO	C-N-CA	6.01	130.90	120.68	6	2
1	A	23	LYS	CA-C-N	6.01	128.25	120.44	5	1
1	A	23	LYS	C-N-CA	6.01	128.25	120.44	5	1
1	A	95	LEU	CD1-CG-CD2	-6.00	97.60	110.80	11	1
1	A	31	GLU	N-CA-CB	6.00	118.88	109.83	5	1
1	A	13	VAL	CA-CB-CG2	5.97	120.55	110.40	13	3
1	A	72	GLU	CA-C-O	-5.97	114.18	120.63	20	1
1	A	118	HIS	CA-CB-CG	5.97	119.77	113.80	18	3
1	A	67	LYS	CA-C-N	5.96	128.27	120.28	2	3
1	A	67	LYS	C-N-CA	5.96	128.27	120.28	2	3
1	A	63	THR	CA-C-N	5.96	128.07	120.56	8	1
1	A	63	THR	C-N-CA	5.96	128.07	120.56	8	1
1	A	49	LEU	CA-C-O	-5.96	114.08	120.75	18	1
1	A	14	LEU	O-C-N	5.95	130.31	122.33	11	1
1	A	31	GLU	CA-C-N	5.95	130.57	122.19	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	GLU	C-N-CA	5.95	130.57	122.19	20	1
1	A	3	LYS	O-C-N	-5.94	115.85	122.86	11	2
1	A	120	LEU	N-CA-CB	5.94	120.25	110.39	1	1
1	A	104	ARG	CD-NE-CZ	5.94	132.71	124.40	11	3
1	A	74	TRP	CA-C-O	-5.94	114.26	120.55	5	1
1	A	81	VAL	CA-C-O	-5.93	113.96	120.84	13	1
1	A	81	VAL	CB-CA-C	5.93	118.26	110.91	4	1
1	A	75	LYS	N-CA-CB	-5.92	101.10	110.22	9	1
1	A	74	TRP	CH2-CZ2-CE2	-5.91	109.82	117.50	9	2
1	A	69	GLN	CG-CD-NE2	5.91	125.26	116.40	5	3
1	A	79	VAL	O-C-N	-5.90	116.94	123.20	9	1
1	A	76	ARG	CD-NE-CZ	5.90	132.66	124.40	10	2
1	A	61	GLY	CA-C-N	5.88	128.16	120.28	12	2
1	A	61	GLY	C-N-CA	5.88	128.16	120.28	12	2
1	A	100	ARG	CA-C-O	-5.88	114.31	120.55	18	2
1	A	88	GLU	O-C-N	-5.88	115.34	122.22	12	1
1	A	23	LYS	CA-C-O	-5.88	114.65	120.82	3	3
1	A	31	GLU	CA-C-O	-5.87	114.49	120.71	16	2
1	A	60	ASP	N-CA-C	5.86	118.98	110.42	12	1
1	A	9	ASP	CA-C-N	5.86	128.41	120.38	6	5
1	A	9	ASP	C-N-CA	5.86	128.41	120.38	6	5
1	A	61	GLY	O-C-N	-5.85	116.10	122.54	9	2
1	A	14	LEU	CA-C-N	5.85	130.49	121.19	9	5
1	A	14	LEU	C-N-CA	5.85	130.49	121.19	9	5
1	A	105	LYS	N-CA-C	5.85	118.15	110.08	15	1
1	A	30	ILE	O-C-N	-5.84	117.04	122.71	6	1
1	A	26	GLY	CA-C-N	5.84	129.77	121.42	3	1
1	A	26	GLY	C-N-CA	5.84	129.77	121.42	3	1
1	A	118	HIS	CB-CG-ND1	5.82	131.43	122.70	10	1
1	A	43	SER	CA-C-O	-5.82	114.67	120.90	10	1
1	A	93	LEU	CA-C-N	5.81	128.07	120.28	9	1
1	A	93	LEU	C-N-CA	5.81	128.07	120.28	9	1
1	A	17	ILE	O-C-N	-5.81	116.21	121.91	14	1
1	A	45	PHE	N-CA-C	5.81	121.28	113.72	14	1
1	A	66	LYS	N-CA-C	5.81	119.63	112.54	2	1
1	A	45	PHE	N-CA-CB	-5.80	101.39	110.44	9	3
1	A	61	GLY	CA-C-O	5.79	126.48	119.65	9	2
1	A	109	PRO	CA-N-CD	-5.79	103.89	112.00	4	1
1	A	61	GLY	N-CA-C	5.79	119.89	112.83	5	2
1	A	105	LYS	CA-CB-CG	5.78	125.66	114.10	10	1
1	A	105	LYS	O-C-N	5.78	127.90	121.43	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	68	LEU	CA-C-N	5.77	128.28	120.38	5	4
1	A	68	LEU	C-N-CA	5.77	128.28	120.38	5	4
1	A	92	SER	N-CA-CB	5.76	118.37	110.01	1	1
1	A	8	VAL	CA-CB-CG2	5.76	120.20	110.40	15	2
1	A	7	LEU	CA-C-N	5.75	128.92	122.59	15	1
1	A	7	LEU	C-N-CA	5.75	128.92	122.59	15	1
1	A	74	TRP	NE1-CE2-CD2	-5.74	99.94	107.40	15	1
1	A	46	THR	CA-C-O	-5.74	115.67	120.26	9	1
1	A	42	LEU	CA-C-N	5.74	127.97	120.28	4	2
1	A	42	LEU	C-N-CA	5.74	127.97	120.28	4	2
1	A	99	ALA	N-CA-CB	-5.74	100.57	109.69	14	1
1	A	64	VAL	CB-CA-C	-5.73	104.53	112.04	7	2
1	A	78	PRO	O-C-N	-5.73	116.68	123.10	3	1
1	A	31	GLU	CB-CG-CD	-5.73	102.86	112.60	6	1
1	A	64	VAL	CA-CB-CG1	5.73	120.14	110.40	18	2
1	A	75	LYS	CA-C-O	5.72	126.42	119.38	8	1
1	A	47	PRO	CB-CA-C	-5.72	103.46	110.95	12	2
1	A	49	LEU	CA-C-N	5.72	130.95	123.06	18	3
1	A	49	LEU	C-N-CA	5.72	130.95	123.06	18	3
1	A	29	VAL	N-CA-C	5.71	117.00	108.54	15	1
1	A	113	ILE	CA-C-O	-5.71	114.80	120.85	14	2
1	A	13	VAL	CB-CA-C	-5.71	104.34	112.22	3	2
1	A	37	ILE	CA-C-N	5.71	128.19	120.65	3	2
1	A	37	ILE	C-N-CA	5.71	128.19	120.65	3	2
1	A	99	ALA	O-C-N	-5.71	115.84	122.87	10	2
1	A	121	ASN	O-C-N	-5.71	115.57	122.71	11	1
1	A	119	LEU	CA-C-O	-5.71	114.82	120.70	8	1
1	A	120	LEU	O-C-N	-5.71	115.25	122.27	5	2
1	A	97	LEU	N-CA-C	5.70	119.32	112.93	7	3
1	A	98	GLY	CA-C-N	5.70	128.94	120.90	17	2
1	A	98	GLY	C-N-CA	5.70	128.94	120.90	17	2
1	A	101	LYS	CB-CA-C	5.70	118.89	109.72	11	1
1	A	81	VAL	CA-CB-CG1	5.70	120.09	110.40	14	1
1	A	103	MET	O-C-N	5.69	128.98	123.29	6	1
1	A	17	ILE	CA-CB-CG1	5.69	120.07	110.40	15	1
1	A	113	ILE	O-C-N	5.67	127.67	121.83	6	1
1	A	62	PHE	O-C-N	-5.65	115.32	122.27	14	2
1	A	52	LEU	N-CA-CB	-5.65	102.25	110.84	19	1
1	A	32	ALA	N-CA-C	5.64	117.59	108.34	6	2
1	A	78	PRO	CA-C-O	5.64	127.45	121.03	3	1
1	A	52	LEU	CA-C-N	5.64	131.10	122.93	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	52	LEU	C-N-CA	5.64	131.10	122.93	8	2
1	A	84	ALA	CA-C-N	5.63	132.30	121.54	11	2
1	A	84	ALA	C-N-CA	5.63	132.30	121.54	11	2
1	A	94	ALA	CA-C-O	-5.63	114.58	120.55	13	1
1	A	21	ASN	CA-C-N	5.63	128.14	120.54	14	1
1	A	21	ASN	C-N-CA	5.63	128.14	120.54	14	1
1	A	114	GLU	CA-C-O	-5.62	114.46	120.42	17	2
1	A	108	SER	CA-C-O	-5.62	115.64	119.29	5	1
1	A	90	ASP	CA-C-N	5.61	127.73	120.44	9	1
1	A	90	ASP	C-N-CA	5.61	127.73	120.44	9	1
1	A	109	PRO	N-CA-C	5.60	121.32	113.53	1	1
1	A	94	ALA	N-CA-C	5.59	117.37	111.28	8	3
1	A	89	GLU	CA-C-N	5.59	128.04	120.44	2	2
1	A	89	GLU	C-N-CA	5.59	128.04	120.44	2	2
1	A	121	ASN	OD1-CG-ND2	-5.59	117.01	122.60	9	2
1	A	24	LYS	CA-C-N	5.59	128.54	120.38	17	1
1	A	24	LYS	C-N-CA	5.59	128.54	120.38	17	1
1	A	59	MET	N-CA-CB	5.58	119.54	110.77	12	1
1	A	14	LEU	N-CA-C	-5.58	106.60	113.41	14	1
1	A	70	GLU	CA-C-O	5.57	126.38	119.97	9	1
1	A	71	LYS	CA-C-O	5.57	126.67	120.43	4	1
1	A	116	VAL	N-CA-CB	-5.57	102.97	110.54	2	1
1	A	67	LYS	O-C-N	5.56	127.80	122.07	19	1
1	A	42	LEU	CA-C-O	-5.56	114.98	120.82	16	1
1	A	59	MET	O-C-N	-5.56	116.40	123.24	18	1
1	A	81	VAL	N-CA-C	5.55	115.78	107.51	12	1
1	A	58	VAL	CB-CA-C	5.54	120.37	111.29	16	1
1	A	44	GLU	CB-CA-C	5.54	119.64	110.90	3	1
1	A	109	PRO	O-C-N	-5.54	115.08	122.22	20	1
1	A	13	VAL	CA-CB-CG1	5.53	119.81	110.40	1	1
1	A	12	ALA	N-CA-CB	-5.53	101.70	110.28	20	1
1	A	102	VAL	O-C-N	-5.53	117.10	123.07	12	2
1	A	51	VAL	N-CA-CB	5.53	118.63	111.83	9	1
1	A	106	PRO	N-CD-CG	5.52	111.48	103.20	3	1
1	A	107	PHE	CA-C-O	5.52	124.88	118.97	20	2
1	A	115	GLU	N-CA-CB	5.52	118.01	110.01	15	1
1	A	27	TYR	CA-C-N	5.52	129.18	121.02	20	2
1	A	27	TYR	C-N-CA	5.52	129.18	121.02	20	2
1	A	83	THR	N-CA-C	5.51	117.40	108.41	1	1
1	A	94	ALA	N-CA-CB	-5.51	102.01	110.12	8	1
1	A	74	TRP	NE1-CE2-CZ2	5.51	138.37	130.10	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	116	VAL	CA-C-O	-5.51	115.68	121.41	20	1
1	A	118	HIS	CA-C-N	5.50	127.66	120.28	2	1
1	A	118	HIS	C-N-CA	5.50	127.66	120.28	2	1
1	A	76	ARG	N-CA-CB	-5.48	101.20	110.41	18	1
1	A	11	SER	CB-CA-C	5.48	118.52	109.70	2	1
1	A	9	ASP	O-C-N	-5.47	117.18	123.42	11	1
1	A	88	GLU	N-CA-C	5.46	118.73	111.75	7	2
1	A	67	LYS	CB-CG-CD	5.45	123.84	111.30	3	1
1	A	115	GLU	N-CA-C	5.45	117.67	111.02	13	1
1	A	63	THR	N-CA-C	-5.45	104.99	111.69	15	2
1	A	50	ILE	CB-CA-C	5.45	119.09	110.81	17	2
1	A	68	LEU	CA-C-O	-5.44	115.11	120.82	10	1
1	A	6	LEU	CA-C-O	5.44	126.20	120.54	3	1
1	A	65	LEU	N-CA-CB	5.44	117.90	110.01	2	1
1	A	116	VAL	CA-CB-CG1	5.44	119.65	110.40	6	2
1	A	30	ILE	CA-CB-CG1	5.44	119.64	110.40	5	2
1	A	25	GLU	CA-C-O	5.44	126.07	119.38	8	1
1	A	3	LYS	N-CA-CB	5.43	117.96	109.97	10	1
1	A	5	VAL	CA-C-O	5.43	125.63	120.31	7	1
1	A	41	LYS	CA-CB-CG	-5.43	103.25	114.10	6	1
1	A	34	ASN	N-CA-C	5.43	117.04	108.96	13	1
1	A	88	GLU	N-CA-CB	5.42	117.87	110.01	16	1
1	A	121	ASN	CA-C-N	5.42	131.46	121.70	11	1
1	A	121	ASN	C-N-CA	5.42	131.46	121.70	11	1
1	A	88	GLU	CB-CG-CD	5.41	121.80	112.60	11	1
1	A	107	PHE	O-C-N	-5.40	115.64	122.17	16	1
1	A	111	GLN	CA-C-N	5.40	127.46	120.44	18	1
1	A	111	GLN	C-N-CA	5.40	127.46	120.44	18	1
1	A	103	MET	N-CA-C	5.39	116.47	108.60	14	2
1	A	117	LYS	CB-CG-CD	5.39	123.70	111.30	18	1
1	A	54	ILE	O-C-N	5.39	128.17	122.67	11	1
1	A	21	ASN	CB-CG-ND2	5.38	124.48	116.40	10	2
1	A	27	TYR	CA-C-O	-5.38	115.62	121.44	6	1
1	A	96	SER	O-C-N	-5.38	115.22	122.43	18	1
1	A	69	GLN	N-CA-C	5.38	117.14	111.28	9	1
1	A	34	ASN	CB-CA-C	5.37	118.96	109.89	17	1
1	A	15	ARG	N-CA-CB	-5.37	102.23	110.12	12	2
1	A	18	VAL	CA-C-N	5.36	127.47	120.28	13	2
1	A	18	VAL	C-N-CA	5.36	127.47	120.28	13	2
1	A	72	GLU	CB-CG-CD	5.36	121.72	112.60	5	1
1	A	49	LEU	O-C-N	-5.36	116.93	123.36	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	VAL	CA-CB-CG2	5.36	119.50	110.40	13	2
1	A	97	LEU	O-C-N	-5.36	115.52	122.37	18	1
1	A	57	PRO	CA-N-CD	-5.35	104.51	112.00	18	1
1	A	19	SER	CB-CA-C	5.35	119.19	110.96	9	1
1	A	11	SER	CA-C-N	5.34	128.43	120.31	15	1
1	A	11	SER	C-N-CA	5.34	128.43	120.31	15	1
1	A	39	LEU	CA-C-O	-5.34	113.49	119.79	1	1
1	A	117	LYS	CA-C-O	-5.33	114.90	120.55	1	2
1	A	28	GLU	CB-CA-C	5.33	118.77	110.67	5	1
1	A	5	VAL	CA-CB-CG1	5.33	119.46	110.40	7	1
1	A	85	LYS	CA-C-O	-5.33	112.95	118.65	10	1
1	A	74	TRP	CB-CG-CD2	5.32	134.25	126.80	19	1
1	A	102	VAL	CA-CB-CG1	5.32	119.44	110.40	19	1
1	A	8	VAL	O-C-N	-5.31	115.18	122.62	4	1
1	A	35	GLY	O-C-N	-5.31	117.08	122.18	14	1
1	A	80	ILE	CA-C-O	-5.31	114.80	120.85	5	1
1	A	73	GLU	CA-C-O	5.31	126.08	119.97	4	2
1	A	115	GLU	CB-CG-CD	-5.30	103.58	112.60	8	1
1	A	65	LEU	CB-CA-C	5.30	119.86	110.85	20	2
1	A	122	GLU	N-CA-CB	-5.29	101.50	110.50	13	1
1	A	46	THR	CB-CA-C	-5.29	107.44	111.20	16	2
1	A	5	VAL	CA-C-N	5.29	129.45	122.42	10	1
1	A	5	VAL	C-N-CA	5.29	129.45	122.42	10	1
1	A	24	LYS	O-C-N	5.28	127.72	122.12	18	1
1	A	104	ARG	NH1-CZ-NH2	-5.28	112.44	119.30	14	1
1	A	16	LYS	N-CA-C	-5.27	105.71	111.82	18	2
1	A	21	ASN	CB-CA-C	5.27	119.81	110.85	5	1
1	A	49	LEU	CD1-CG-CD2	-5.27	99.21	110.80	3	1
1	A	44	GLU	CA-CB-CG	5.27	124.63	114.10	9	2
1	A	89	GLU	N-CA-CB	-5.27	102.43	110.07	1	1
1	A	48	ASP	O-C-N	-5.26	116.11	122.48	16	1
1	A	71	LYS	CA-CB-CG	5.26	124.62	114.10	19	1
1	A	74	TRP	CG-CD1-NE1	5.26	117.04	110.20	19	1
1	A	40	GLU	CA-C-O	-5.26	115.27	120.90	20	1
1	A	19	SER	CA-C-O	-5.26	114.98	120.55	13	1
1	A	121	ASN	CB-CA-C	5.25	119.13	110.88	2	2
1	A	44	GLU	CA-C-N	5.25	130.84	121.75	5	1
1	A	44	GLU	C-N-CA	5.25	130.84	121.75	5	1
1	A	44	GLU	N-CA-CB	5.25	117.62	110.01	18	2
1	A	33	GLU	N-CA-C	5.24	117.90	111.82	20	1
1	A	40	GLU	CB-CG-CD	5.23	121.49	112.60	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	8	VAL	CG1-CB-CG2	-5.23	99.30	110.80	10	1
1	A	40	GLU	N-CA-CB	-5.23	102.43	110.01	16	1
1	A	62	PHE	CA-C-N	5.23	127.23	120.44	20	1
1	A	62	PHE	C-N-CA	5.23	127.23	120.44	20	1
1	A	84	ALA	N-CA-CB	-5.22	101.89	110.40	1	1
1	A	109	PRO	CA-C-N	5.22	127.54	120.44	10	1
1	A	109	PRO	C-N-CA	5.22	127.54	120.44	10	1
1	A	117	LYS	CB-CA-C	-5.22	101.81	110.68	10	1
1	A	78	PRO	CB-CA-C	5.21	117.24	111.56	8	1
1	A	95	LEU	CB-CA-C	5.21	119.06	110.88	19	1
1	A	24	LYS	N-CA-CB	5.21	117.73	109.82	13	1
1	A	48	ASP	CA-C-N	5.20	131.10	121.94	1	1
1	A	48	ASP	C-N-CA	5.20	131.10	121.94	1	1
1	A	13	VAL	CA-C-O	-5.20	116.00	121.41	1	2
1	A	28	GLU	CA-C-N	-5.20	114.52	121.80	1	1
1	A	28	GLU	C-N-CA	-5.20	114.52	121.80	1	1
1	A	10	ASP	N-CA-C	5.20	121.87	110.80	8	1
1	A	80	ILE	CB-CG1-CD1	5.19	124.71	113.80	12	1
1	A	121	ASN	CB-CG-OD1	5.19	131.19	120.80	19	1
1	A	22	LEU	N-CA-CB	5.19	117.84	110.16	15	1
1	A	18	VAL	N-CA-C	5.18	115.33	110.30	12	1
1	A	14	LEU	N-CA-CB	-5.17	103.49	110.67	3	1
1	A	59	MET	CA-C-N	5.17	128.55	120.75	10	2
1	A	59	MET	C-N-CA	5.17	128.55	120.75	10	2
1	A	58	VAL	CA-C-N	5.16	131.03	121.94	4	1
1	A	58	VAL	C-N-CA	5.16	131.03	121.94	4	1
1	A	82	LEU	N-CA-CB	-5.16	102.22	110.63	5	1
1	A	77	ILE	CA-CB-CG2	5.15	119.26	110.50	3	1
1	A	32	ALA	O-C-N	-5.15	117.24	123.27	16	1
1	A	36	GLN	O-C-N	-5.15	116.28	122.15	4	1
1	A	42	LEU	CB-CG-CD1	5.14	126.13	110.70	11	1
1	A	106	PRO	N-CA-C	5.14	118.57	110.50	13	1
1	A	31	GLU	CB-CA-C	5.14	118.36	110.14	13	1
1	A	37	ILE	CA-CB-CG1	5.13	119.12	110.40	18	1
1	A	73	GLU	N-CA-CB	-5.13	102.30	109.94	18	1
1	A	23	LYS	CB-CG-CD	5.12	123.07	111.30	20	1
1	A	108	SER	O-C-N	-5.11	115.29	121.12	9	1
1	A	93	LEU	CB-CA-C	5.11	118.83	110.96	17	1
1	A	85	LYS	N-CA-C	5.11	121.68	110.80	11	1
1	A	26	GLY	O-C-N	-5.11	116.06	122.70	15	1
1	A	74	TRP	CE2-CD2-CG	5.11	113.33	107.20	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	99	ALA	CA-C-O	5.09	126.79	121.19	10	1
1	A	30	ILE	N-CA-CB	5.09	117.18	111.89	12	1
1	A	71	LYS	CG-CD-CE	5.08	123.00	111.30	10	1
1	A	87	GLY	O-C-N	5.07	128.07	122.84	18	1
1	A	65	LEU	O-C-N	-5.07	116.37	122.15	20	1
1	A	101	LYS	CA-C-O	5.07	126.17	119.98	20	1
1	A	102	VAL	N-CA-C	5.07	115.58	108.17	9	1
1	A	76	ARG	CA-CB-CG	-5.07	103.96	114.10	3	1
1	A	71	LYS	N-CA-C	5.06	117.86	109.46	5	1
1	A	92	SER	CA-C-N	5.06	127.82	120.79	13	1
1	A	92	SER	C-N-CA	5.06	127.82	120.79	13	1
1	A	55	MET	O-C-N	-5.05	115.88	122.59	17	1
1	A	5	VAL	CB-CA-C	5.04	117.69	110.33	2	1
1	A	97	LEU	N-CA-CB	-5.04	103.18	110.70	3	1
1	A	36	GLN	N-CA-C	-5.04	106.29	112.90	13	1
1	A	84	ALA	CB-CA-C	5.04	119.18	110.86	4	1
1	A	19	SER	N-CA-C	5.04	116.46	111.07	6	1
1	A	7	LEU	N-CA-CB	-5.04	102.38	110.69	4	1
1	A	109	PRO	CB-CA-C	-5.04	104.31	112.62	1	1
1	A	57	PRO	N-CD-CG	5.03	110.75	103.20	4	1
1	A	103	MET	N-CA-CB	-5.03	103.61	111.56	10	1
1	A	79	VAL	CA-CB-CG2	5.03	118.95	110.40	17	1
1	A	28	GLU	O-C-N	-5.03	115.98	122.77	5	1
1	A	79	VAL	CA-C-N	5.03	128.60	121.66	16	1
1	A	79	VAL	C-N-CA	5.03	128.60	121.66	16	1
1	A	12	ALA	O-C-N	-5.03	115.59	122.33	17	1
1	A	113	ILE	CA-C-N	5.02	126.97	120.44	13	1
1	A	113	ILE	C-N-CA	5.02	126.97	120.44	13	1
1	A	69	GLN	CB-CG-CD	5.02	121.14	112.60	20	1
1	A	43	SER	N-CA-C	5.01	117.13	111.11	10	1
1	A	21	ASN	N-CA-CB	-5.01	102.75	110.16	12	1
1	A	105	LYS	N-CA-CB	5.01	117.11	109.75	2	1
1	A	101	LYS	N-CA-CB	-5.00	101.94	111.00	3	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	76	ARG	Sidechain	7
1	A	62	PHE	Sidechain,Mainchain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	20	PHE	Sidechain	3
1	A	27	TYR	Sidechain	3
1	A	12	ALA	Peptide	3
1	A	15	ARG	Sidechain	3
1	A	97	LEU	Peptide	2
1	A	104	ARG	Sidechain	2
1	A	70	GLU	Sidechain	1
1	A	93	LEU	Mainchain	1
1	A	108	SER	Mainchain	1
1	A	64	VAL	Mainchain	1
1	A	24	LYS	Mainchain	1
1	A	38	ALA	Mainchain	1
1	A	85	LYS	Peptide	1
1	A	115	GLU	Sidechain	1
1	A	118	HIS	Sidechain	1
1	A	58	VAL	Peptide	1
1	A	112	PHE	Sidechain	1
1	A	98	GLY	Mainchain	1
1	A	120	LEU	Peptide	1
1	A	45	PHE	Sidechain	1
1	A	107	PHE	Sidechain	1
1	A	4	LYS	Mainchain	1
1	A	65	LEU	Mainchain	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	956	1008	1008	1±1
All	All	19140	20160	20160	16

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:MET:HE3	1:A:64:VAL:HG22	0.75	1.58	16	1
1:A:91:GLU:HA	1:A:102:VAL:HG11	0.59	1.75	5	3
1:A:101:LYS:HE2	1:A:103:MET:SD	0.54	2.43	7	1
1:A:35:GLY:HA3	1:A:64:VAL:HG21	0.51	1.80	5	1
1:A:66:LYS:HG3	1:A:97:LEU:HD22	0.46	1.88	6	1
1:A:50:ILE:HD13	1:A:68:LEU:HD11	0.45	1.89	8	1
1:A:8:VAL:HG12	1:A:56:MET:HE1	0.45	1.88	15	1
1:A:66:LYS:HD2	1:A:97:LEU:HD22	0.45	1.87	4	1
1:A:30:ILE:N	1:A:30:ILE:HD12	0.43	2.28	13	1
1:A:35:GLY:O	1:A:38:ALA:HB3	0.41	2.16	11	1
1:A:80:ILE:HD11	1:A:119:LEU:CD1	0.41	2.45	12	1
1:A:85:LYS:C	1:A:104:ARG:HE	0.41	2.24	15	1
1:A:35:GLY:HA3	1:A:64:VAL:CG2	0.40	2.46	5	1
1:A:19:SER:OG	1:A:23:LYS:HE3	0.40	2.17	20	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/122 (98%)	111±2 (93±2%)	6±2 (5±1%)	2±1 (1±1%)	12	60
All	All	2380/2440 (98%)	2221 (93%)	128 (5%)	31 (1%)	12	60

All 5 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	55	MET	16
1	A	58	VAL	11
1	A	13	VAL	2
1	A	57	PRO	1
1	A	85	LYS	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	108/110 (98%)	106±2 (98±1%)	2±2 (2±1%)	46 90
All	All	2160/2200 (98%)	2115 (98%)	45 (2%)	46 90

All 32 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	34	ASN	5
1	A	42	LEU	4
1	A	29	VAL	2
1	A	85	LYS	2
1	A	24	LYS	2
1	A	89	GLU	2
1	A	13	VAL	2
1	A	63	THR	2
1	A	68	LEU	1
1	A	93	LEU	1
1	A	58	VAL	1
1	A	97	LEU	1
1	A	110	SER	1
1	A	115	GLU	1
1	A	66	LYS	1
1	A	44	GLU	1
1	A	105	LYS	1
1	A	48	ASP	1
1	A	8	VAL	1
1	A	119	LEU	1
1	A	107	PHE	1
1	A	70	GLU	1
1	A	53	ASP	1
1	A	30	ILE	1
1	A	100	ARG	1
1	A	121	ASN	1
1	A	122	GLU	1
1	A	54	ILE	1
1	A	55	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	69	GLN	1
1	A	37	ILE	1
1	A	113	ILE	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 70% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

Total number of shifts	1209
Number of shifts mapped to atoms	1209
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	114	2.51 ± 0.10	Should be applied
$^{13}\text{C}_\beta$	107	2.73 ± 0.13	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	114	0.62 ± 0.38	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 70%, i.e. 1202 atoms were assigned a chemical shift out of a possible 1712. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	452/596 (76%)	226/241 (94%)	113/240 (47%)	113/115 (98%)
Sidechain	750/1038 (72%)	508/676 (75%)	242/330 (73%)	0/32 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/78 (0%)	0/39 (0%)	0/37 (0%)	0/2 (0%)
Overall	1202/1712 (70%)	734/956 (77%)	355/607 (58%)	113/149 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1209 atoms were assigned a chemical shift out of a possible 1735. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	456/606 (75%)	228/245 (93%)	114/244 (47%)	114/117 (97%)
Sidechain	753/1051 (72%)	510/685 (74%)	243/334 (73%)	0/32 (0%)
Aromatic	0/78 (0%)	0/39 (0%)	0/37 (0%)	0/2 (0%)
Overall	1209/1735 (70%)	738/969 (76%)	357/615 (58%)	114/151 (75%)

7.1.4 Statistically unusual chemical shifts [i](#)

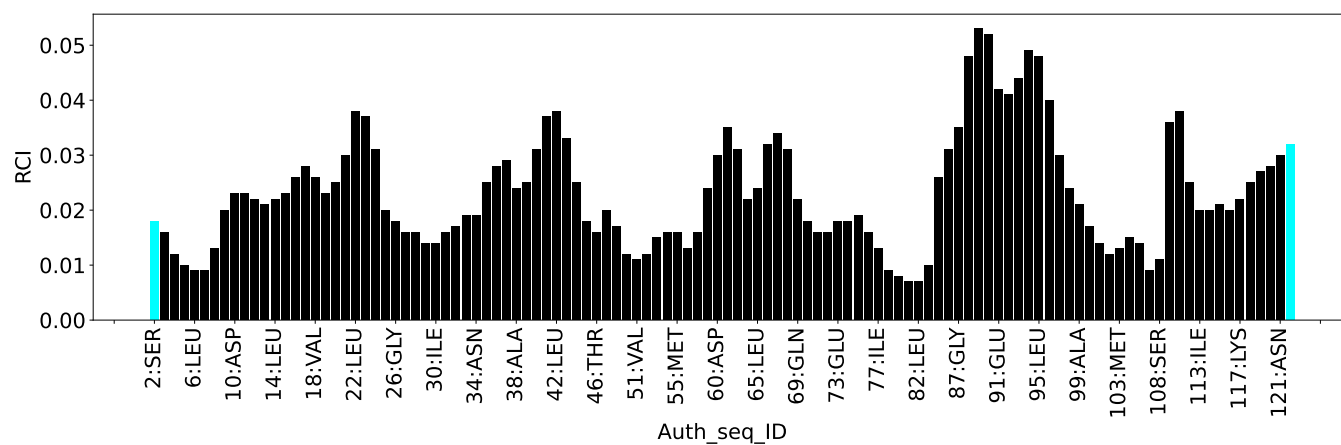
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	71	LYS	HD3	0.11	0.54 – 2.65	-7.1
1	A	71	LYS	HD2	0.26	0.58 – 2.64	-6.5

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:



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	427
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	164
Medium range ($ i-j >1$ and $ i-j <5$)	39
Long range ($ i-j \geq 5$)	106
Inter-chain	0
Hydrogen bond restraints	118
Disulfide bond restraints	0
Total dihedral-angle restraints	214
Number of unmapped restraints	0
Number of restraints per residue	5.2
Number of long range restraints per residue ¹	1.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	44.1	0.2
0.2-0.5 (Medium)	49.5	0.5
>0.5 (Large)	40.2	3.89

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)	24.1	9.91
10.0-20.0 (Medium)	8.5	20.0
>20.0 (Large)	16.4	160.12

9 Distance violation analysis ⓘ

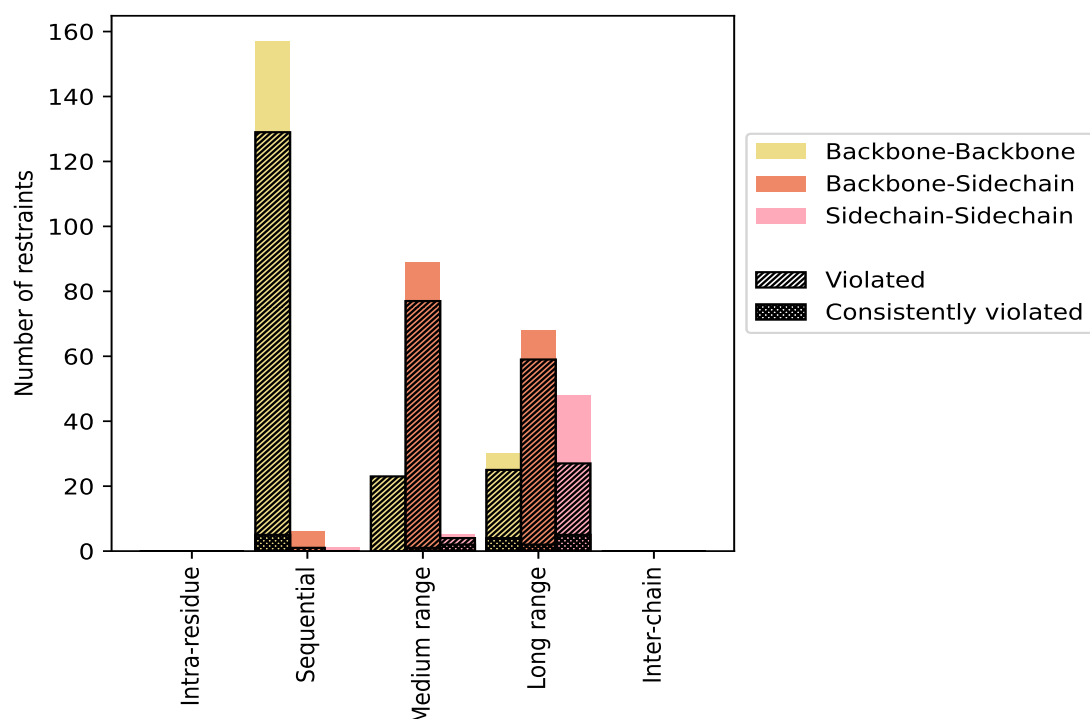
9.1 Summary of distance violations ⓘ

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$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	164	38.4	130	79.3	30.4	5	3.0	1.2
Backbone-Backbone	157	36.8	129	82.2	30.2	5	3.2	1.2
Backbone-Sidechain	6	1.4	1	16.7	0.2	0	0.0	0.0
Sidechain-Sidechain	1	0.2	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	39	9.1	33	84.6	7.7	3	7.7	0.7
Backbone-Backbone	23	5.4	23	100.0	5.4	0	0.0	0.0
Backbone-Sidechain	11	2.6	6	54.5	1.4	1	9.1	0.2
Sidechain-Sidechain	5	1.2	4	80.0	0.9	2	40.0	0.5
Long range ($ i-j \geq 5$)	106	24.8	74	69.8	17.3	11	10.4	2.6
Backbone-Backbone	30	7.0	25	83.3	5.9	4	13.3	0.9
Backbone-Sidechain	28	6.6	22	78.6	5.2	2	7.1	0.5
Sidechain-Sidechain	48	11.2	27	56.2	6.3	5	10.4	1.2
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	118	27.6	108	91.5	25.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	427	100.0	345	80.8	80.8	19	4.4	4.4
Backbone-Backbone	210	49.2	177	84.3	41.5	9	4.3	2.1
Backbone-Sidechain	163	38.2	137	84.0	32.1	3	1.8	0.7
Sidechain-Sidechain	54	12.6	31	57.4	7.3	7	13.0	1.6

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	48	45	43	0	136	0.49	3.3	0.52	0.28
2	0	43	49	43	0	135	0.53	3.24	0.55	0.33
3	0	33	34	54	0	121	0.54	3.35	0.61	0.27
4	0	46	35	41	0	122	0.52	3.52	0.56	0.32
5	0	53	44	49	0	146	0.46	3.89	0.61	0.23
6	0	41	49	43	0	133	0.49	3.42	0.53	0.26
7	0	49	50	61	0	160	0.53	3.64	0.61	0.32
8	0	44	42	49	0	135	0.49	3.59	0.58	0.26
9	0	43	49	49	0	141	0.48	2.81	0.5	0.29
10	0	40	40	53	0	133	0.59	3.54	0.62	0.35

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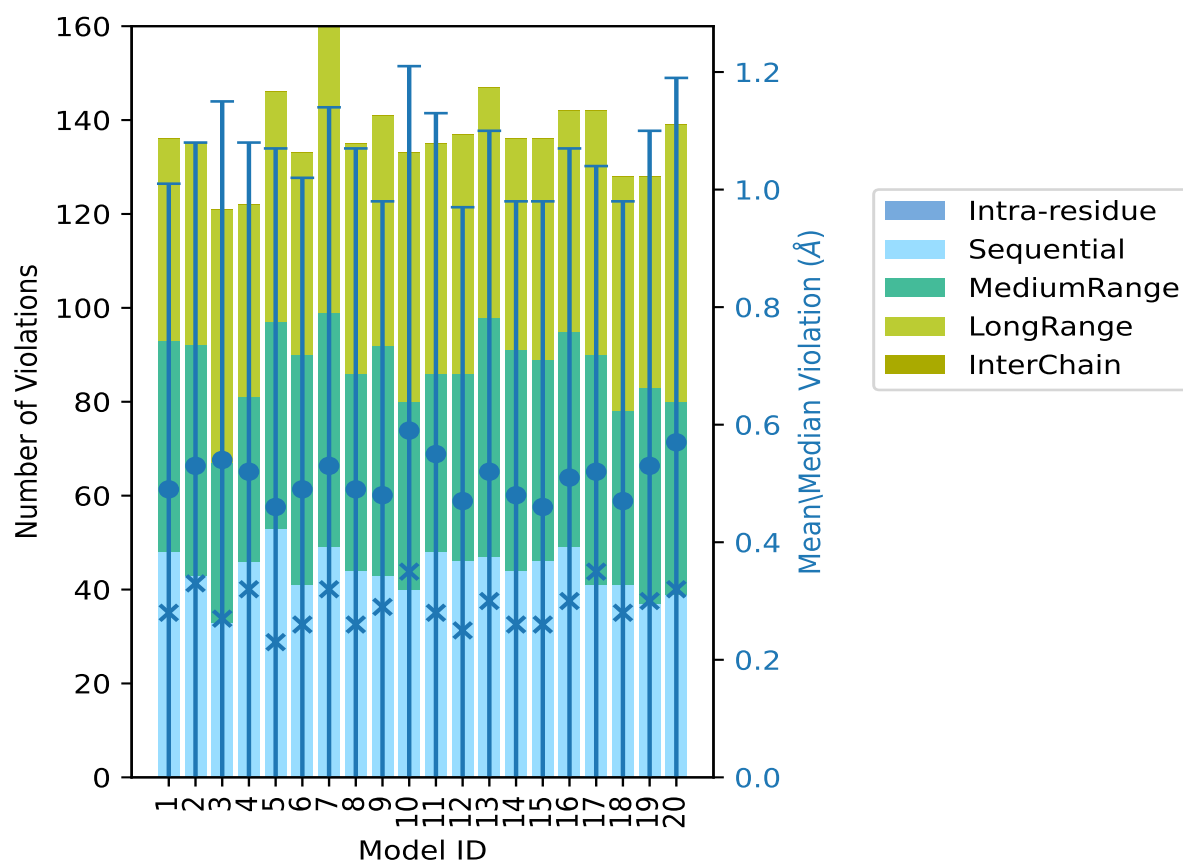
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	48	38	49	0	135	0.55	3.45	0.58	0.28
12	0	46	40	51	0	137	0.47	2.6	0.5	0.25
13	0	47	51	49	0	147	0.52	3.34	0.58	0.3
14	0	44	47	45	0	136	0.48	3.3	0.5	0.26
15	0	46	43	47	0	136	0.46	3.83	0.52	0.26
16	0	49	46	47	0	142	0.51	3.83	0.56	0.3
17	0	41	49	52	0	142	0.52	3.52	0.52	0.35
18	0	41	37	50	0	128	0.47	3.07	0.51	0.28
19	0	37	46	45	0	128	0.53	3.53	0.57	0.3
20	0	39	41	59	0	139	0.57	3.08	0.62	0.32

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

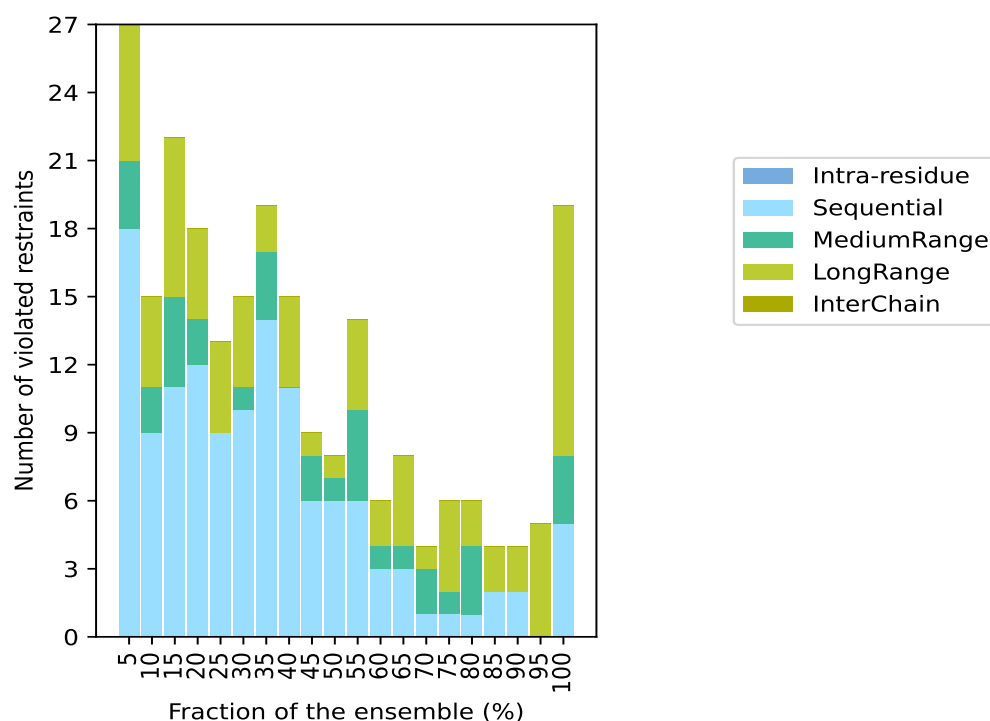
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 72(IR:0, SQ:34, MR:6, LR:32, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	18	3	6	0	27	1	5.0
0	9	2	4	0	15	2	10.0
0	11	4	7	0	22	3	15.0
0	12	2	4	0	18	4	20.0
0	9	0	4	0	13	5	25.0
0	10	1	4	0	15	6	30.0
0	14	3	2	0	19	7	35.0
0	11	0	4	0	15	8	40.0
0	6	2	1	0	9	9	45.0
0	6	1	1	0	8	10	50.0
0	6	4	4	0	14	11	55.0
0	3	1	2	0	6	12	60.0
0	3	1	4	0	8	13	65.0
0	1	2	1	0	4	14	70.0
0	1	1	4	0	6	15	75.0
0	1	3	2	0	6	16	80.0
0	2	0	2	0	4	17	85.0
0	2	0	2	0	4	18	90.0
0	0	0	5	0	5	19	95.0
0	5	3	11	0	19	20	100.0

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

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

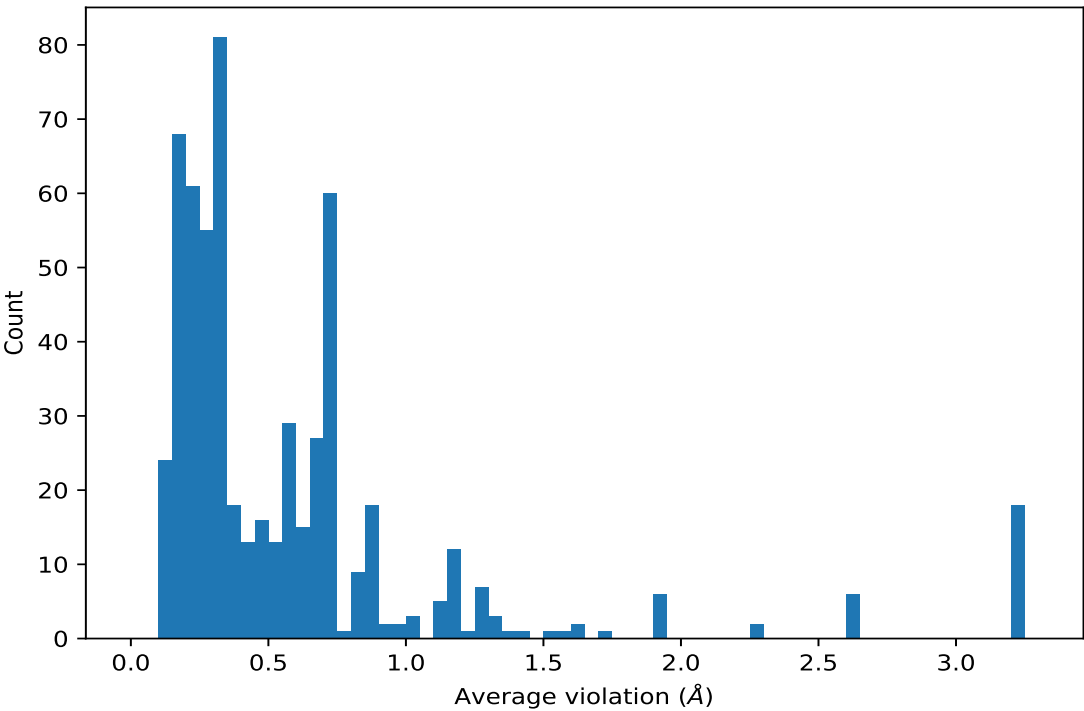
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



9.4.2 Table: Most violated distance restraints ⓘ

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)
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	20	3.24	0.58	3.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	20	3.24	0.58	3.44
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	20	3.24	0.58	3.44
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	20	2.61	0.43	2.64
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	20	2.61	0.43	2.64
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	20	2.61	0.43	2.64
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	20	2.61	0.43	2.64
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	20	2.61	0.43	2.64
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	20	2.61	0.43	2.64
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	20	2.27	0.54	2.38
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	20	2.27	0.54	2.38
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	20	1.9	0.46	1.76
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	20	1.9	0.46	1.76
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	20	1.9	0.46	1.76
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	20	1.9	0.46	1.76
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	20	1.9	0.46	1.76
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	20	1.9	0.46	1.76
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	20	1.72	0.31	1.78
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	20	1.52	0.16	1.55
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	20	1.26	0.1	1.28
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	20	1.23	0.21	1.23
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	20	0.95	0.43	0.98
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	20	0.95	0.43	0.98
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	20	0.84	0.15	0.82
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	20	0.84	0.15	0.82
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	20	0.75	0.19	0.71
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	20	0.73	0.19	0.69

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	20	0.73	0.19	0.69
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	20	0.73	0.19	0.69
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	20	0.72	0.23	0.68
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	20	0.72	0.23	0.68
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	20	0.72	0.23	0.68
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	20	0.72	0.23	0.68
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	20	0.72	0.23	0.68
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	20	0.72	0.23	0.68
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	20	0.71	0.35	0.71
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	20	0.56	0.19	0.6
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	20	0.56	0.19	0.6
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	20	0.56	0.19	0.6
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	20	0.56	0.19	0.6
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	20	0.56	0.19	0.6
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	20	0.56	0.19	0.6
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	20	0.51	0.27	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	20	0.48	0.18	0.51
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	20	0.48	0.18	0.51
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	20	0.48	0.18	0.51
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	20	0.48	0.18	0.51
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	20	0.48	0.18	0.51
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	20	0.48	0.18	0.51
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	20	0.48	0.21	0.43
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	20	0.46	0.19	0.43
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	19	1.56	0.7	1.57
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	19	1.44	0.53	1.32
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	19	1.35	0.54	1.25
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	19	0.71	0.49	0.56
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	19	0.71	0.49	0.56
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	19	0.71	0.49	0.56
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	19	0.64	0.09	0.61

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	19	0.64	0.09	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	19	0.64	0.09	0.61
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	19	0.53	0.32	0.48
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	19	0.49	0.18	0.45
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	19	0.34	0.23	0.26
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	18	1.62	0.58	1.92
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	18	1.62	0.58	1.92
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	18	1.16	0.44	1.1
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	18	1.16	0.44	1.1
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	18	0.3	0.12	0.3
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	18	0.27	0.11	0.26
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	18	0.27	0.11	0.26
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	18	0.27	0.11	0.26
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	17	1.12	0.49	1.06
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	17	0.51	0.28	0.49
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	17	0.48	0.22	0.53
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	17	0.4	0.19	0.44
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	17	0.2	0.06	0.19
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	17	0.2	0.06	0.19
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	16	1.18	0.42	1.25
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	16	1.18	0.42	1.25
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	16	1.18	0.42	1.25
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	16	0.9	0.52	0.84
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	16	0.9	0.52	0.84
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	16	0.53	0.2	0.5
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	16	0.46	0.3	0.38
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	16	0.39	0.15	0.36
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	16	0.32	0.16	0.29
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	16	0.3	0.11	0.28
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	16	0.29	0.13	0.26
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	16	0.29	0.14	0.26

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	16	0.26	0.13	0.23
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	15	1.13	0.12	1.11
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	15	0.71	0.31	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	15	0.71	0.31	0.65
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	15	0.56	0.41	0.43
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	15	0.56	0.41	0.43
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	15	0.56	0.41	0.43
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	15	0.54	0.22	0.59
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	15	0.43	0.34	0.26
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	15	0.4	0.16	0.36
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	15	0.36	0.12	0.32
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	15	0.22	0.09	0.17
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	14	0.61	0.33	0.63
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	14	0.54	0.34	0.4
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	14	0.48	0.29	0.36
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	14	0.42	0.24	0.36
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	14	0.4	0.13	0.38
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	14	0.33	0.2	0.3
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	14	0.28	0.12	0.26
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	14	0.26	0.09	0.26
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	14	0.24	0.06	0.22
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	13	1.27	0.6	1.15
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	13	1.27	0.6	1.15
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	13	1.27	0.6	1.15
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	13	1.27	0.6	1.15
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	13	1.27	0.6	1.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	13	1.27	0.6	1.15
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	13	1.0	0.37	1.08
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	13	1.0	0.37	1.08
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	13	1.0	0.37	1.08
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	13	0.85	0.47	0.73
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	13	0.85	0.47	0.73
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	13	0.85	0.47	0.73
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	13	0.73	0.48	0.75
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	13	0.73	0.48	0.75
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	13	0.73	0.48	0.75
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	13	0.51	0.28	0.45
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	13	0.33	0.18	0.27
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	13	0.33	0.17	0.3
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	13	0.27	0.11	0.27
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	13	0.26	0.05	0.26
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	13	0.21	0.06	0.2
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	13	0.15	0.05	0.13
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	12	0.53	0.26	0.54
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	12	0.51	0.2	0.48
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	12	0.48	0.45	0.2
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	12	0.31	0.16	0.32
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	12	0.29	0.19	0.22
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	12	0.27	0.13	0.24
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	12	0.26	0.12	0.24
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	12	0.26	0.12	0.25
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	12	0.24	0.14	0.18
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	12	0.24	0.08	0.23
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	12	0.22	0.1	0.2
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	12	0.18	0.05	0.18
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	11	1.31	0.46	1.31
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	11	1.31	0.46	1.31
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	11	0.87	0.45	0.88
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	11	0.87	0.45	0.88
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	11	0.87	0.45	0.88
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	11	0.68	0.44	0.72
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	11	0.68	0.44	0.72
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	11	0.68	0.44	0.72
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	11	0.62	0.61	0.31
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	11	0.42	0.27	0.47
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	11	0.42	0.27	0.47
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	11	0.42	0.27	0.47
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	11	0.42	0.27	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	11	0.42	0.27	0.47
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	11	0.42	0.27	0.47
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	11	0.38	0.24	0.38
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	11	0.35	0.22	0.32
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	11	0.31	0.17	0.26
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	11	0.29	0.11	0.24
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	11	0.28	0.18	0.24
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	11	0.27	0.11	0.25
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	11	0.27	0.12	0.27
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	11	0.26	0.12	0.24
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	11	0.26	0.12	0.23
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	11	0.22	0.11	0.2
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	11	0.21	0.08	0.2
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	11	0.21	0.09	0.16
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	11	0.21	0.08	0.2
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	11	0.18	0.07	0.16
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	10	0.57	0.28	0.51
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	10	0.57	0.28	0.51
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	10	0.5	0.6	0.3
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	10	0.29	0.14	0.26
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	10	0.28	0.1	0.26
(2,93)	1:92:A:SER:O	1:96:A:SER:H	10	0.27	0.11	0.31
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	10	0.23	0.1	0.26
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	10	0.22	0.07	0.21
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	10	0.21	0.09	0.2
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	10	0.2	0.08	0.16
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	10	0.19	0.05	0.19
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	10	0.17	0.07	0.16
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	10	0.17	0.06	0.16
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	10	0.16	0.05	0.15
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	9	0.39	0.23	0.28
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	9	0.39	0.23	0.28
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	9	0.33	0.18	0.33
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	9	0.29	0.16	0.26
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	9	0.27	0.09	0.27
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	9	0.26	0.13	0.25
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	9	0.26	0.1	0.27
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	9	0.23	0.11	0.23
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	9	0.22	0.09	0.21
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	9	0.21	0.07	0.19
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	9	0.16	0.06	0.13
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	9	0.15	0.04	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	9	0.15	0.04	0.16
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	9	0.14	0.05	0.12
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	8	0.86	0.31	0.96
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	8	0.86	0.31	0.96
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	8	0.86	0.31	0.96
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	8	0.86	0.31	0.96
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	8	0.86	0.31	0.96
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	8	0.86	0.31	0.96
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	8	0.61	0.58	0.48
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	8	0.59	0.32	0.58
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	8	0.59	0.32	0.58
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	8	0.36	0.19	0.3
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	8	0.32	0.18	0.32
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	8	0.3	0.12	0.32
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	8	0.3	0.12	0.32
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	8	0.3	0.12	0.32
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	8	0.27	0.16	0.24
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	8	0.26	0.06	0.26
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	8	0.23	0.12	0.18
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	8	0.19	0.06	0.19
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	8	0.19	0.08	0.16
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	8	0.18	0.05	0.18
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	8	0.18	0.07	0.16
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	8	0.18	0.06	0.16
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	8	0.18	0.08	0.15
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	8	0.17	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	8	0.16	0.05	0.15
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	8	0.16	0.03	0.16
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	8	0.15	0.03	0.15
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	8	0.14	0.03	0.14
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	8	0.13	0.04	0.12
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	7	0.65	0.37	0.57
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	7	0.65	0.37	0.57
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	7	0.39	0.26	0.41
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	7	0.35	0.18	0.26
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	7	0.32	0.2	0.21
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	7	0.3	0.12	0.31
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	7	0.29	0.13	0.28
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	7	0.27	0.16	0.2
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	7	0.27	0.12	0.25
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	7	0.27	0.12	0.25
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	7	0.27	0.12	0.25
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	7	0.27	0.12	0.25
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	7	0.27	0.21	0.15
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	7	0.26	0.13	0.21
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	7	0.26	0.15	0.25
(2,94)	1:92:A:SER:O	1:96:A:SER:N	7	0.25	0.06	0.26
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	7	0.24	0.06	0.23
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	7	0.24	0.12	0.21
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	7	0.23	0.05	0.24
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	7	0.22	0.08	0.2
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	7	0.21	0.07	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	7	0.17	0.05	0.14
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	7	0.17	0.05	0.16
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	7	0.17	0.04	0.16
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	7	0.17	0.05	0.16
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	7	0.16	0.04	0.15
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	7	0.16	0.04	0.13
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	7	0.16	0.05	0.14
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	7	0.14	0.04	0.13
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	7	0.14	0.04	0.12
(2,58)	1:21:A:ASN:O	1:25:A:GLU:N	6	0.54	0.35	0.5
(2,5)	1:5:A:VAL:O	1:30:A:ILE:H	6	0.38	0.17	0.4
(1,70)	1:83:A:THR:H	1:105:A:LYS:H	6	0.37	0.17	0.44
(1,308)	1:95:A:LEU:HD11	1:101:A:LYS:H	6	0.32	0.09	0.32
(1,308)	1:95:A:LEU:HD12	1:101:A:LYS:H	6	0.32	0.09	0.32
(1,308)	1:95:A:LEU:HD13	1:101:A:LYS:H	6	0.32	0.09	0.32
(1,308)	1:95:A:LEU:HD21	1:101:A:LYS:H	6	0.32	0.09	0.32
(1,308)	1:95:A:LEU:HD22	1:101:A:LYS:H	6	0.32	0.09	0.32
(1,308)	1:95:A:LEU:HD23	1:101:A:LYS:H	6	0.32	0.09	0.32
(1,122)	1:52:A:LEU:H	1:81:A:VAL:HA	6	0.26	0.09	0.26
(1,258)	1:114:A:GLU:H	1:115:A:GLU:H	6	0.24	0.09	0.21
(1,208)	1:17:A:ILE:H	1:18:A:VAL:H	6	0.23	0.09	0.22
(1,201)	1:95:A:LEU:HA	1:98:A:GLY:H	6	0.22	0.09	0.2
(2,103)	1:110:A:SER:O	1:114:A:GLU:H	6	0.21	0.05	0.21
(1,268)	1:5:A:VAL:H	1:28:A:GLU:H	6	0.21	0.08	0.2
(2,112)	1:114:A:GLU:O	1:118:A:HIS:N	6	0.21	0.05	0.2
(1,147)	1:37:A:ILE:HA	1:38:A:ALA:H	6	0.19	0.07	0.19
(2,34)	1:81:A:VAL:N	1:101:A:LYS:O	6	0.18	0.03	0.16
(1,136)	1:19:A:SER:HA	1:20:A:PHE:H	6	0.17	0.04	0.16
(1,71)	1:86:A:GLY:HA2	1:87:A:GLY:H	6	0.17	0.06	0.16
(1,71)	1:86:A:GLY:HA3	1:87:A:GLY:H	6	0.17	0.06	0.16
(1,137)	1:20:A:PHE:HA	1:21:A:ASN:H	6	0.16	0.03	0.16
(2,52)	1:18:A:VAL:O	1:22:A:LEU:N	6	0.15	0.03	0.15
(1,154)	1:44:A:GLU:HA	1:45:A:PHE:H	6	0.15	0.04	0.14
(1,244)	1:89:A:GLU:H	1:90:A:ASP:H	6	0.15	0.04	0.13
(1,169)	1:68:A:LEU:HA	1:69:A:GLN:H	6	0.15	0.02	0.15
(1,163)	1:62:A:PHE:HA	1:63:A:THR:H	6	0.12	0.02	0.12
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD11	5	0.86	0.48	0.82
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD12	5	0.86	0.48	0.82
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD13	5	0.86	0.48	0.82
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD11	5	0.86	0.48	0.82
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD12	5	0.86	0.48	0.82
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD13	5	0.86	0.48	0.82

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD11	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD12	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD13	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD11	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD12	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD13	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD11	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD12	5	0.7	0.61	0.36
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD13	5	0.7	0.61	0.36
(2,32)	1:79:A:VAL:O	1:100:A:ARG:N	5	0.39	0.19	0.39
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD11	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD12	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD13	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD21	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD22	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD23	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD11	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD12	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD13	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD21	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD22	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD23	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD11	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD12	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD13	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD21	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD22	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD23	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD11	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD12	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD13	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD21	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD22	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD23	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD11	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD12	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD13	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD21	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD22	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD23	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD11	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD12	5	0.3	0.1	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD13	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD21	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD22	5	0.3	0.1	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD23	5	0.3	0.1	0.28
(1,212)	1:21:A:ASN:H	1:22:A:LEU:H	5	0.3	0.15	0.25
(2,56)	1:20:A:PHE:O	1:24:A:LYS:N	5	0.29	0.2	0.15
(2,81)	1:65:A:LEU:O	1:69:A:GLN:H	5	0.25	0.13	0.24
(2,39)	1:12:A:ALA:O	1:16:A:LYS:H	5	0.23	0.13	0.17
(2,75)	1:62:A:PHE:O	1:66:A:LYS:H	5	0.22	0.12	0.15
(2,104)	1:110:A:SER:O	1:114:A:GLU:N	5	0.22	0.04	0.2
(1,297)	1:51:A:VAL:HG11	1:80:A:ILE:H	5	0.21	0.1	0.19
(1,297)	1:51:A:VAL:HG12	1:80:A:ILE:H	5	0.21	0.1	0.19
(1,297)	1:51:A:VAL:HG13	1:80:A:ILE:H	5	0.21	0.1	0.19
(1,297)	1:51:A:VAL:HG21	1:80:A:ILE:H	5	0.21	0.1	0.19
(1,297)	1:51:A:VAL:HG22	1:80:A:ILE:H	5	0.21	0.1	0.19
(1,297)	1:51:A:VAL:HG23	1:80:A:ILE:H	5	0.21	0.1	0.19
(1,149)	1:39:A:LEU:HA	1:40:A:GLU:H	5	0.19	0.04	0.21
(1,222)	1:40:A:GLU:H	1:41:A:LYS:H	5	0.19	0.03	0.21
(1,207)	1:16:A:LYS:H	1:17:A:ILE:H	5	0.19	0.05	0.18
(2,24)	1:50:A:ILE:N	1:78:A:PRO:O	5	0.19	0.05	0.2
(1,146)	1:36:A:GLN:HA	1:37:A:ILE:H	5	0.18	0.04	0.2
(1,167)	1:66:A:LYS:HA	1:67:A:LYS:H	5	0.17	0.04	0.17
(1,172)	1:73:A:GLU:HA	1:74:A:TRP:H	5	0.15	0.04	0.15
(1,84)	1:11:A:SER:HA	1:12:A:ALA:H	5	0.15	0.02	0.14
(1,140)	1:23:A:LYS:HA	1:24:A:LYS:H	5	0.14	0.03	0.13
(1,34)	1:80:A:ILE:HD11	1:116:A:VAL:HA	4	1.1	0.91	1.14
(1,34)	1:80:A:ILE:HD12	1:116:A:VAL:HA	4	1.1	0.91	1.14
(1,34)	1:80:A:ILE:HD13	1:116:A:VAL:HA	4	1.1	0.91	1.14
(2,6)	1:5:A:VAL:O	1:30:A:ILE:N	4	0.44	0.11	0.42
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG21	4	0.37	0.25	0.26
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG22	4	0.37	0.25	0.26
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG23	4	0.37	0.25	0.26
(2,96)	1:95:A:LEU:O	1:98:A:GLY:N	4	0.34	0.09	0.33
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB2	4	0.3	0.09	0.28
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB3	4	0.3	0.09	0.28
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB2	4	0.3	0.09	0.28
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB3	4	0.3	0.09	0.28
(2,37)	1:83:A:THR:H	1:103:A:MET:O	4	0.28	0.12	0.24
(1,225)	1:43:A:SER:H	1:44:A:GLU:H	4	0.28	0.08	0.24
(1,158)	1:37:A:ILE:HA	1:40:A:GLU:H	4	0.27	0.14	0.25
(1,160)	1:39:A:LEU:HA	1:42:A:LEU:H	4	0.26	0.11	0.25
(1,238)	1:69:A:GLN:H	1:70:A:GLU:H	4	0.24	0.1	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,266)	1:6:A:LEU:H	1:51:A:VAL:H	4	0.22	0.05	0.21
(2,76)	1:62:A:PHE:O	1:66:A:LYS:N	4	0.21	0.12	0.16
(2,27)	1:52:A:LEU:H	1:80:A:ILE:O	4	0.2	0.13	0.13
(1,221)	1:39:A:LEU:H	1:40:A:GLU:H	4	0.2	0.07	0.19
(2,25)	1:50:A:ILE:O	1:80:A:ILE:H	4	0.2	0.09	0.2
(2,43)	1:14:A:LEU:O	1:18:A:VAL:H	4	0.19	0.07	0.18
(2,53)	1:19:A:SER:O	1:23:A:LYS:H	4	0.18	0.05	0.19
(1,243)	1:88:A:GLU:H	1:89:A:GLU:H	4	0.18	0.05	0.15
(2,78)	1:63:A:THR:O	1:67:A:LYS:N	4	0.17	0.02	0.18
(1,257)	1:113:A:ILE:H	1:114:A:GLU:H	4	0.16	0.02	0.16
(2,13)	1:7:A:LEU:O	1:32:A:ALA:H	4	0.16	0.05	0.14
(1,135)	1:18:A:VAL:HA	1:19:A:SER:H	4	0.15	0.05	0.14
(2,7)	1:6:A:LEU:H	1:49:A:LEU:O	4	0.14	0.05	0.12
(1,100)	1:58:A:VAL:HA	1:59:A:MET:H	4	0.14	0.02	0.14
(1,131)	1:14:A:LEU:HA	1:15:A:ARG:H	4	0.14	0.02	0.14
(1,214)	1:23:A:LYS:H	1:24:A:LYS:H	4	0.14	0.02	0.15
(1,193)	1:100:A:ARG:HA	1:101:A:LYS:H	4	0.14	0.01	0.14
(1,174)	1:76:A:ARG:HA	1:77:A:ILE:H	4	0.13	0.01	0.13
(2,21)	1:4:A:LYS:O	1:48:A:ASP:H	4	0.13	0.02	0.12
(1,181)	1:88:A:GLU:HA	1:89:A:GLU:H	4	0.12	0.02	0.12
(1,6)	1:6:A:LEU:H	1:30:A:ILE:HB	3	1.34	1.26	0.8
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG2	3	0.69	0.24	0.83
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG2	3	0.69	0.24	0.83
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG2	3	0.69	0.24	0.83
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG3	3	0.69	0.24	0.83
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG3	3	0.69	0.24	0.83
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG3	3	0.69	0.24	0.83
(1,23)	1:42:A:LEU:HB2	1:47:A:PRO:HD3	3	0.51	0.29	0.66
(1,23)	1:42:A:LEU:HB3	1:47:A:PRO:HD3	3	0.51	0.29	0.66
(1,19)	1:42:A:LEU:HB2	1:47:A:PRO:HD2	3	0.48	0.31	0.28
(1,19)	1:42:A:LEU:HB3	1:47:A:PRO:HD2	3	0.48	0.31	0.28
(2,11)	1:7:A:LEU:H	1:30:A:ILE:O	3	0.41	0.37	0.19
(1,59)	1:71:A:LYS:HG2	1:73:A:GLU:H	3	0.37	0.11	0.43
(1,59)	1:71:A:LYS:HG3	1:73:A:GLU:H	3	0.37	0.11	0.43
(1,294)	1:49:A:LEU:HD11	1:80:A:ILE:H	3	0.32	0.11	0.36
(1,294)	1:49:A:LEU:HD12	1:80:A:ILE:H	3	0.32	0.11	0.36
(1,294)	1:49:A:LEU:HD13	1:80:A:ILE:H	3	0.32	0.11	0.36
(1,294)	1:49:A:LEU:HD21	1:80:A:ILE:H	3	0.32	0.11	0.36
(1,294)	1:49:A:LEU:HD22	1:80:A:ILE:H	3	0.32	0.11	0.36
(1,294)	1:49:A:LEU:HD23	1:80:A:ILE:H	3	0.32	0.11	0.36
(2,67)	1:38:A:ALA:O	1:42:A:LEU:H	3	0.3	0.15	0.24
(2,29)	1:52:A:LEU:O	1:82:A:LEU:H	3	0.27	0.12	0.31

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,61)	1:71:A:LYS:HG2	1:74:A:TRP:H	3	0.27	0.16	0.19
(1,61)	1:71:A:LYS:HG3	1:74:A:TRP:H	3	0.27	0.16	0.19
(2,9)	1:6:A:LEU:O	1:51:A:VAL:H	3	0.26	0.07	0.26
(2,12)	1:7:A:LEU:N	1:30:A:ILE:O	3	0.25	0.17	0.13
(2,40)	1:12:A:ALA:O	1:16:A:LYS:N	3	0.25	0.15	0.17
(1,274)	1:52:A:LEU:H	1:80:A:ILE:H	3	0.23	0.1	0.19
(1,162)	1:41:A:LYS:HA	1:44:A:GLU:H	3	0.23	0.09	0.18
(2,10)	1:6:A:LEU:O	1:51:A:VAL:N	3	0.21	0.1	0.16
(1,252)	1:97:A:LEU:H	1:98:A:GLY:H	3	0.21	0.07	0.21
(2,65)	1:37:A:ILE:O	1:41:A:LYS:H	3	0.21	0.11	0.15
(1,107)	1:83:A:THR:HA	1:84:A:ALA:H	3	0.21	0.06	0.19
(2,28)	1:52:A:LEU:N	1:80:A:ILE:O	3	0.2	0.12	0.13
(2,44)	1:14:A:LEU:O	1:18:A:VAL:N	3	0.2	0.07	0.24
(2,26)	1:50:A:ILE:O	1:80:A:ILE:N	3	0.2	0.07	0.22
(1,223)	1:41:A:LYS:H	1:42:A:LEU:H	3	0.2	0.05	0.23
(1,170)	1:69:A:GLN:HA	1:70:A:GLU:H	3	0.19	0.11	0.13
(1,209)	1:18:A:VAL:H	1:19:A:SER:H	3	0.19	0.07	0.19
(2,3)	1:5:A:VAL:H	1:28:A:GLU:O	3	0.19	0.07	0.18
(1,173)	1:75:A:LYS:HA	1:76:A:ARG:H	3	0.17	0.05	0.14
(1,179)	1:67:A:LYS:HA	1:70:A:GLU:H	3	0.17	0.03	0.18
(2,107)	1:112:A:PHE:O	1:116:A:VAL:H	3	0.17	0.06	0.14
(1,256)	1:112:A:PHE:H	1:113:A:ILE:H	3	0.16	0.05	0.16
(1,213)	1:22:A:LEU:H	1:23:A:LYS:H	3	0.15	0.03	0.13
(2,8)	1:6:A:LEU:N	1:49:A:LEU:O	3	0.14	0.04	0.13
(2,54)	1:19:A:SER:O	1:23:A:LYS:N	3	0.14	0.02	0.15
(1,263)	1:119:A:LEU:H	1:120:A:LEU:H	3	0.14	0.02	0.14
(1,276)	1:81:A:VAL:H	1:103:A:MET:H	3	0.13	0.01	0.13
(1,86)	1:28:A:GLU:HA	1:29:A:VAL:H	3	0.12	0.01	0.12
(1,88)	1:30:A:ILE:HA	1:31:A:GLU:H	3	0.12	0.0	0.12
(2,108)	1:112:A:PHE:O	1:116:A:VAL:N	3	0.12	0.02	0.12
(1,62)	1:71:A:LYS:HD2	1:74:A:TRP:H	2	0.7	0.04	0.7
(1,62)	1:71:A:LYS:HD3	1:74:A:TRP:H	2	0.7	0.04	0.7
(2,47)	1:16:A:LYS:O	1:20:A:PHE:H	2	0.45	0.05	0.45
(1,269)	1:5:A:VAL:H	1:30:A:ILE:H	2	0.35	0.11	0.35
(2,48)	1:16:A:LYS:O	1:20:A:PHE:N	2	0.33	0.08	0.33
(1,277)	1:83:A:THR:H	1:103:A:MET:H	2	0.32	0.04	0.32
(2,85)	1:88:A:GLU:O	1:92:A:SER:H	2	0.32	0.05	0.32
(2,86)	1:88:A:GLU:O	1:92:A:SER:N	2	0.3	0.05	0.3
(1,285)	1:22:A:LEU:HD11	1:116:A:VAL:HB	2	0.3	0.13	0.3
(1,285)	1:22:A:LEU:HD12	1:116:A:VAL:HB	2	0.3	0.13	0.3
(1,285)	1:22:A:LEU:HD13	1:116:A:VAL:HB	2	0.3	0.13	0.3
(1,285)	1:22:A:LEU:HD21	1:116:A:VAL:HB	2	0.3	0.13	0.3

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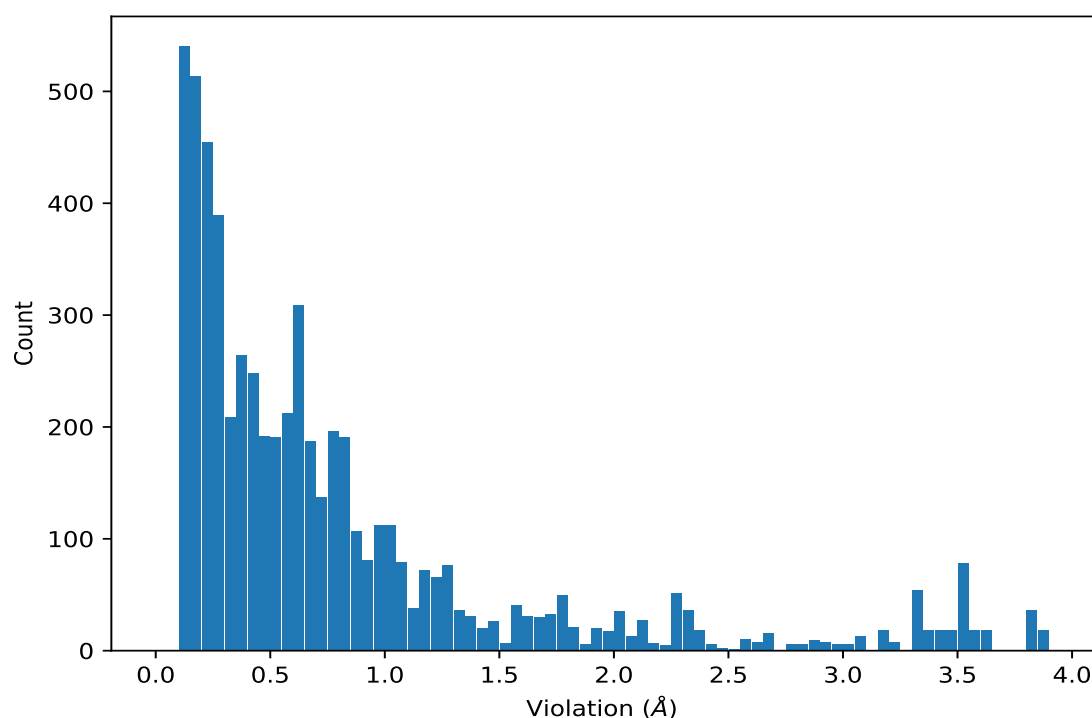
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,285)	1:22:A:LEU:HD22	1:116:A:VAL:HB	2	0.3	0.13	0.3
(1,285)	1:22:A:LEU:HD23	1:116:A:VAL:HB	2	0.3	0.13	0.3
(1,203)	1:12:A:ALA:H	1:13:A:VAL:H	2	0.26	0.04	0.26
(2,30)	1:52:A:LEU:O	1:82:A:LEU:N	2	0.26	0.08	0.26
(2,82)	1:65:A:LEU:O	1:69:A:GLN:N	2	0.26	0.04	0.26
(2,79)	1:64:A:VAL:O	1:68:A:LEU:H	2	0.24	0.05	0.24
(2,66)	1:37:A:ILE:O	1:41:A:LYS:N	2	0.21	0.07	0.21
(1,264)	1:120:A:LEU:H	1:121:A:ASN:H	2	0.2	0.06	0.2
(1,272)	1:9:A:ASP:H	1:32:A:ALA:H	2	0.2	0.0	0.2
(1,215)	1:33:A:GLU:H	1:34:A:ASN:H	2	0.2	0.01	0.2
(1,151)	1:41:A:LYS:HA	1:42:A:LEU:H	2	0.19	0.0	0.19
(2,80)	1:64:A:VAL:O	1:68:A:LEU:N	2	0.19	0.06	0.19
(1,93)	1:50:A:ILE:HA	1:51:A:VAL:H	2	0.18	0.04	0.18
(1,175)	1:63:A:THR:HA	1:66:A:LYS:H	2	0.18	0.04	0.18
(1,142)	1:25:A:GLU:HA	1:26:A:GLY:H	2	0.17	0.03	0.17
(1,92)	1:49:A:LEU:HA	1:50:A:ILE:H	2	0.16	0.04	0.16
(2,38)	1:83:A:THR:N	1:103:A:MET:O	2	0.16	0.05	0.16
(1,251)	1:96:A:SER:H	1:97:A:LEU:H	2	0.16	0.05	0.16
(1,218)	1:36:A:GLN:H	1:37:A:ILE:H	2	0.14	0.04	0.14
(2,4)	1:5:A:VAL:N	1:28:A:GLU:O	2	0.14	0.02	0.14

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)
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	5	3.89
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	5	3.89
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	5	3.89
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	5	3.89
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	5	3.89
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	5	3.89
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	5	3.89
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	5	3.89
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	5	3.89
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	5	3.89
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	5	3.89
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	5	3.89
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	5	3.89
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	5	3.89
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	5	3.89
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	5	3.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	5	3.89
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	5	3.89
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	15	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	15	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	15	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	15	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	15	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	15	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	15	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	15	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	15	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	15	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	15	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	15	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	15	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	15	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	15	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	15	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	15	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	15	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	16	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	16	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	16	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	16	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	16	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	16	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	16	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	16	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	16	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	16	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	16	3.83
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	16	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	16	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	16	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	16	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	16	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	16	3.83
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	16	3.83
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	7	3.64
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	7	3.64
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	7	3.64
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	7	3.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	7	3.64
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	7	3.64
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	7	3.64
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	7	3.64
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	7	3.64
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	7	3.64
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	7	3.64
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	7	3.64
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	7	3.64
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	7	3.64
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	7	3.64
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	7	3.64
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	7	3.64
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	7	3.64
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	8	3.59
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	8	3.59
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	8	3.59
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	8	3.59
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	8	3.59
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	8	3.59
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	8	3.59
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	8	3.59
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	8	3.59
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	8	3.59
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	8	3.59
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	8	3.59
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	8	3.59
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	8	3.59
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	8	3.59
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	8	3.59
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	8	3.59
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	8	3.59
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	10	3.54
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	10	3.54
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	10	3.54
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	10	3.54
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	10	3.54
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	10	3.54
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	10	3.54
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	10	3.54
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	10	3.54
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	10	3.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	10	3.54
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	10	3.54
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	10	3.54
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	10	3.54
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	10	3.54
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	10	3.54
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	10	3.54
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	10	3.54
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	19	3.53
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	19	3.53
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	19	3.53
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	19	3.53
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	19	3.53
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	19	3.53
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	19	3.53
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	19	3.53
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	19	3.53
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	19	3.53
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	19	3.53
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	19	3.53
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	19	3.53
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	19	3.53
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	19	3.53
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	19	3.53
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	19	3.53
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	19	3.53
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	4	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	4	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	4	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	4	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	4	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	4	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	4	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	4	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	4	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	4	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	4	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	4	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	4	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	4	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	4	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	4	3.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	4	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	4	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	17	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	17	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	17	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	17	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	17	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	17	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	17	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	17	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	17	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	17	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	17	3.52
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	17	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	17	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	17	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	17	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	17	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	17	3.52
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	17	3.52
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	5	3.52
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	5	3.52
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	5	3.52
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	5	3.52
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	5	3.52
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	5	3.52
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	11	3.45
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	11	3.45
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	11	3.45
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	11	3.45
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	11	3.45
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	11	3.45
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	11	3.45
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	11	3.45
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	11	3.45
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	11	3.45
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	11	3.45
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	11	3.45
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	11	3.45
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	11	3.45
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	11	3.45
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	11	3.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	11	3.45
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	11	3.45
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	6	3.42
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	6	3.42
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	6	3.42
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	6	3.42
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	6	3.42
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	6	3.42
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	6	3.42
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	6	3.42
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	6	3.42
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	6	3.42
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	6	3.42
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	6	3.42
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	6	3.42
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	6	3.42
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	6	3.42
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	6	3.42
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	6	3.42
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	6	3.42
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	3	3.35
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	3	3.35
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	3	3.35
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	3	3.35
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	3	3.35
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	3	3.35
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	3	3.35
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	3	3.35
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	3	3.35
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	3	3.35
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	3	3.35
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	3	3.35
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	3	3.35
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	3	3.35
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	3	3.35
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	3	3.35
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	3	3.35
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	3	3.35
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	13	3.34
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	13	3.34
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	13	3.34
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	13	3.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	13	3.34
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	13	3.34
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	13	3.34
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	13	3.34
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	13	3.34
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	13	3.34
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	13	3.34
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	13	3.34
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	13	3.34
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	13	3.34
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	13	3.34
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	13	3.34
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	13	3.34
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	13	3.34
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	1	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	1	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	1	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	1	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	1	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	1	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	1	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	1	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	1	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	1	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	1	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	1	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	1	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	1	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	1	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	1	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	1	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	1	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	14	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	14	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	14	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	14	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	14	3.3
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	14	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	14	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	14	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	14	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	14	3.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	14	3.3
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	14	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	14	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	14	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	14	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	14	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	14	3.3
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	14	3.3
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	2	3.24
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	2	3.24
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	2	3.24
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	2	3.24
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	2	3.24
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	2	3.24
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	13	3.21
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	13	3.21
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	2	3.16
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	2	3.16
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	2	3.16
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	2	3.16
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	2	3.16
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	2	3.16
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	2	3.16
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	2	3.16
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	2	3.16
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	2	3.16
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	2	3.16
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	2	3.16
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	2	3.16
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	2	3.16
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	2	3.16
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	2	3.16
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	2	3.16
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	2	3.16
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	20	3.08
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	20	3.08
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	20	3.08
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	20	3.08
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	20	3.08
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	20	3.08
(1,6)	1:6:A:LEU:H	1:30:A:ILE:HB	17	3.08
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	18	3.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	18	3.07
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	18	3.07
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	18	3.07
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	18	3.07
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	18	3.07
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	5	3.04
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	5	3.04
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	5	3.04
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	5	3.04
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	5	3.04
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	5	3.04
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	7	2.95
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	7	2.95
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	7	2.95
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	7	2.95
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	7	2.95
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	7	2.95
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	3	2.93
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	3	2.93
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	3	2.93
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	3	2.93
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	3	2.93
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	3	2.93
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	20	2.92
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	20	2.92
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	7	2.89
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	7	2.89
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	7	2.89
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	7	2.89
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	7	2.89
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	7	2.89
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	20	2.87
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	4	2.85
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	4	2.85
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	9	2.81
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	9	2.81
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	9	2.81
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	9	2.81
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	9	2.81
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	9	2.81
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	11	2.75
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	11	2.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	11	2.75
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	11	2.75
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	11	2.75
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	11	2.75
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	1	2.68
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	1	2.68
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	1	2.68
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	1	2.68
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	1	2.68
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	1	2.68
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	7	2.67
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	16	2.67
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	16	2.67
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	16	2.67
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	16	2.67
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	16	2.67
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	16	2.67
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	7	2.66
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	10	2.65
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	10	2.65
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	5	2.64
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	5	2.64
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	12	2.6
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	12	2.6
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	12	2.6
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	12	2.6
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	12	2.6
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	12	2.6
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	7	2.58
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	7	2.58
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	13	2.56
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	13	2.56
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	13	2.56
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	13	2.56
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	13	2.56
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	13	2.56
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	8	2.55
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	8	2.55
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	10	2.53
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	3	2.47
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	3	2.47
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	19	2.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	19	2.44
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	19	2.44
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	19	2.44
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	19	2.44
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	19	2.44
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	16	2.38
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	16	2.38
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	19	2.38
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	19	2.38
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	19	2.38
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	19	2.38
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	19	2.38
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	19	2.38
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	19	2.38
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	19	2.38
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	18	2.37
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	18	2.37
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	1	2.37
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	1	2.37
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	1	2.37
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	1	2.37
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	1	2.37
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	1	2.37
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	12	2.34
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	12	2.34
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	9	2.32
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	9	2.32
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	9	2.32
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	9	2.32
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	9	2.32
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	9	2.32
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	9	2.32
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	9	2.32
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	9	2.32
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	9	2.32
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	9	2.32
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	9	2.32
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	9	2.32
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	9	2.32
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	9	2.32
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	9	2.32
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	9	2.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	9	2.32
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	19	2.31
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	19	2.31
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	6	2.31
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	6	2.31
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	6	2.31
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	6	2.31
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	6	2.31
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	6	2.31
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	14	2.3
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	14	2.3
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	14	2.3
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	14	2.3
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	14	2.3
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	14	2.3
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	14	2.3
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	14	2.3
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	4	2.28
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	18	2.28
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	18	2.28
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	18	2.28
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	18	2.28
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	18	2.28
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	18	2.28
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	20	2.27
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	20	2.27
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	20	2.27
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	20	2.27
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	20	2.27
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	20	2.27
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	20	2.27
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	20	2.27
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	20	2.27
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	20	2.27
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	20	2.27
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	20	2.27
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	20	2.27
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	20	2.27
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	20	2.27
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	20	2.27
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	20	2.27
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	20	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	15	2.27
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	15	2.27
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	15	2.27
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	15	2.27
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	15	2.27
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	15	2.27
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	20	2.26
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	12	2.25
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	12	2.25
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	12	2.25
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	12	2.25
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	12	2.25
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	12	2.25
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	12	2.25
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	12	2.25
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	12	2.25
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	12	2.25
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	12	2.25
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	12	2.25
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	12	2.25
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	12	2.25
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	12	2.25
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	12	2.25
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	12	2.25
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	12	2.25
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	11	2.25
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	20	2.24
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	9	2.23
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	9	2.23
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	8	2.22
(1,5)	1:6:A:LEU:HA	1:30:A:ILE:HB	17	2.22
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	2	2.15
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	8	2.15
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	8	2.15
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	8	2.15
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	8	2.15
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	8	2.15
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	8	2.15
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	8	2.14
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	15	2.13
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	15	2.13
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	7	2.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	3	2.12
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	3	2.12
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	2	2.12
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	2	2.12
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	2	2.12
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	2	2.12
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	2	2.12
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	2	2.12
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	4	2.12
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	4	2.12
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	4	2.12
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	4	2.12
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	4	2.12
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	4	2.12
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	2	2.11
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	5	2.1
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	5	2.1
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	11	2.1
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	11	2.1
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	11	2.1
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	11	2.1
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	11	2.1
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	11	2.1
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	10	2.08
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	11	2.08
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	11	2.08
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	20	2.08
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	13	2.07
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	13	2.07
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	10	2.06
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	10	2.06
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	10	2.06
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	10	2.06
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	10	2.06
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	10	2.06
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	10	2.06
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	10	2.04
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	10	2.04
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	13	2.04
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	12	2.03
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	12	2.03
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	6	2.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	6	2.03
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	6	2.03
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	6	2.03
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	6	2.03
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	6	2.03
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	10	2.03
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	10	2.03
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	10	2.03
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	10	2.03
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	10	2.03
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	10	2.03
(1,34)	1:80:A:ILE:HD11	1:116:A:VAL:HA	2	2.02
(1,34)	1:80:A:ILE:HD12	1:116:A:VAL:HA	2	2.02
(1,34)	1:80:A:ILE:HD13	1:116:A:VAL:HA	2	2.02
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	12	2.02
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	12	2.02
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	12	2.02
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	11	2.01
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	11	2.01
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	20	2.0
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	5	2.0
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	5	2.0
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	5	2.0
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	5	2.0
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	5	2.0
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	5	2.0
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	5	2.0
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	5	2.0
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	5	2.0
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	3	1.99
(1,34)	1:80:A:ILE:HD11	1:116:A:VAL:HA	20	1.99
(1,34)	1:80:A:ILE:HD12	1:116:A:VAL:HA	20	1.99
(1,34)	1:80:A:ILE:HD13	1:116:A:VAL:HA	20	1.99
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	5	1.98
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	5	1.98
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	5	1.98
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	16	1.96
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	7	1.95
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	7	1.95
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	7	1.95
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	7	1.95
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	7	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	7	1.95
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	7	1.95
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	7	1.95
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	7	1.95
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	20	1.94
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	16	1.94
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	16	1.94
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	6	1.93
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	6	1.93
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	10	1.93
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	10	1.93
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	10	1.93
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	9	1.93
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	9	1.93
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	9	1.93
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	9	1.93
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	9	1.93
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	9	1.93
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	3	1.92
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	3	1.92
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	9	1.91
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	9	1.91
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	15	1.91
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	15	1.91
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	3	1.88
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	7	1.88
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	7	1.88
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	5	1.87
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	6	1.85
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	6	1.85
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	14	1.84
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	16	1.83
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	16	1.83
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	16	1.83
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	16	1.83
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	16	1.83
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	16	1.83
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	18	1.8
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	8	1.8
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	11	1.8
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	2	1.8
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	2	1.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD11	11	1.8
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD12	11	1.8
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD13	11	1.8
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD11	11	1.8
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD12	11	1.8
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD13	11	1.8
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD11	11	1.8
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD12	11	1.8
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD13	11	1.8
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	20	1.79
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	20	1.79
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	20	1.79
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	20	1.79
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	20	1.79
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	20	1.79
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB2	17	1.79
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB2	17	1.79
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB2	17	1.79
(1,9)	1:37:A:ILE:HD11	1:41:A:LYS:HB3	17	1.79
(1,9)	1:37:A:ILE:HD12	1:41:A:LYS:HB3	17	1.79
(1,9)	1:37:A:ILE:HD13	1:41:A:LYS:HB3	17	1.79
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD11	18	1.78
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD12	18	1.78
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD13	18	1.78
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD21	18	1.78
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD22	18	1.78
(1,300)	1:54:A:ILE:HG21	1:82:A:LEU:HD23	18	1.78
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD11	18	1.78
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD12	18	1.78
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD13	18	1.78
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD21	18	1.78
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD22	18	1.78
(1,300)	1:54:A:ILE:HG22	1:82:A:LEU:HD23	18	1.78
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD11	18	1.78
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD12	18	1.78
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD13	18	1.78
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD21	18	1.78
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD22	18	1.78
(1,300)	1:54:A:ILE:HG23	1:82:A:LEU:HD23	18	1.78
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	10	1.78
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	18	1.78
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	12	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	16	1.77
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	16	1.77
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	16	1.77
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	15	1.77
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	15	1.77
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	15	1.77
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	15	1.77
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	15	1.77
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	15	1.77
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	15	1.77
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	15	1.77
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	15	1.77
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	8	1.76
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	8	1.76
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	8	1.76
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	20	1.75
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	3	1.75
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	3	1.73
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	7	1.72
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	8	1.72
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	8	1.72
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	8	1.72
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	8	1.72
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	8	1.72
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	8	1.72
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	10	1.71
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	10	1.71
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	9	1.71
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	9	1.71
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	7	1.71
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	7	1.71
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	11	1.71
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	11	1.71
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	11	1.71
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	11	1.71
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	11	1.71
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	11	1.71
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	19	1.71
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	19	1.71
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	19	1.71
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	19	1.71
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	19	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	19	1.71
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	1	1.7
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	8	1.7
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	8	1.7
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	8	1.7
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	8	1.7
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	8	1.7
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	8	1.7
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD11	11	1.69
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD12	11	1.69
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD13	11	1.69
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD11	11	1.69
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD12	11	1.69
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD13	11	1.69
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	2	1.69
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	2	1.69
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	4	1.69
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	17	1.69
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	12	1.69
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	6	1.69
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	6	1.69
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	6	1.69
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	6	1.69
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	6	1.69
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	6	1.69
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	13	1.68
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	13	1.68
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	11	1.68
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	8	1.67
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	13	1.67
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	10	1.67
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	10	1.67
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	10	1.67
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	1	1.66
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	1	1.66
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	6	1.65
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	14	1.65
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	14	1.65
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	18	1.64
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	17	1.64
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	17	1.64
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	17	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	17	1.64
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	17	1.64
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	17	1.64
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	1	1.63
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	19	1.63
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	5	1.62
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	14	1.62
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	11	1.61
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	11	1.61
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	11	1.61
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	11	1.61
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	11	1.61
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	11	1.61
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	11	1.61
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	11	1.61
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	11	1.61
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	11	1.61
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	11	1.61
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	11	1.61
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	1	1.6
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	1	1.6
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	14	1.6
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	14	1.6
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	14	1.6
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	14	1.6
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	14	1.6
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	14	1.6
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	13	1.59
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	13	1.59
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	13	1.59
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	13	1.59
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	13	1.59
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	13	1.59
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	13	1.59
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	19	1.58
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	7	1.58
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	3	1.58
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	3	1.58
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	3	1.58
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	3	1.58
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	3	1.58
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	3	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	10	1.57
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	10	1.57
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	10	1.57
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	9	1.57
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	18	1.57
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	4	1.57
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	4	1.57
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	4	1.57
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	4	1.57
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	4	1.57
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	4	1.57
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	13	1.56
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	2	1.56
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	2	1.56
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	13	1.56
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	16	1.56
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	20	1.56
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	20	1.56
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	20	1.56
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	13	1.55
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	18	1.55
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	10	1.55
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	10	1.55
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	16	1.55
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	16	1.55
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	16	1.55
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	12	1.54
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	4	1.53
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	13	1.51
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	13	1.51
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	13	1.51
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	3	1.51
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	15	1.5
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	20	1.49
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	20	1.49
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	20	1.49
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	8	1.49
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	1	1.49
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	1	1.49
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	1	1.49
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	1	1.49
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	1	1.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	1	1.49
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	15	1.48
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	20	1.47
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	20	1.47
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	19	1.47
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	19	1.47
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	19	1.47
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	15	1.47
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	15	1.47
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	15	1.47
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	15	1.47
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	15	1.47
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	15	1.47
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	9	1.45
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	16	1.45
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	17	1.45
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	8	1.45
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	9	1.44
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	4	1.44
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	8	1.44
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	16	1.44
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	16	1.44
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	16	1.44
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	13	1.44
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	13	1.44
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	13	1.44
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	10	1.43
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	10	1.43
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	10	1.43
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	14	1.41
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	14	1.41
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	11	1.41
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	11	1.41
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	18	1.41
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	12	1.41
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	12	1.41
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	12	1.41
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	13	1.39
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	18	1.39
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	18	1.39
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	3	1.38
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	3	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	3	1.38
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	1	1.37
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	20	1.37
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	20	1.37
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	20	1.37
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	20	1.37
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	20	1.37
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	20	1.37
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	20	1.37
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	20	1.37
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	20	1.37
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	20	1.37
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	20	1.37
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	20	1.37
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	20	1.37
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	20	1.37
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	20	1.37
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	20	1.37
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	20	1.37
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	20	1.37
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	17	1.37
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	17	1.37
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	17	1.37
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	6	1.35
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	19	1.35
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	18	1.35
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	6	1.34
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	6	1.34
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	2	1.34
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	4	1.34
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	16	1.34
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	18	1.34
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	19	1.33
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	1	1.33
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	4	1.32
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	6	1.32
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	10	1.32
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	10	1.32
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	10	1.32
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	1	1.31
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	12	1.31
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	12	1.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	7	1.31
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	15	1.31
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	16	1.31
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	7	1.31
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	7	1.31
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	8	1.31
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	8	1.31
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	12	1.31
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	12	1.31
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	12	1.31
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	12	1.31
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	12	1.31
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	12	1.31
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	20	1.3
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	3	1.3
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	17	1.3
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	20	1.3
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	15	1.3
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	15	1.3
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	15	1.3
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	1	1.29
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	3	1.29
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	5	1.29
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	17	1.28
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	17	1.28
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	17	1.28
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	1	1.27
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	20	1.27
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	10	1.27
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	11	1.27
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	11	1.27
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	11	1.27
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	9	1.27
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	9	1.27
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	9	1.27
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	6	1.26
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	16	1.26
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	20	1.26
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	13	1.26
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	13	1.26
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	3	1.25
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	16	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	18	1.25
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	18	1.25
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	18	1.25
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	18	1.25
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	18	1.25
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	18	1.25
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	18	1.25
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	18	1.25
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	18	1.25
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	18	1.25
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	18	1.25
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	18	1.25
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	18	1.25
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	18	1.25
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	18	1.25
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	18	1.25
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	18	1.25
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	18	1.25
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	3	1.25
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	6	1.25
(1,216)	1:34:A:ASN:H	1:35:A:GLY:H	17	1.25
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	6	1.25
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	6	1.25
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	4	1.25
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	4	1.25
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	4	1.25
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	4	1.25
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	4	1.25
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	4	1.25
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	4	1.25
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	4	1.25
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	4	1.25
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	4	1.25
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	4	1.25
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	4	1.25
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	4	1.25
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	4	1.25
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	4	1.25
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	4	1.25
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	4	1.25
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	4	1.25
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	4	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	12	1.25
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	12	1.25
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	12	1.25
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD2	4	1.25
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD2	4	1.25
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD2	4	1.25
(1,10)	1:37:A:ILE:HD11	1:41:A:LYS:HD3	4	1.25
(1,10)	1:37:A:ILE:HD12	1:41:A:LYS:HD3	4	1.25
(1,10)	1:37:A:ILE:HD13	1:41:A:LYS:HD3	4	1.25
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	19	1.25
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	19	1.25
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	19	1.25
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	17	1.24
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	17	1.24
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	17	1.24
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	17	1.24
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	17	1.24
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	17	1.24
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	17	1.24
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	17	1.24
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	17	1.24
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	17	1.24
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	17	1.24
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	17	1.24
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	17	1.24
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	17	1.24
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	17	1.24
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	17	1.24
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	17	1.24
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	17	1.24
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	6	1.24
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	6	1.24
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	6	1.24
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	6	1.24
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	6	1.24
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	6	1.24
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	2	1.23
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	8	1.23
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	19	1.23
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	19	1.23
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	2	1.23
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	9	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	9	1.23
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	9	1.23
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	15	1.22
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	1	1.22
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	1	1.22
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	20	1.21
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	20	1.21
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	12	1.21
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	12	1.21
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	12	1.21
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	12	1.21
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	12	1.21
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	12	1.21
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	12	1.21
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	3	1.21
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	3	1.21
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	9	1.21
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	9	1.21
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	9	1.21
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	19	1.21
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	19	1.21
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	19	1.21
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	19	1.21
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	19	1.21
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	19	1.21
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	19	1.21
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	19	1.21
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	19	1.21
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	13	1.2
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	7	1.2
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	16	1.2
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	16	1.2
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	3	1.2
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	3	1.2
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	3	1.2
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	14	1.2
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	17	1.19
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	14	1.19
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	13	1.18
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	17	1.18
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	14	1.18
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	19	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	14	1.18
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	14	1.18
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	14	1.18
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	14	1.18
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	14	1.18
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	14	1.18
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	14	1.18
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	14	1.18
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	14	1.18
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	12	1.17
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	11	1.17
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	11	1.17
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	11	1.17
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	8	1.17
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	8	1.17
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	8	1.17
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	8	1.17
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	8	1.17
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	8	1.17
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	8	1.17
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	8	1.17
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	8	1.17
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	1	1.16
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	17	1.16
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	13	1.16
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	4	1.16
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	4	1.16
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	10	1.16
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	10	1.16
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	10	1.16
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	10	1.16
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	10	1.16
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	10	1.16
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	10	1.16
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	10	1.16
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	10	1.16
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	12	1.15
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	11	1.15
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	4	1.15
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	4	1.15
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	4	1.15
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	4	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	4	1.15
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	4	1.15
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	16	1.15
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	16	1.15
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	16	1.15
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	16	1.15
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	16	1.15
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	16	1.15
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	16	1.15
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	16	1.15
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	16	1.15
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	15	1.15
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	5	1.15
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	5	1.15
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	5	1.15
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	2	1.15
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	2	1.15
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	2	1.15
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	2	1.15
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	2	1.15
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	2	1.15
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	16	1.15
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	16	1.15
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	16	1.15
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	10	1.14
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	9	1.14
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	4	1.14
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	15	1.13
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	19	1.13
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	19	1.13
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	4	1.12
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	9	1.12
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	14	1.12
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	4	1.11
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	4	1.11
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	9	1.11
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	10	1.11
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	5	1.11
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	5	1.11
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	5	1.11
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	13	1.11
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	13	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	13	1.11
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	13	1.11
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	13	1.11
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	13	1.11
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	13	1.11
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	13	1.11
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	13	1.11
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	13	1.1
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	13	1.1
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	13	1.1
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	13	1.1
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	17	1.1
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	17	1.1
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	17	1.1
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	17	1.1
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	17	1.1
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	17	1.1
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	17	1.1
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	17	1.1
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	17	1.1
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	1	1.09
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	12	1.09
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	12	1.09
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	6	1.09
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	17	1.09
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	17	1.09
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	15	1.09
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	4	1.09
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	4	1.09
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	4	1.09
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	4	1.09
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	4	1.09
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	4	1.09
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	4	1.09
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	4	1.09
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	4	1.09
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	6	1.09
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	6	1.09
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	6	1.09
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	6	1.09
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	6	1.09
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	6	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	6	1.09
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	6	1.09
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	6	1.09
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	7	1.09
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	7	1.09
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	7	1.09
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	14	1.08
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	14	1.08
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	8	1.08
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	15	1.08
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	10	1.08
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	10	1.08
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	10	1.08
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	12	1.08
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	12	1.08
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	12	1.08
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	7	1.07
(1,108)	1:84:A:ALA:HA	1:85:A:LYS:H	10	1.07
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	16	1.07
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	9	1.07
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	9	1.07
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	9	1.07
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	13	1.07
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	13	1.07
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	13	1.07
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	13	1.07
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	13	1.07
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	13	1.07
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	13	1.07
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	13	1.07
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	13	1.07
(2,58)	1:21:A:ASN:O	1:25:A:GLU:N	13	1.06
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	14	1.06
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	14	1.06
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	14	1.06
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	14	1.06
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	14	1.06
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	14	1.06
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	14	1.06
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	14	1.06
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	14	1.06
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	14	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	14	1.06
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	14	1.06
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	14	1.06
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	14	1.06
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	14	1.06
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	14	1.06
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	14	1.06
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	14	1.06
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	4	1.06
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	4	1.06
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	4	1.06
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	9	1.06
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	6	1.05
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	8	1.05
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	8	1.05
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	17	1.04
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	16	1.04
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	9	1.04
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	13	1.03
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	8	1.03
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	1	1.03
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	1	1.03
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	2	1.03
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	15	1.03
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	1	1.03
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	1	1.03
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	1	1.03
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	10	1.03
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	10	1.03
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	10	1.03
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	10	1.03
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	10	1.03
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	10	1.03
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	11	1.03
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	11	1.03
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	11	1.03
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	2	1.02
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	2	1.02
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	2	1.02
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	2	1.02
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	2	1.02
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	2	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	2	1.02
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	2	1.02
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	2	1.02
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	2	1.02
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	2	1.02
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	2	1.02
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	2	1.02
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	2	1.02
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	2	1.02
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	2	1.02
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	2	1.02
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	2	1.02
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD11	2	1.02
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD12	2	1.02
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD13	2	1.02
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD11	2	1.02
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD12	2	1.02
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD13	2	1.02
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	14	1.02
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	14	1.02
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	14	1.02
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	14	1.02
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	14	1.02
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	14	1.02
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	20	1.02
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	3	1.01
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	9	1.01
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	9	1.01
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	9	1.01
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	9	1.01
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	9	1.01
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	9	1.01
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	9	1.01
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	9	1.01
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	9	1.01
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	9	1.01
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	9	1.01
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	9	1.01
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	9	1.01
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	9	1.01
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	9	1.01
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	9	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	9	1.01
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	9	1.01
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	11	1.01
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	16	1.01
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	2	1.01
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	2	1.01
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	2	1.01
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	2	1.01
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	2	1.01
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	2	1.01
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	2	1.01
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	2	1.01
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	2	1.01
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	19	1.0
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	17	1.0
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	14	1.0
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	14	1.0
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	14	1.0
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	14	1.0
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	14	1.0
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	14	1.0
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	14	1.0
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	14	1.0
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	14	1.0
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	14	1.0
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	14	1.0
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	14	1.0
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	14	1.0
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	14	1.0
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	14	1.0
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	14	1.0
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	14	1.0
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	14	1.0
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	15	1.0
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	12	1.0
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	12	1.0
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	12	1.0
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	12	1.0
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	12	1.0
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	12	1.0
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	12	1.0
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	12	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	12	1.0
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	17	0.99
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	5	0.99
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	2	0.99
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	11	0.99
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	19	0.99
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	19	0.99
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	19	0.99
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	19	0.99
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	19	0.99
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	19	0.99
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	19	0.99
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	19	0.99
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	19	0.99
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	2	0.99
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	2	0.99
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	2	0.99
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	13	0.99
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	13	0.99
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	13	0.99
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	13	0.99
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	13	0.99
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	13	0.99
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	3	0.99
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	3	0.99
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	3	0.99
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	8	0.98
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	8	0.98
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	14	0.98
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	10	0.98
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	10	0.98
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	10	0.98
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	10	0.98
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	10	0.98
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	10	0.98
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	10	0.98
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	10	0.98
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	10	0.98
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	5	0.97
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	5	0.97
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	5	0.97
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	5	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	5	0.97
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	5	0.97
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	5	0.97
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	5	0.97
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	5	0.97
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	5	0.97
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	5	0.97
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	5	0.97
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	5	0.97
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	5	0.97
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	5	0.97
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	5	0.97
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	5	0.97
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	5	0.97
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	16	0.97
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	16	0.97
(1,91)	1:45:A:PHE:HA	1:46:A:THR:H	11	0.97
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	3	0.97
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	3	0.97
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	3	0.97
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	3	0.97
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	3	0.97
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	3	0.97
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	3	0.97
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	3	0.97
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	3	0.97
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	7	0.96
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	10	0.96
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	10	0.96
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	15	0.96
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	17	0.96
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	17	0.96
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	17	0.96
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	17	0.96
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	17	0.96
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	17	0.96
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	18	0.96
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	18	0.96
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	18	0.96
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	18	0.96
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	18	0.96
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	18	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	3	0.96
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	3	0.96
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	3	0.96
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	17	0.96
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	17	0.96
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	17	0.96
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	17	0.96
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	17	0.96
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	17	0.96
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	17	0.96
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	17	0.96
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	17	0.96
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	8	0.95
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	7	0.95
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	1	0.95
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	11	0.95
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	11	0.95
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	11	0.95
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	11	0.95
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	11	0.95
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	11	0.95
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	11	0.95
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	11	0.95
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	2	0.95
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	2	0.95
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	2	0.95
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	2	0.95
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	2	0.95
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	2	0.95
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	6	0.94
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	13	0.94
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	13	0.94
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	13	0.94
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	13	0.94
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	13	0.94
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	13	0.94
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	19	0.94
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	19	0.94
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	19	0.94
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	19	0.94
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	19	0.94
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	19	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	7	0.94
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	19	0.94
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	19	0.94
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	19	0.94
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	19	0.94
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	19	0.94
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	19	0.94
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	19	0.94
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	19	0.94
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	19	0.94
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	19	0.94
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	19	0.94
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	19	0.94
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	19	0.94
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	19	0.94
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	19	0.94
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	19	0.94
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	19	0.94
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	19	0.94
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	16	0.94
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	16	0.94
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	16	0.94
(2,11)	1:7:A:LEU:H	1:30:A:ILE:O	7	0.93
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	20	0.93
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	20	0.93
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	20	0.93
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	5	0.92
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	2	0.92
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	8	0.92
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	15	0.92
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	10	0.92
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	11	0.92
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	11	0.92
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	11	0.92
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	11	0.92
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	11	0.92
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	11	0.92
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	11	0.92
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	11	0.92
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	11	0.92
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	10	0.92
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	19	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	19	0.92
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	19	0.92
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	19	0.92
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	19	0.92
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	19	0.92
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	12	0.91
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	11	0.91
(2,58)	1:21:A:ASN:O	1:25:A:GLU:N	2	0.91
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	6	0.91
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	6	0.91
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	7	0.91
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	15	0.91
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	7	0.91
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	7	0.91
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	7	0.91
(1,19)	1:42:A:LEU:HB2	1:47:A:PRO:HD2	7	0.91
(1,19)	1:42:A:LEU:HB3	1:47:A:PRO:HD2	7	0.91
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	14	0.9
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	16	0.9
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	16	0.9
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	16	0.9
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	16	0.9
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	16	0.9
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	16	0.9
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB2	17	0.9
(1,287)	1:39:A:LEU:HG	1:74:A:TRP:HB3	17	0.9
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	7	0.89
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	2	0.89
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	5	0.89
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	14	0.89
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	14	0.89
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	14	0.89
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	19	0.88
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	19	0.88
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	19	0.88
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	19	0.88
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	19	0.88
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	19	0.88
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	1	0.88
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	16	0.88
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	4	0.88
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	4	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	7	0.88
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	7	0.88
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	7	0.88
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	7	0.88
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	7	0.88
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	7	0.88
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG2	19	0.88
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG2	19	0.88
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG2	19	0.88
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG3	19	0.88
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG3	19	0.88
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG3	19	0.88
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD11	12	0.88
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD12	12	0.88
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD13	12	0.88
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD11	12	0.88
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD12	12	0.88
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD13	12	0.88
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD11	12	0.88
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD12	12	0.88
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD13	12	0.88
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	5	0.87
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	7	0.87
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	7	0.87
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	7	0.87
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	7	0.87
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	7	0.87
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	7	0.87
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	7	0.87
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	7	0.87
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	7	0.87
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	7	0.87
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	7	0.87
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	7	0.87
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	7	0.87
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	7	0.87
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	7	0.87
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	7	0.87
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	7	0.87
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	7	0.87
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	15	0.87
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	14	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	14	0.87
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	14	0.87
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	14	0.87
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	14	0.87
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	14	0.87
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	20	0.87
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	20	0.87
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	20	0.87
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	8	0.87
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	8	0.87
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	8	0.87
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	8	0.87
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	8	0.87
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	8	0.87
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	8	0.87
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	8	0.87
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	8	0.87
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	15	0.86
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	7	0.86
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	7	0.86
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	7	0.86
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	7	0.86
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	7	0.86
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	7	0.86
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	7	0.86
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	7	0.86
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	7	0.86
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	2	0.86
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	7	0.85
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	2	0.85
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	6	0.85
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	6	0.85
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	6	0.85
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	6	0.85
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	6	0.85
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	6	0.85
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	6	0.85
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	6	0.85
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	6	0.85
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	6	0.85
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	6	0.85
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	6	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	6	0.85
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	6	0.85
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	6	0.85
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	6	0.85
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	6	0.85
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	6	0.85
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	19	0.85
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	15	0.84
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	15	0.84
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	15	0.84
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	15	0.84
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	15	0.84
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	15	0.84
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	15	0.84
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	15	0.84
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	15	0.84
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	12	0.84
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	12	0.84
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	12	0.84
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	12	0.84
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	12	0.84
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	12	0.84
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	12	0.84
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	12	0.84
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	12	0.84
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	12	0.84
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	12	0.84
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	12	0.84
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	12	0.84
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	12	0.84
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	12	0.84
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	12	0.84
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	12	0.84
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	12	0.84
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	11	0.83
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	9	0.83
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	20	0.83
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	6	0.83
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	14	0.83
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	14	0.83
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	17	0.83
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	17	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	17	0.83
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	17	0.83
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	17	0.83
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	17	0.83
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	17	0.83
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	17	0.83
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	17	0.83
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	17	0.83
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	17	0.83
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	17	0.83
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	17	0.83
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	17	0.83
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	17	0.83
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	17	0.83
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	17	0.83
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	17	0.83
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	9	0.83
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	9	0.83
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	9	0.83
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	9	0.83
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	9	0.83
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	9	0.83
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	9	0.83
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	9	0.83
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	9	0.83
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG2	8	0.83
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG2	8	0.83
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG2	8	0.83
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG3	8	0.83
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG3	8	0.83
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG3	8	0.83
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	16	0.83
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	16	0.83
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	16	0.83
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	16	0.83
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	16	0.83
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	16	0.83
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	16	0.83
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	16	0.83
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	16	0.83
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	5	0.83
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	5	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	5	0.83
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	19	0.82
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD11	10	0.82
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD12	10	0.82
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD13	10	0.82
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD11	10	0.82
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD12	10	0.82
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD13	10	0.82
(1,229)	1:59:A:MET:H	1:60:A:ASP:H	7	0.82
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	1	0.82
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	1	0.82
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	2	0.82
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	2	0.82
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	2	0.82
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	2	0.82
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	2	0.82
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	2	0.82
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	2	0.82
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	2	0.82
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	2	0.82
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	1	0.82
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	1	0.82
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	1	0.82
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	9	0.81
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	12	0.81
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	7	0.81
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	7	0.81
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	7	0.81
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	7	0.81
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	7	0.81
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	7	0.81
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	7	0.81
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	7	0.81
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	7	0.81
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	7	0.81
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	7	0.81
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	7	0.81
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	2	0.81
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	2	0.81
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	2	0.81
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	2	0.81
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	2	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	2	0.81
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	2	0.81
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	2	0.81
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	2	0.81
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	2	0.81
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	2	0.81
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	2	0.81
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	2	0.81
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	2	0.81
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	2	0.81
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	2	0.81
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	2	0.81
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	2	0.81
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	5	0.81
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	5	0.81
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	5	0.81
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	5	0.81
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	5	0.81
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	5	0.81
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	11	0.81
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	10	0.81
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	6	0.81
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	6	0.81
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	18	0.81
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	18	0.81
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	18	0.81
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	18	0.81
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	18	0.81
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	18	0.81
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	18	0.81
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	18	0.81
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	18	0.81
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	18	0.81
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	18	0.81
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	18	0.81
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	18	0.81
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	18	0.81
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	18	0.81
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	18	0.81
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	18	0.81
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	18	0.81
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	9	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	8	0.8
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	8	0.8
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	8	0.8
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	8	0.8
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	8	0.8
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	8	0.8
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	8	0.8
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	8	0.8
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	8	0.8
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	8	0.8
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	8	0.8
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	8	0.8
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	8	0.8
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	8	0.8
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	8	0.8
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	8	0.8
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	8	0.8
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	8	0.8
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	10	0.8
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	16	0.8
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG21	6	0.8
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG22	6	0.8
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG23	6	0.8
(1,6)	1:6:A:LEU:H	1:30:A:ILE:HB	20	0.8
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	12	0.8
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	12	0.8
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	12	0.8
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	12	0.8
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	12	0.8
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	12	0.8
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	9	0.79
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	14	0.79
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	11	0.79
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	11	0.79
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	5	0.79
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	5	0.79
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	5	0.79
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	5	0.79
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	5	0.79
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	5	0.79
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	13	0.79
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	13	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	13	0.79
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	13	0.79
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	13	0.79
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	13	0.79
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	13	0.79
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	13	0.79
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	13	0.79
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	13	0.79
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	13	0.79
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	13	0.79
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	4	0.79
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	9	0.79
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	17	0.79
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	17	0.79
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	3	0.79
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	3	0.79
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	3	0.79
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	3	0.79
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	3	0.79
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	3	0.79
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	3	0.79
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	3	0.79
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	3	0.79
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	4	0.79
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	4	0.79
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	4	0.79
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	4	0.79
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	4	0.79
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	4	0.79
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	4	0.79
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	4	0.79
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	4	0.79
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	10	0.79
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	10	0.79
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	10	0.79
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	13	0.78
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	20	0.78
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	20	0.78
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	20	0.78
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	20	0.78
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	20	0.78
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	20	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	20	0.78
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	20	0.78
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	20	0.78
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	20	0.78
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	20	0.78
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	20	0.78
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	3	0.78
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	3	0.78
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	3	0.78
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	3	0.78
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	3	0.78
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	3	0.78
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	3	0.78
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	3	0.78
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	3	0.78
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	3	0.78
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	3	0.78
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	3	0.78
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	3	0.78
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	3	0.78
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	3	0.78
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	3	0.78
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	3	0.78
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	3	0.78
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	13	0.78
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	13	0.78
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	13	0.78
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	13	0.78
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	13	0.78
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	13	0.78
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	13	0.78
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	13	0.78
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	13	0.78
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	13	0.78
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	13	0.78
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	13	0.78
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	13	0.78
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	13	0.78
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	13	0.78
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	13	0.78
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	13	0.78
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	13	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	10	0.78
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	20	0.78
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	20	0.78
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	9	0.78
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	9	0.78
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	9	0.78
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	9	0.78
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	9	0.78
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	9	0.78
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	18	0.77
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	20	0.77
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	10	0.77
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	16	0.77
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	16	0.77
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	16	0.77
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	16	0.77
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	16	0.77
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	16	0.77
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	16	0.77
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	16	0.77
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	16	0.77
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	16	0.77
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	16	0.77
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	16	0.77
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	16	0.77
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	16	0.77
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	16	0.77
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	16	0.77
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	16	0.77
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	16	0.77
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	20	0.77
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	20	0.77
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	20	0.77
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	20	0.77
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	20	0.77
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	20	0.77
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	18	0.77
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	6	0.77
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	6	0.77
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	6	0.77
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	6	0.77
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	6	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	6	0.77
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	6	0.77
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	6	0.77
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	6	0.77
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	6	0.77
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	6	0.77
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	6	0.77
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	6	0.77
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	6	0.77
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	6	0.77
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	6	0.77
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	6	0.77
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	6	0.77
(1,23)	1:42:A:LEU:HB2	1:47:A:PRO:HD3	7	0.77
(1,23)	1:42:A:LEU:HB3	1:47:A:PRO:HD3	7	0.77
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	12	0.76
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	18	0.76
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	20	0.76
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	20	0.76
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	20	0.76
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	20	0.76
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	20	0.76
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	20	0.76
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	20	0.76
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	20	0.76
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	20	0.76
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	20	0.76
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	20	0.76
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	20	0.76
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	20	0.76
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	20	0.76
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	20	0.76
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	20	0.76
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	20	0.76
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	20	0.76
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	15	0.76
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	19	0.76
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	7	0.76
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	7	0.76
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	5	0.76
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	5	0.76
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	5	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	2	0.75
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	10	0.75
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	8	0.75
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	4	0.75
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	5	0.75
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	5	0.75
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	5	0.75
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	5	0.75
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	5	0.75
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	5	0.75
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	5	0.75
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	5	0.75
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	5	0.75
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	6	0.75
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	6	0.75
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	6	0.75
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	4	0.74
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	11	0.74
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	13	0.74
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	3	0.74
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	6	0.74
(1,62)	1:71:A:LYS:HD2	1:74:A:TRP:H	19	0.74
(1,62)	1:71:A:LYS:HD3	1:74:A:TRP:H	19	0.74
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	5	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	5	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	5	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	5	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	5	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	5	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	5	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	5	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	5	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	5	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	5	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	5	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	5	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	10	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	10	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	10	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	10	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	10	0.73
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	10	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	10	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	10	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	10	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	10	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	10	0.73
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	10	0.73
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	15	0.73
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	15	0.73
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	17	0.73
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	17	0.73
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	17	0.73
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	17	0.73
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	17	0.73
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	17	0.73
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	20	0.73
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	3	0.73
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	3	0.73
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	3	0.73
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	13	0.73
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	13	0.73
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	13	0.73
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	13	0.73
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	13	0.73
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	13	0.73
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	2	0.72
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	1	0.72
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	1	0.72
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	1	0.72
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	1	0.72
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	1	0.72
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	1	0.72
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	1	0.72
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	1	0.72
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	1	0.72
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	1	0.72
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	1	0.72
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	1	0.72
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	19	0.72
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	19	0.72
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	17	0.72
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	17	0.72
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	18	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	18	0.72
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	18	0.72
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	18	0.72
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	18	0.72
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	18	0.72
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	18	0.72
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	18	0.72
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	18	0.72
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	4	0.72
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	4	0.72
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	4	0.72
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	4	0.72
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	4	0.72
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	4	0.72
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	8	0.72
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	8	0.72
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	8	0.72
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	11	0.72
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	19	0.71
(2,32)	1:79:A:VAL:O	1:100:A:ARG:N	19	0.71
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	9	0.71
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	9	0.71
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	9	0.71
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	9	0.71
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	9	0.71
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	9	0.71
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	9	0.71
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	9	0.71
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	9	0.71
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	9	0.71
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	9	0.71
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	9	0.71
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	8	0.71
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	1	0.71
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	1	0.71
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	13	0.71
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	4	0.71
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	6	0.71
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	6	0.71
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	1	0.71
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	1	0.71
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	1	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	1	0.71
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	1	0.71
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	1	0.71
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	1	0.71
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	1	0.71
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	1	0.71
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	11	0.7
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	10	0.7
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	10	0.7
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	10	0.7
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	10	0.7
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	10	0.7
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	10	0.7
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	10	0.7
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	10	0.7
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	10	0.7
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	10	0.7
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	10	0.7
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	10	0.7
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	10	0.7
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	10	0.7
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	10	0.7
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	10	0.7
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	10	0.7
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	10	0.7
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	3	0.7
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	13	0.7
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	9	0.69
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	7	0.69
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	3	0.69
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	3	0.69
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	3	0.69
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	3	0.69
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	3	0.69
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	3	0.69
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	7	0.69
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	7	0.69
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	7	0.69
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	7	0.69
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	7	0.69
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	7	0.69
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	14	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	16	0.69
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	15	0.69
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	19	0.69
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	13	0.69
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	13	0.69
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	13	0.69
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	3	0.69
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	3	0.69
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	3	0.69
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	3	0.69
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	3	0.69
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	3	0.69
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	18	0.69
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	18	0.69
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	18	0.69
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	18	0.69
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	18	0.69
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	18	0.69
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	20	0.69
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	20	0.69
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	20	0.69
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	20	0.69
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	20	0.69
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	20	0.69
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	20	0.69
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	20	0.69
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	20	0.69
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	4	0.68
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	4	0.68
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	4	0.68
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	4	0.68
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	4	0.68
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	4	0.68
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	4	0.68
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	4	0.68
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	4	0.68
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	4	0.68
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	4	0.68
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	4	0.68
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	4	0.68
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	4	0.68
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	4	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	4	0.68
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	4	0.68
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	4	0.68
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	7	0.68
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	7	0.68
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	7	0.68
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	7	0.68
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	7	0.68
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	7	0.68
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	7	0.68
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	7	0.68
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	7	0.68
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	7	0.68
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	7	0.68
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	7	0.68
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	7	0.68
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	7	0.68
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	7	0.68
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	7	0.68
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	7	0.68
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	7	0.68
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	13	0.68
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	10	0.68
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	5	0.68
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	20	0.68
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	20	0.68
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	20	0.68
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	7	0.67
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	7	0.67
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	7	0.67
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	7	0.67
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	7	0.67
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	7	0.67
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	18	0.67
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	18	0.67
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	18	0.67
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	18	0.67
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	18	0.67
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	18	0.67
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	20	0.67
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	20	0.67
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	20	0.67
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	20	0.67
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	20	0.67
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	3	0.67
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	3	0.67
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	3	0.67
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	3	0.67
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	3	0.67
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	3	0.67
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	17	0.67
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	18	0.67
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	10	0.67
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	10	0.67
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	6	0.67
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	6	0.67
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	6	0.67
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	6	0.67
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	6	0.67
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	6	0.67
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	6	0.67
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	6	0.67
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	6	0.67
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	10	0.66
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	10	0.66
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	4	0.66
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	1	0.66
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	9	0.66
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	9	0.66
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	9	0.66
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	9	0.66
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	9	0.66
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	9	0.66
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	9	0.66
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	9	0.66
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	9	0.66
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	9	0.66
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	9	0.66
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	9	0.66
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	16	0.66
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	1	0.66
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	6	0.66
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	19	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,62)	1:71:A:LYS:HD2	1:74:A:TRP:H	17	0.66
(1,62)	1:71:A:LYS:HD3	1:74:A:TRP:H	17	0.66
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	13	0.66
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	17	0.66
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	17	0.66
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	17	0.66
(1,23)	1:42:A:LEU:HB2	1:47:A:PRO:HD3	20	0.66
(1,23)	1:42:A:LEU:HB3	1:47:A:PRO:HD3	20	0.66
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	2	0.65
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	5	0.65
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	11	0.65
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	11	0.65
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	11	0.65
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	11	0.65
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	11	0.65
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	11	0.65
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	1	0.65
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	16	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	11	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	11	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	11	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	11	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	11	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	11	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	11	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	11	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	11	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	11	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	11	0.65
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	11	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	11	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	11	0.65
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	11	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	11	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	11	0.65
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	11	0.65
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	14	0.65
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	14	0.65
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	14	0.65
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	14	0.65
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	14	0.65
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	14	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	12	0.65
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	2	0.65
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	2	0.65
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	2	0.65
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	1	0.64
(2,56)	1:20:A:PHE:O	1:24:A:LYS:N	2	0.64
(2,5)	1:5:A:VAL:O	1:30:A:ILE:H	20	0.64
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	1	0.64
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	1	0.64
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	1	0.64
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	1	0.64
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	1	0.64
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	1	0.64
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	1	0.64
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	1	0.64
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	1	0.64
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	1	0.64
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	1	0.64
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	1	0.64
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	1	0.64
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	1	0.64
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	1	0.64
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	1	0.64
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	1	0.64
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	1	0.64
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	12	0.64
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	12	0.64
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	12	0.64
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	12	0.64
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	12	0.64
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	12	0.64
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	12	0.64
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	12	0.64
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	12	0.64
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	12	0.64
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	12	0.64
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	12	0.64
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	12	0.64
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	12	0.64
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	12	0.64
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	12	0.64
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	12	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	12	0.64
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	6	0.64
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	6	0.64
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	6	0.64
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	6	0.64
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	6	0.64
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	6	0.64
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	18	0.64
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	18	0.64
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	18	0.64
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	18	0.64
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	18	0.64
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	18	0.64
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	14	0.64
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	3	0.64
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	3	0.64
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	3	0.64
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	1	0.64
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	1	0.64
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	1	0.64
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	1	0.64
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	1	0.64
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	1	0.64
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	1	0.64
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	1	0.64
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	1	0.64
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	15	0.64
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	15	0.64
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	15	0.64
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	15	0.64
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	15	0.64
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	15	0.64
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	15	0.64
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	15	0.64
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	15	0.64
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	17	0.64
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	17	0.64
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	17	0.64
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	17	0.64
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	17	0.64
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	17	0.64
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	11	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	15	0.63
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	5	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	11	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	11	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	11	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	11	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	11	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	11	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	11	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	11	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	11	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	11	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	11	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	11	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	11	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	11	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	11	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	11	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	11	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	11	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	14	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	14	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	14	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	14	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	14	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	14	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	14	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	14	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	14	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	14	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	14	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	14	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	14	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	14	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	14	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	14	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	14	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	14	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	15	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	15	0.63
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	15	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	15	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	15	0.63
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	15	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	15	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	15	0.63
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	15	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	15	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	15	0.63
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	15	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	15	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	15	0.63
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	15	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	15	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	15	0.63
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	15	0.63
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	2	0.63
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	2	0.63
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	2	0.63
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	2	0.63
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	2	0.63
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	2	0.63
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	11	0.63
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	12	0.63
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	5	0.63
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	16	0.63
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	8	0.63
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	8	0.63
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	2	0.63
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	2	0.63
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	2	0.63
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	14	0.63
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	14	0.63
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	14	0.63
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	14	0.63
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	14	0.63
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	14	0.63
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	14	0.63
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	14	0.63
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	14	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	9	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	9	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	9	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	9	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	9	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	9	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	16	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	16	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	16	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	16	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	16	0.63
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	16	0.63
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	14	0.63
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	14	0.63
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	14	0.63
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	14	0.63
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	14	0.63
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	14	0.63
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	20	0.62
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	3	0.62
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	2	0.62
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	2	0.62
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	2	0.62
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	2	0.62
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	2	0.62
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	2	0.62
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	2	0.62
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	2	0.62
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	2	0.62
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	2	0.62
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	2	0.62
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	2	0.62
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	19	0.62
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	19	0.62
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	19	0.62
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	19	0.62
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	19	0.62
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	19	0.62
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	19	0.62
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	19	0.62
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	19	0.62
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	19	0.62
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	19	0.62
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	19	0.62
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	19	0.62
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	19	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	19	0.62
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	19	0.62
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	19	0.62
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	19	0.62
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	10	0.62
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	1	0.62
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	6	0.62
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	6	0.62
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	6	0.62
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG21	20	0.62
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG22	20	0.62
(1,39)	1:50:A:ILE:HG21	1:77:A:ILE:HG23	20	0.62
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG21	20	0.62
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG22	20	0.62
(1,39)	1:50:A:ILE:HG22	1:77:A:ILE:HG23	20	0.62
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG21	20	0.62
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG22	20	0.62
(1,39)	1:50:A:ILE:HG23	1:77:A:ILE:HG23	20	0.62
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	14	0.61
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	20	0.61
(2,6)	1:5:A:VAL:O	1:30:A:ILE:N	20	0.61
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	1	0.61
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	1	0.61
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	1	0.61
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	1	0.61
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	1	0.61
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	1	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	6	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	6	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	6	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	6	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	6	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	6	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	6	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	6	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	6	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	6	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	6	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	6	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	14	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	14	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	14	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	14	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	14	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	14	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	14	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	14	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	14	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	14	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	14	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	14	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	15	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	15	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	15	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	15	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	15	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	15	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	15	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	15	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	15	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	15	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	15	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	15	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	18	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	18	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	18	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	18	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	18	0.61
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	18	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	18	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	18	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	18	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	18	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	18	0.61
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	18	0.61
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	10	0.61
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	10	0.61
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	10	0.61
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	10	0.61
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	10	0.61
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	10	0.61
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	6	0.61
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	11	0.61
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	9	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	10	0.61
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG2	2	0.61
(1,56)	1:10:A:ASP:H	1:56:A:MET:HG3	2	0.61
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	14	0.6
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	16	0.6
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	16	0.6
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	8	0.6
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	8	0.6
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	8	0.6
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	8	0.6
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	8	0.6
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	8	0.6
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	7	0.6
(1,70)	1:83:A:THR:H	1:105:A:LYS:H	3	0.6
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	14	0.6
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	14	0.6
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	11	0.6
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	11	0.6
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	11	0.6
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	2	0.59
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	11	0.59
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	11	0.59
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	11	0.59
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	11	0.59
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	11	0.59
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	11	0.59
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	11	0.59
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	11	0.59
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	11	0.59
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	11	0.59
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	11	0.59
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	11	0.59
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	9	0.59
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	9	0.59
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	9	0.59
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	9	0.59
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	9	0.59
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	9	0.59
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	9	0.59
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	9	0.59
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	9	0.59
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	9	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	9	0.59
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	9	0.59
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	9	0.59
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	9	0.59
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	9	0.59
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	9	0.59
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	9	0.59
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	9	0.59
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	9	0.59
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	9	0.59
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	17	0.59
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	4	0.59
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	11	0.59
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	14	0.59
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	1	0.59
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	2	0.59
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	5	0.59
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	9	0.59
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	20	0.59
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	1	0.59
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	1	0.59
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	10	0.59
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	3	0.59
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	3	0.59
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	12	0.59
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	14	0.59
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	14	0.59
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	14	0.59
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	14	0.59
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	14	0.59
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	14	0.59
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	14	0.59
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	14	0.59
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	14	0.59
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	14	0.59
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	14	0.59
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	14	0.59
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	14	0.59
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	14	0.59
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	14	0.59
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	14	0.59
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	14	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	14	0.59
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	19	0.59
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	19	0.59
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	19	0.59
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	12	0.58
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	18	0.58
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	7	0.58
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	4	0.58
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	3	0.58
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	3	0.58
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	11	0.58
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	10	0.58
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	1	0.58
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	4	0.58
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	17	0.58
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	13	0.58
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	13	0.58
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	13	0.58
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	13	0.58
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	13	0.58
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	17	0.57
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	2	0.57
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	15	0.57
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	9	0.57
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	2	0.57
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	14	0.57
(2,58)	1:21:A:ASN:O	1:25:A:GLU:N	7	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	8	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	8	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	8	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	8	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	8	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	8	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	8	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	8	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	8	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	8	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	8	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	8	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	16	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	16	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	16	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	16	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	16	0.57
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	16	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	16	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	16	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	16	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	16	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	16	0.57
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	16	0.57
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	17	0.57
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	17	0.57
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	17	0.57
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	17	0.57
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	17	0.57
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	17	0.57
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	17	0.57
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	17	0.57
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	17	0.57
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	17	0.57
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	17	0.57
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	17	0.57
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	17	0.57
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	17	0.57
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	17	0.57
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	17	0.57
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	17	0.57
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	17	0.57
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	8	0.57
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	14	0.57
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	19	0.57
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	14	0.57
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	5	0.57
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	17	0.57
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	3	0.57
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	3	0.57
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	3	0.57
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	3	0.57
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	3	0.57
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	3	0.57
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	3	0.57
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	3	0.57
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	3	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	3	0.57
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	3	0.57
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	3	0.57
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	3	0.57
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	3	0.57
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	3	0.57
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	3	0.57
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	3	0.57
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	3	0.57
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	1	0.57
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	1	0.57
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	1	0.57
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	1	0.57
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	1	0.57
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	1	0.57
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	10	0.57
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	10	0.57
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	10	0.57
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	19	0.56
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	2	0.56
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	18	0.56
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	1	0.56
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	14	0.56
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	14	0.56
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	4	0.56
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	13	0.56
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	15	0.56
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	15	0.56
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	15	0.56
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	1	0.55
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	4	0.55
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	6	0.55
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	6	0.55
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	6	0.55
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	6	0.55
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	6	0.55
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	6	0.55
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	3	0.55
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	3	0.55
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	3	0.55
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	3	0.55
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	3	0.55
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	3	0.55
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	3	0.55
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	3	0.55
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	3	0.55
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	3	0.55
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	3	0.55
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	4	0.55
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	17	0.55
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	10	0.55
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	2	0.55
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	1	0.55
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	16	0.55
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	16	0.55
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	2	0.55
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	15	0.55
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	15	0.55
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	15	0.55
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	15	0.55
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	15	0.55
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	15	0.55
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	4	0.54
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	9	0.54
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	15	0.54
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	1	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	4	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	4	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	4	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	4	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	4	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	4	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	4	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	4	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	4	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	4	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	4	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	4	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	17	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	17	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	17	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	17	0.54
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	17	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	17	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	17	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	17	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	17	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	17	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	17	0.54
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	17	0.54
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	4	0.54
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	18	0.54
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	10	0.54
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	3	0.54
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	5	0.53
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	13	0.53
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	1	0.53
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	5	0.53
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	16	0.53
(2,41)	1:13:A:VAL:O	1:17:A:ILE:H	20	0.53
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG11	12	0.53
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG12	12	0.53
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG13	12	0.53
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG21	12	0.53
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG22	12	0.53
(1,306)	1:95:A:LEU:HB2	1:102:A:VAL:HG23	12	0.53
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG11	12	0.53
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG12	12	0.53
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG13	12	0.53
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG21	12	0.53
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG22	12	0.53
(1,306)	1:95:A:LEU:HB3	1:102:A:VAL:HG23	12	0.53
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	8	0.53
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	8	0.53
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	8	0.53
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	8	0.53
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	8	0.53
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	8	0.53
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	4	0.53
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	11	0.53
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	5	0.53
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	2	0.53
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	18	0.53
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	18	0.53
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	18	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	7	0.53
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	7	0.53
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	7	0.53
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	7	0.53
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	7	0.53
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	7	0.53
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	7	0.53
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	7	0.53
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	7	0.53
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	7	0.53
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	7	0.53
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	7	0.53
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	7	0.53
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	7	0.53
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	7	0.53
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	7	0.53
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	7	0.53
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	7	0.53
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	14	0.53
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	14	0.53
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	14	0.53
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	7	0.53
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	7	0.53
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	7	0.53
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	7	0.53
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	7	0.53
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	7	0.53
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	5	0.52
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	5	0.52
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	17	0.52
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	12	0.52
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	20	0.52
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	20	0.52
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	1	0.52
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	1	0.52
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	1	0.52
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	10	0.52
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	10	0.52
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	10	0.52
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	10	0.52
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	10	0.52
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	6	0.51
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	15	0.51
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	14	0.51
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	14	0.51
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	12	0.51
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	8	0.51
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	2	0.51
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	20	0.51
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	1	0.51
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	1	0.51
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	1	0.51
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	1	0.51
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	1	0.51
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	1	0.51
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	1	0.51
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	1	0.51
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	1	0.51
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	1	0.51
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	1	0.51
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	1	0.51
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	1	0.51
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	1	0.51
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	1	0.51
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	1	0.51
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	1	0.51
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	1	0.51
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	17	0.51
(1,232)	1:63:A:THR:H	1:64:A:VAL:H	20	0.51
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	4	0.51
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	5	0.51
(1,212)	1:21:A:ASN:H	1:22:A:LEU:H	6	0.51
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	4	0.51
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	5	0.51
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	8	0.51
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	8	0.51
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	8	0.51
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	8	0.51
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	8	0.51
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	8	0.51
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	8	0.51
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	4	0.5
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	20	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,67)	1:38:A:ALA:O	1:42:A:LEU:H	20	0.5
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	15	0.5
(2,47)	1:16:A:LYS:O	1:20:A:PHE:H	6	0.5
(2,12)	1:7:A:LEU:N	1:30:A:ILE:O	7	0.5
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	19	0.5
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	7	0.5
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	7	0.5
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	12	0.5
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	14	0.5
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	18	0.5
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	8	0.5
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	6	0.5
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	15	0.5
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	3	0.5
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	12	0.5
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	12	0.5
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	12	0.5
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	2	0.5
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	2	0.5
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	2	0.5
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	2	0.5
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	2	0.5
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	2	0.5
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	2	0.5
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	2	0.5
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	2	0.5
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	2	0.5
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	2	0.5
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	2	0.5
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	2	0.5
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	2	0.5
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	2	0.5
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	2	0.5
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	2	0.5
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	2	0.5
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	18	0.5
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	18	0.5
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	18	0.5
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	18	0.5
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	18	0.5
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	18	0.5
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	16	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	16	0.5
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	16	0.5
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	8	0.49
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	15	0.49
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	14	0.49
(2,42)	1:13:A:VAL:O	1:17:A:ILE:N	20	0.49
(2,5)	1:5:A:VAL:O	1:30:A:ILE:H	17	0.49
(1,308)	1:95:A:LEU:HD11	1:101:A:LYS:H	3	0.49
(1,308)	1:95:A:LEU:HD12	1:101:A:LYS:H	3	0.49
(1,308)	1:95:A:LEU:HD13	1:101:A:LYS:H	3	0.49
(1,308)	1:95:A:LEU:HD21	1:101:A:LYS:H	3	0.49
(1,308)	1:95:A:LEU:HD22	1:101:A:LYS:H	3	0.49
(1,308)	1:95:A:LEU:HD23	1:101:A:LYS:H	3	0.49
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	4	0.49
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	4	0.49
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	4	0.49
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	4	0.49
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	4	0.49
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	4	0.49
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	14	0.49
(1,265)	1:4:A:LYS:H	1:48:A:ASP:H	18	0.49
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	3	0.49
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	19	0.49
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	12	0.49
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	5	0.49
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	20	0.49
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	9	0.49
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	2	0.49
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	16	0.49
(1,70)	1:83:A:THR:H	1:105:A:LYS:H	4	0.49
(1,61)	1:71:A:LYS:HG2	1:74:A:TRP:H	17	0.49
(1,61)	1:71:A:LYS:HG3	1:74:A:TRP:H	17	0.49
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	4	0.48
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	8	0.48
(2,81)	1:65:A:LEU:O	1:69:A:GLN:H	7	0.48
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	7	0.48
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	17	0.48
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	2	0.48
(2,37)	1:83:A:THR:H	1:103:A:MET:O	10	0.48
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	4	0.48
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	15	0.48
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	15	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	15	0.48
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	15	0.48
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	18	0.48
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	18	0.48
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	18	0.48
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	18	0.48
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	18	0.48
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	18	0.48
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	18	0.48
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	18	0.48
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	18	0.48
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	18	0.48
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	18	0.48
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	18	0.48
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	18	0.48
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	18	0.48
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	18	0.48
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	18	0.48
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	18	0.48
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	18	0.48
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	10	0.48
(1,227)	1:54:A:ILE:H	1:55:A:MET:H	15	0.48
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	12	0.48
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	7	0.48
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	17	0.48
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	11	0.48
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	4	0.48
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	13	0.48
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	9	0.48
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	3	0.48
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	19	0.48
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	19	0.48
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	19	0.48
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	16	0.48
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	16	0.48
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	16	0.48
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	17	0.48
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	6	0.47
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	9	0.47
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	9	0.47
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	6	0.47
(2,40)	1:12:A:ALA:O	1:16:A:LYS:N	6	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,39)	1:12:A:ALA:O	1:16:A:LYS:H	6	0.47
(2,32)	1:79:A:VAL:O	1:100:A:ARG:N	18	0.47
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	5	0.47
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	17	0.47
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	17	0.47
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	6	0.47
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	4	0.47
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	18	0.47
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	13	0.47
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	14	0.47
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	4	0.47
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	4	0.47
(1,13)	1:54:A:ILE:HD11	1:94:A:ALA:HB1	18	0.47
(1,13)	1:54:A:ILE:HD11	1:94:A:ALA:HB2	18	0.47
(1,13)	1:54:A:ILE:HD11	1:94:A:ALA:HB3	18	0.47
(1,13)	1:54:A:ILE:HD12	1:94:A:ALA:HB1	18	0.47
(1,13)	1:54:A:ILE:HD12	1:94:A:ALA:HB2	18	0.47
(1,13)	1:54:A:ILE:HD12	1:94:A:ALA:HB3	18	0.47
(1,13)	1:54:A:ILE:HD13	1:94:A:ALA:HB1	18	0.47
(1,13)	1:54:A:ILE:HD13	1:94:A:ALA:HB2	18	0.47
(1,13)	1:54:A:ILE:HD13	1:94:A:ALA:HB3	18	0.47
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	15	0.47
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	15	0.47
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	15	0.47
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	15	0.47
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	15	0.47
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	15	0.47
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	3	0.47
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	3	0.47
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	3	0.47
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	3	0.47
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	3	0.47
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	3	0.47
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	11	0.47
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	11	0.47
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	11	0.47
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	11	0.47
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	11	0.47
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	11	0.47
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	16	0.46
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	9	0.46
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	1	0.46
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	1	0.46
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	13	0.46
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	13	0.46
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	13	0.46
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	13	0.46
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	13	0.46
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	13	0.46
(1,269)	1:5:A:VAL:H	1:30:A:ILE:H	20	0.46
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	12	0.46
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	16	0.46
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	17	0.46
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	12	0.46
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	13	0.46
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	10	0.46
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	18	0.46
(1,59)	1:71:A:LYS:HG2	1:73:A:GLU:H	17	0.46
(1,59)	1:71:A:LYS:HG3	1:73:A:GLU:H	17	0.46
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	2	0.46
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	2	0.46
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	2	0.46
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	5	0.46
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	5	0.46
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	5	0.46
(1,8)	1:37:A:ILE:HG21	1:41:A:LYS:HE2	7	0.46
(1,8)	1:37:A:ILE:HG22	1:41:A:LYS:HE2	7	0.46
(1,8)	1:37:A:ILE:HG23	1:41:A:LYS:HE2	7	0.46
(1,8)	1:37:A:ILE:HG21	1:41:A:LYS:HE3	7	0.46
(1,8)	1:37:A:ILE:HG22	1:41:A:LYS:HE3	7	0.46
(1,8)	1:37:A:ILE:HG23	1:41:A:LYS:HE3	7	0.46
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	15	0.46
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	15	0.46
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	15	0.46
(2,96)	1:95:A:LEU:O	1:98:A:GLY:N	12	0.45
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	2	0.45
(2,75)	1:62:A:PHE:O	1:66:A:LYS:H	9	0.45
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	18	0.45
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	7	0.45
(2,5)	1:5:A:VAL:O	1:30:A:ILE:H	9	0.45
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	15	0.45
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	15	0.45
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	15	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	15	0.45
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	15	0.45
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	15	0.45
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB2	10	0.45
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB3	10	0.45
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB2	10	0.45
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB3	10	0.45
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	19	0.45
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	9	0.45
(1,158)	1:37:A:ILE:HA	1:40:A:GLU:H	20	0.45
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	6	0.45
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	7	0.45
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	16	0.45
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	19	0.45
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	17	0.45
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	9	0.45
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	9	0.45
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	18	0.45
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	18	0.45
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	18	0.45
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	12	0.45
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	12	0.45
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	12	0.45
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	12	0.45
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	12	0.45
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	12	0.45
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	16	0.44
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	18	0.44
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	2	0.44
(2,6)	1:5:A:VAL:O	1:30:A:ILE:N	9	0.44
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD11	6	0.44
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD12	6	0.44
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD13	6	0.44
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD21	6	0.44
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD22	6	0.44
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD23	6	0.44
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD11	6	0.44
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD12	6	0.44
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD13	6	0.44
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD21	6	0.44
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD22	6	0.44
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD23	6	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD11	6	0.44
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD12	6	0.44
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD13	6	0.44
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD21	6	0.44
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD22	6	0.44
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD23	6	0.44
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD11	6	0.44
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD12	6	0.44
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD13	6	0.44
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD21	6	0.44
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD22	6	0.44
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD23	6	0.44
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD11	6	0.44
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD12	6	0.44
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD13	6	0.44
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD21	6	0.44
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD22	6	0.44
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD23	6	0.44
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD11	6	0.44
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD12	6	0.44
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD13	6	0.44
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD21	6	0.44
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD22	6	0.44
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD23	6	0.44
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	13	0.44
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	6	0.44
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	18	0.44
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	7	0.44
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	9	0.44
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	12	0.44
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	18	0.44
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	17	0.44
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	6	0.44
(1,70)	1:83:A:THR:H	1:105:A:LYS:H	5	0.44
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	17	0.44
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	18	0.44
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	18	0.44
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	17	0.43
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	5	0.43
(2,58)	1:21:A:ASN:O	1:25:A:GLU:N	19	0.43
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	16	0.43
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	16	0.43
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	16	0.43
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	16	0.43
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	16	0.43
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	16	0.43
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	16	0.43
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	16	0.43
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	16	0.43
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	16	0.43
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	16	0.43
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	16	0.43
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	16	0.43
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	16	0.43
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	16	0.43
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	16	0.43
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	16	0.43
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	16	0.43
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	16	0.43
(1,294)	1:49:A:LEU:HD11	1:80:A:ILE:H	10	0.43
(1,294)	1:49:A:LEU:HD12	1:80:A:ILE:H	10	0.43
(1,294)	1:49:A:LEU:HD13	1:80:A:ILE:H	10	0.43
(1,294)	1:49:A:LEU:HD21	1:80:A:ILE:H	10	0.43
(1,294)	1:49:A:LEU:HD22	1:80:A:ILE:H	10	0.43
(1,294)	1:49:A:LEU:HD23	1:80:A:ILE:H	10	0.43
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD11	13	0.43
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD12	13	0.43
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD13	13	0.43
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD11	13	0.43
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD12	13	0.43
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD13	13	0.43
(1,285)	1:22:A:LEU:HD11	1:116:A:VAL:HB	20	0.43
(1,285)	1:22:A:LEU:HD12	1:116:A:VAL:HB	20	0.43
(1,285)	1:22:A:LEU:HD13	1:116:A:VAL:HB	20	0.43
(1,285)	1:22:A:LEU:HD21	1:116:A:VAL:HB	20	0.43
(1,285)	1:22:A:LEU:HD22	1:116:A:VAL:HB	20	0.43
(1,285)	1:22:A:LEU:HD23	1:116:A:VAL:HB	20	0.43
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	16	0.43
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	16	0.43
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	16	0.43
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	16	0.43
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	16	0.43
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	16	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	19	0.43
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	15	0.43
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	2	0.43
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	17	0.43
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	19	0.43
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	2	0.43
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	11	0.43
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	15	0.43
(1,70)	1:83:A:THR:H	1:105:A:LYS:H	17	0.43
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	3	0.43
(1,59)	1:71:A:LYS:HG2	1:73:A:GLU:H	13	0.43
(1,59)	1:71:A:LYS:HG3	1:73:A:GLU:H	13	0.43
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	11	0.43
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	11	0.43
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	11	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	6	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	6	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	6	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	6	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	6	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	6	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	7	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	7	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	7	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	7	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	7	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	7	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	19	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	19	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	19	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	19	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	19	0.43
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	19	0.43
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	7	0.43
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	7	0.43
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	7	0.43
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	1	0.43
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	6	0.43
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	6	0.43
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	6	0.43
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	17	0.42
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	7	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	10	0.42
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	5	0.42
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	16	0.42
(2,27)	1:52:A:LEU:H	1:80:A:ILE:O	4	0.42
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	17	0.42
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	6	0.42
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	7	0.42
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	11	0.42
(1,225)	1:43:A:SER:H	1:44:A:GLU:H	10	0.42
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	8	0.42
(1,212)	1:21:A:ASN:H	1:22:A:LEU:H	1	0.42
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	7	0.42
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	3	0.42
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	19	0.42
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	5	0.42
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	6	0.42
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	12	0.42
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	1	0.42
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	3	0.42
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	1	0.42
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	7	0.42
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	7	0.42
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	19	0.42
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	19	0.42
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	19	0.42
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	7	0.41
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	20	0.41
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	11	0.41
(2,93)	1:92:A:SER:O	1:96:A:SER:H	9	0.41
(2,93)	1:92:A:SER:O	1:96:A:SER:H	14	0.41
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	17	0.41
(2,56)	1:20:A:PHE:O	1:24:A:LYS:N	14	0.41
(2,48)	1:16:A:LYS:O	1:20:A:PHE:N	6	0.41
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	20	0.41
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	3	0.41
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	5	0.41
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	2	0.41
(1,201)	1:95:A:LEU:HA	1:98:A:GLY:H	13	0.41
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	2	0.41
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	10	0.41
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	3	0.41
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	4	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	11	0.41
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	17	0.41
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	17	0.41
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	17	0.41
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	5	0.41
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	5	0.41
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE1	9	0.41
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE1	9	0.41
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE1	9	0.41
(1,4)	1:30:A:ILE:HD11	1:45:A:PHE:HE2	9	0.41
(1,4)	1:30:A:ILE:HD12	1:45:A:PHE:HE2	9	0.41
(1,4)	1:30:A:ILE:HD13	1:45:A:PHE:HE2	9	0.41
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	9	0.4
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	17	0.4
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	12	0.4
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	10	0.4
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	20	0.4
(2,76)	1:62:A:PHE:O	1:66:A:LYS:N	9	0.4
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	13	0.4
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	18	0.4
(2,47)	1:16:A:LYS:O	1:20:A:PHE:H	13	0.4
(2,6)	1:5:A:VAL:O	1:30:A:ILE:N	17	0.4
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	14	0.4
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	14	0.4
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	14	0.4
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	14	0.4
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	14	0.4
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	14	0.4
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	15	0.4
(1,258)	1:114:A:GLU:H	1:115:A:GLU:H	20	0.4
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	10	0.4
(1,238)	1:69:A:GLN:H	1:70:A:GLU:H	16	0.4
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	13	0.4
(1,228)	1:58:A:VAL:H	1:59:A:MET:H	16	0.4
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	5	0.4
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	7	0.4
(1,122)	1:52:A:LEU:H	1:81:A:VAL:HA	12	0.4
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	2	0.4
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	18	0.4
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	11	0.4
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	13	0.4
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	19	0.4
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	16	0.4
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	16	0.4
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	16	0.4
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	16	0.4
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	16	0.4
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	16	0.4
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	16	0.4
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	16	0.4
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	16	0.4
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	16	0.4
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	16	0.4
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	16	0.4
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	16	0.4
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	16	0.4
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	16	0.4
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	16	0.4
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	16	0.4
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	16	0.4
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	13	0.4
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	13	0.4
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	13	0.4
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	20	0.39
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	7	0.39
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	6	0.39
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	20	0.39
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	11	0.39
(2,32)	1:79:A:VAL:O	1:100:A:ARG:N	1	0.39
(2,29)	1:52:A:LEU:O	1:82:A:LEU:H	2	0.39
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	4	0.39
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	4	0.39
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	4	0.39
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	4	0.39
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	4	0.39
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	4	0.39
(1,297)	1:51:A:VAL:HG11	1:80:A:ILE:H	9	0.39
(1,297)	1:51:A:VAL:HG12	1:80:A:ILE:H	9	0.39
(1,297)	1:51:A:VAL:HG13	1:80:A:ILE:H	9	0.39
(1,297)	1:51:A:VAL:HG21	1:80:A:ILE:H	9	0.39
(1,297)	1:51:A:VAL:HG22	1:80:A:ILE:H	9	0.39
(1,297)	1:51:A:VAL:HG23	1:80:A:ILE:H	9	0.39
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	17	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	13	0.39
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	13	0.39
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	16	0.39
(1,208)	1:17:A:ILE:H	1:18:A:VAL:H	2	0.39
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	14	0.39
(1,160)	1:39:A:LEU:HA	1:42:A:LEU:H	10	0.39
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	16	0.39
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	8	0.39
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	9	0.39
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	14	0.39
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	14	0.39
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	14	0.39
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	14	0.39
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	11	0.38
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	12	0.38
(2,96)	1:95:A:LEU:O	1:98:A:GLY:N	13	0.38
(2,85)	1:88:A:GLU:O	1:92:A:SER:H	18	0.38
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	10	0.38
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	1	0.38
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	18	0.38
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	16	0.38
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	4	0.38
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	12	0.38
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD11	5	0.38
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD12	5	0.38
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD13	5	0.38
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD21	5	0.38
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD22	5	0.38
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD23	5	0.38
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD11	5	0.38
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD12	5	0.38
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD13	5	0.38
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD21	5	0.38
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD22	5	0.38
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD23	5	0.38
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD11	5	0.38
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD12	5	0.38
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD13	5	0.38
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD21	5	0.38
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD22	5	0.38
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD23	5	0.38
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD11	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD12	5	0.38
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD13	5	0.38
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD21	5	0.38
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD22	5	0.38
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD23	5	0.38
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD11	5	0.38
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD12	5	0.38
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD13	5	0.38
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD21	5	0.38
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD22	5	0.38
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD23	5	0.38
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD11	5	0.38
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD12	5	0.38
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD13	5	0.38
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD21	5	0.38
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD22	5	0.38
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD23	5	0.38
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	13	0.38
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	16	0.38
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	2	0.38
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	2	0.38
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	9	0.38
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	14	0.38
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	6	0.38
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	12	0.38
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	12	0.38
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	5	0.38
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	5	0.38
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	5	0.38
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	12	0.38
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	12	0.38
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	12	0.38
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	19	0.37
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	5	0.37
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	4	0.37
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	16	0.37
(2,93)	1:92:A:SER:O	1:96:A:SER:H	5	0.37
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	1	0.37
(2,65)	1:37:A:ILE:O	1:41:A:LYS:H	20	0.37
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	19	0.37
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	8	0.37
(2,28)	1:52:A:LEU:N	1:80:A:ILE:O	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	20	0.37
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB1	18	0.37
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB2	18	0.37
(1,299)	1:52:A:LEU:HD11	1:94:A:ALA:HB3	18	0.37
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB1	18	0.37
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB2	18	0.37
(1,299)	1:52:A:LEU:HD12	1:94:A:ALA:HB3	18	0.37
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB1	18	0.37
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB2	18	0.37
(1,299)	1:52:A:LEU:HD13	1:94:A:ALA:HB3	18	0.37
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB1	18	0.37
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB2	18	0.37
(1,299)	1:52:A:LEU:HD21	1:94:A:ALA:HB3	18	0.37
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB1	18	0.37
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB2	18	0.37
(1,299)	1:52:A:LEU:HD22	1:94:A:ALA:HB3	18	0.37
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB1	18	0.37
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB2	18	0.37
(1,299)	1:52:A:LEU:HD23	1:94:A:ALA:HB3	18	0.37
(1,277)	1:83:A:THR:H	1:103:A:MET:H	10	0.37
(1,274)	1:52:A:LEU:H	1:80:A:ILE:H	5	0.37
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	7	0.37
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	8	0.37
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	8	0.37
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	3	0.37
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	18	0.37
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	13	0.37
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	13	0.37
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	14	0.37
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	17	0.37
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	11	0.37
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	13	0.37
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	7	0.37
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	20	0.37
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	10	0.37
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	10	0.37
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	10	0.37
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	10	0.36
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	14	0.36
(2,93)	1:92:A:SER:O	1:96:A:SER:H	7	0.36
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	6	0.36
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	13	0.36
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	9	0.36
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	13	0.36
(2,10)	1:6:A:LEU:O	1:51:A:VAL:N	7	0.36
(2,5)	1:5:A:VAL:O	1:30:A:ILE:H	18	0.36
(1,294)	1:49:A:LEU:HD11	1:80:A:ILE:H	7	0.36
(1,294)	1:49:A:LEU:HD12	1:80:A:ILE:H	7	0.36
(1,294)	1:49:A:LEU:HD13	1:80:A:ILE:H	7	0.36
(1,294)	1:49:A:LEU:HD21	1:80:A:ILE:H	7	0.36
(1,294)	1:49:A:LEU:HD22	1:80:A:ILE:H	7	0.36
(1,294)	1:49:A:LEU:HD23	1:80:A:ILE:H	7	0.36
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD11	12	0.36
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD12	12	0.36
(1,293)	1:47:A:PRO:HD2	1:77:A:ILE:HD13	12	0.36
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD11	12	0.36
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD12	12	0.36
(1,293)	1:47:A:PRO:HD3	1:77:A:ILE:HD13	12	0.36
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	18	0.36
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	18	0.36
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	20	0.36
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	10	0.36
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	8	0.36
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	8	0.36
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	16	0.36
(1,158)	1:37:A:ILE:HA	1:40:A:GLU:H	2	0.36
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	8	0.36
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	15	0.36
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	16	0.36
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	2	0.36
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	6	0.36
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	9	0.36
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	9	0.36
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	9	0.36
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	9	0.36
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	9	0.36
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	9	0.36
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	9	0.36
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	9	0.36
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	9	0.36
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	9	0.36
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	9	0.36
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	9	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	9	0.36
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	9	0.36
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	9	0.36
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	9	0.36
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	9	0.36
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	9	0.36
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	5	0.36
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD11	16	0.36
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD12	16	0.36
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD13	16	0.36
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD11	16	0.36
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD12	16	0.36
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD13	16	0.36
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD11	16	0.36
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD12	16	0.36
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD13	16	0.36
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	20	0.35
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	17	0.35
(2,86)	1:88:A:GLU:O	1:92:A:SER:N	18	0.35
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	17	0.35
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	17	0.35
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	18	0.35
(2,9)	1:6:A:LEU:O	1:51:A:VAL:H	7	0.35
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	2	0.35
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	2	0.35
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	2	0.35
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	2	0.35
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	2	0.35
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	2	0.35
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	10	0.35
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	10	0.35
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	10	0.35
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	10	0.35
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	10	0.35
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	10	0.35
(1,268)	1:5:A:VAL:H	1:28:A:GLU:H	9	0.35
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	2	0.35
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	9	0.35
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	8	0.35
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	13	0.35
(1,170)	1:69:A:GLN:HA	1:70:A:GLU:H	3	0.35
(1,162)	1:41:A:LYS:HA	1:44:A:GLU:H	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	9	0.35
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	18	0.35
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	20	0.35
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	10	0.35
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	7	0.35
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	15	0.35
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	7	0.35
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	4	0.35
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	7	0.35
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	12	0.35
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	15	0.35
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	15	0.35
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	15	0.35
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE1	17	0.35
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE2	17	0.35
(1,41)	1:35:A:GLY:HA3	1:56:A:MET:HE3	17	0.35
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	10	0.35
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	10	0.35
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	10	0.35
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG2	17	0.35
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG2	17	0.35
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG2	17	0.35
(1,35)	1:80:A:ILE:HD11	1:115:A:GLU:HG3	17	0.35
(1,35)	1:80:A:ILE:HD12	1:115:A:GLU:HG3	17	0.35
(1,35)	1:80:A:ILE:HD13	1:115:A:GLU:HG3	17	0.35
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	8	0.35
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	8	0.35
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	8	0.35
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	15	0.35
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	15	0.35
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	15	0.35
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	17	0.35
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	17	0.35
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	17	0.35
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	1	0.34
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	2	0.34
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	7	0.34
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	19	0.34
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	17	0.34
(2,94)	1:92:A:SER:O	1:96:A:SER:N	14	0.34
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	2	0.34
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	13	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	8	0.34
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	11	0.34
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	10	0.34
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	3	0.34
(1,308)	1:95:A:LEU:HD11	1:101:A:LYS:H	19	0.34
(1,308)	1:95:A:LEU:HD12	1:101:A:LYS:H	19	0.34
(1,308)	1:95:A:LEU:HD13	1:101:A:LYS:H	19	0.34
(1,308)	1:95:A:LEU:HD21	1:101:A:LYS:H	19	0.34
(1,308)	1:95:A:LEU:HD22	1:101:A:LYS:H	19	0.34
(1,308)	1:95:A:LEU:HD23	1:101:A:LYS:H	19	0.34
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	17	0.34
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	17	0.34
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	17	0.34
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	17	0.34
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	17	0.34
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	17	0.34
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	18	0.34
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	18	0.34
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	18	0.34
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	18	0.34
(1,255)	1:111:A:GLN:H	1:112:A:PHE:H	6	0.34
(1,253)	1:100:A:ARG:H	1:101:A:LYS:H	1	0.34
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	11	0.34
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	4	0.34
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	7	0.34
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	7	0.34
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	20	0.34
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	16	0.34
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	16	0.34
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	7	0.34
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	1	0.34
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	7	0.34
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	9	0.34
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	9	0.34
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	9	0.34
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	4	0.34
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	4	0.34
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	4	0.34
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	16	0.34
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	16	0.34
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	16	0.34
(1,20)	1:42:A:LEU:HG	1:47:A:PRO:HD2	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	19	0.33
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	2	0.33
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	16	0.33
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	17	0.33
(2,93)	1:92:A:SER:O	1:96:A:SER:H	16	0.33
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	8	0.33
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	1	0.33
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	2	0.33
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	2	0.33
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	7	0.33
(2,30)	1:52:A:LEU:O	1:82:A:LEU:N	2	0.33
(1,308)	1:95:A:LEU:HD11	1:101:A:LYS:H	16	0.33
(1,308)	1:95:A:LEU:HD12	1:101:A:LYS:H	16	0.33
(1,308)	1:95:A:LEU:HD13	1:101:A:LYS:H	16	0.33
(1,308)	1:95:A:LEU:HD21	1:101:A:LYS:H	16	0.33
(1,308)	1:95:A:LEU:HD22	1:101:A:LYS:H	16	0.33
(1,308)	1:95:A:LEU:HD23	1:101:A:LYS:H	16	0.33
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	13	0.33
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	11	0.33
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	7	0.33
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	4	0.33
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	10	0.33
(1,160)	1:39:A:LEU:HA	1:42:A:LEU:H	17	0.33
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	4	0.33
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	8	0.33
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	3	0.33
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	13	0.33
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	11	0.33
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	3	0.33
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	3	0.33
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	3	0.33
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	9	0.32
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	15	0.32
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	19	0.32
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	19	0.32
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	14	0.32
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	7	0.32
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	12	0.32
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	17	0.32
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	4	0.32
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	9	0.32
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	9	0.32
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	16	0.32
(2,6)	1:5:A:VAL:O	1:30:A:ILE:N	18	0.32
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	16	0.32
(1,308)	1:95:A:LEU:HD11	1:101:A:LYS:H	7	0.32
(1,308)	1:95:A:LEU:HD12	1:101:A:LYS:H	7	0.32
(1,308)	1:95:A:LEU:HD13	1:101:A:LYS:H	7	0.32
(1,308)	1:95:A:LEU:HD21	1:101:A:LYS:H	7	0.32
(1,308)	1:95:A:LEU:HD22	1:101:A:LYS:H	7	0.32
(1,308)	1:95:A:LEU:HD23	1:101:A:LYS:H	7	0.32
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	13	0.32
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	13	0.32
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	13	0.32
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	13	0.32
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	5	0.32
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	5	0.32
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB2	17	0.32
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB3	17	0.32
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB2	17	0.32
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB3	17	0.32
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	3	0.32
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	18	0.32
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	13	0.32
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	20	0.32
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	14	0.32
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	16	0.32
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	20	0.32
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	19	0.32
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	6	0.32
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	20	0.32
(1,122)	1:52:A:LEU:H	1:81:A:VAL:HA	9	0.32
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	12	0.32
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	12	0.32
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	8	0.32
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	8	0.32
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	7	0.32
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	7	0.32
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	7	0.32
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE1	19	0.32
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE2	19	0.32
(1,45)	1:34:A:ASN:HA	1:56:A:MET:HE3	19	0.32
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	18	0.32
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	18	0.32
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD11	20	0.32
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD12	20	0.32
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD13	20	0.32
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD11	20	0.32
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD12	20	0.32
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD13	20	0.32
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD11	20	0.32
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD12	20	0.32
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD13	20	0.32
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	4	0.31
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	5	0.31
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	11	0.31
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	18	0.31
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	18	0.31
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	8	0.31
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	7	0.31
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	19	0.31
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	15	0.31
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	13	0.31
(2,29)	1:52:A:LEU:O	1:82:A:LEU:H	7	0.31
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	19	0.31
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	13	0.31
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	17	0.31
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	9	0.31
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	17	0.31
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	17	0.31
(1,221)	1:39:A:LEU:H	1:40:A:GLU:H	17	0.31
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	11	0.31
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	4	0.31
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	12	0.31
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	12	0.31
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	9	0.31
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	14	0.31
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	13	0.31
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	12	0.31
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	10	0.31
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	5	0.31
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	3	0.31
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE1	7	0.31
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE2	7	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:35:A:GLY:H	1:56:A:MET:HE3	7	0.31
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	19	0.31
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	19	0.31
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	19	0.31
(2,94)	1:92:A:SER:O	1:96:A:SER:N	16	0.3
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	1	0.3
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	15	0.3
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	1	0.3
(2,82)	1:65:A:LEU:O	1:69:A:GLN:N	7	0.3
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	2	0.3
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	17	0.3
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	15	0.3
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	13	0.3
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	3	0.3
(2,25)	1:50:A:ILE:O	1:80:A:ILE:H	16	0.3
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	7	0.3
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	3	0.3
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	17	0.3
(1,252)	1:97:A:LEU:H	1:98:A:GLY:H	11	0.3
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	9	0.3
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	15	0.3
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	18	0.3
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	15	0.3
(1,203)	1:12:A:ALA:H	1:13:A:VAL:H	10	0.3
(1,147)	1:37:A:ILE:HA	1:38:A:ALA:H	19	0.3
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	19	0.3
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	20	0.3
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	2	0.3
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	2	0.3
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	6	0.3
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	12	0.3
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	12	0.3
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	12	0.3
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	16	0.29
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	20	0.29
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	14	0.29
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	1	0.29
(2,94)	1:92:A:SER:O	1:96:A:SER:N	9	0.29
(2,93)	1:92:A:SER:O	1:96:A:SER:H	20	0.29
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	18	0.29
(2,79)	1:64:A:VAL:O	1:68:A:LEU:H	13	0.29
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,43)	1:14:A:LEU:O	1:18:A:VAL:H	7	0.29
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	14	0.29
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	16	0.29
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	15	0.29
(1,288)	1:39:A:LEU:HD11	1:74:A:TRP:HB2	17	0.29
(1,288)	1:39:A:LEU:HD11	1:74:A:TRP:HB3	17	0.29
(1,288)	1:39:A:LEU:HD12	1:74:A:TRP:HB2	17	0.29
(1,288)	1:39:A:LEU:HD12	1:74:A:TRP:HB3	17	0.29
(1,288)	1:39:A:LEU:HD13	1:74:A:TRP:HB2	17	0.29
(1,288)	1:39:A:LEU:HD13	1:74:A:TRP:HB3	17	0.29
(1,288)	1:39:A:LEU:HD21	1:74:A:TRP:HB2	17	0.29
(1,288)	1:39:A:LEU:HD21	1:74:A:TRP:HB3	17	0.29
(1,288)	1:39:A:LEU:HD22	1:74:A:TRP:HB2	17	0.29
(1,288)	1:39:A:LEU:HD22	1:74:A:TRP:HB3	17	0.29
(1,288)	1:39:A:LEU:HD23	1:74:A:TRP:HB2	17	0.29
(1,288)	1:39:A:LEU:HD23	1:74:A:TRP:HB3	17	0.29
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	3	0.29
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	3	0.29
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	3	0.29
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	3	0.29
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	3	0.29
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	3	0.29
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	3	0.29
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	3	0.29
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	3	0.29
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	3	0.29
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	3	0.29
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	3	0.29
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	3	0.29
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	3	0.29
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	3	0.29
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	3	0.29
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	3	0.29
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	3	0.29
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	7	0.29
(1,266)	1:6:A:LEU:H	1:51:A:VAL:H	8	0.29
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	5	0.29
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	18	0.29
(1,258)	1:114:A:GLU:H	1:115:A:GLU:H	17	0.29
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	2	0.29
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	6	0.29
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	12	0.29
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	1	0.29
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	15	0.29
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	1	0.29
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	13	0.29
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	5	0.29
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	19	0.29
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	7	0.29
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	11	0.29
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	16	0.29
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	8	0.29
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	13	0.29
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	9	0.29
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	1	0.29
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	10	0.29
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	11	0.29
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	11	0.29
(1,107)	1:83:A:THR:HA	1:84:A:ALA:H	7	0.29
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	6	0.29
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	6	0.29
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	8	0.29
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	15	0.29
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	15	0.29
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	16	0.29
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	16	0.29
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	16	0.29
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	11	0.29
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	11	0.29
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	11	0.29
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	2	0.28
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	16	0.28
(2,112)	1:114:A:GLU:O	1:118:A:HIS:N	12	0.28
(2,104)	1:110:A:SER:O	1:114:A:GLU:N	11	0.28
(2,96)	1:95:A:LEU:O	1:98:A:GLY:N	5	0.28
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	3	0.28
(2,66)	1:37:A:ILE:O	1:41:A:LYS:N	20	0.28
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	12	0.28
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	12	0.28
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	6	0.28
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	1	0.28
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	1	0.28
(2,39)	1:12:A:ALA:O	1:16:A:LYS:H	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	13	0.28
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	7	0.28
(2,25)	1:50:A:ILE:O	1:80:A:ILE:H	20	0.28
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	19	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD11	15	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD12	15	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD13	15	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD21	15	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD22	15	0.28
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD23	15	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD11	15	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD12	15	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD13	15	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD21	15	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD22	15	0.28
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD23	15	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD11	15	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD12	15	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD13	15	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD21	15	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD22	15	0.28
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD23	15	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD11	15	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD12	15	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD13	15	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD21	15	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD22	15	0.28
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD23	15	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD11	15	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD12	15	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD13	15	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD21	15	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD22	15	0.28
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD23	15	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD11	15	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD12	15	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD13	15	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD21	15	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD22	15	0.28
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD23	15	0.28
(1,277)	1:83:A:THR:H	1:103:A:MET:H	15	0.28
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	8	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	12	0.28
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	2	0.28
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	12	0.28
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	18	0.28
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	14	0.28
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	17	0.28
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	13	0.28
(1,208)	1:17:A:ILE:H	1:18:A:VAL:H	14	0.28
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	19	0.28
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	8	0.28
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	8	0.28
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	16	0.28
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	14	0.28
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	15	0.28
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	19	0.28
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	15	0.28
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	18	0.28
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	20	0.28
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	18	0.28
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	14	0.28
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	14	0.28
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	2	0.28
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	11	0.28
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	11	0.28
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	11	0.28
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	19	0.28
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	19	0.28
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	19	0.28
(1,34)	1:80:A:ILE:HD11	1:116:A:VAL:HA	9	0.28
(1,34)	1:80:A:ILE:HD12	1:116:A:VAL:HA	9	0.28
(1,34)	1:80:A:ILE:HD13	1:116:A:VAL:HA	9	0.28
(1,19)	1:42:A:LEU:HB2	1:47:A:PRO:HD2	20	0.28
(1,19)	1:42:A:LEU:HB3	1:47:A:PRO:HD2	20	0.28
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	8	0.28
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	8	0.28
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	8	0.28
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	13	0.28
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	13	0.28
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	13	0.28
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG21	1	0.28
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG22	1	0.28
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG23	1	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	16	0.27
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	5	0.27
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	10	0.27
(2,103)	1:110:A:SER:O	1:114:A:GLU:H	11	0.27
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	16	0.27
(2,85)	1:88:A:GLU:O	1:92:A:SER:H	7	0.27
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	2	0.27
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	10	0.27
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	9	0.27
(2,37)	1:83:A:THR:H	1:103:A:MET:O	18	0.27
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	3	0.27
(2,26)	1:50:A:ILE:O	1:80:A:ILE:N	20	0.27
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	16	0.27
(2,3)	1:5:A:VAL:H	1:28:A:GLU:O	11	0.27
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	3	0.27
(1,264)	1:120:A:LEU:H	1:121:A:ASN:H	18	0.27
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	19	0.27
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	9	0.27
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	13	0.27
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	4	0.27
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	20	0.27
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	18	0.27
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	1	0.27
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	18	0.27
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	19	0.27
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	18	0.27
(1,209)	1:18:A:VAL:H	1:19:A:SER:H	11	0.27
(1,207)	1:16:A:LYS:H	1:17:A:ILE:H	9	0.27
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	10	0.27
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	8	0.27
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	17	0.27
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	8	0.27
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	17	0.27
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	8	0.27
(1,122)	1:52:A:LEU:H	1:81:A:VAL:HA	7	0.27
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	2	0.27
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	19	0.27
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	10	0.27
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	10	0.27
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	10	0.27
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	18	0.27
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	17	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	17	0.27
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	17	0.27
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	19	0.26
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	14	0.26
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	19	0.26
(2,112)	1:114:A:GLU:O	1:118:A:HIS:N	6	0.26
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	15	0.26
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	12	0.26
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	19	0.26
(2,103)	1:110:A:SER:O	1:114:A:GLU:H	17	0.26
(2,94)	1:92:A:SER:O	1:96:A:SER:N	20	0.26
(2,81)	1:65:A:LEU:O	1:69:A:GLN:H	12	0.26
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	8	0.26
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	2	0.26
(2,44)	1:14:A:LEU:O	1:18:A:VAL:N	7	0.26
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	14	0.26
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	19	0.26
(2,9)	1:6:A:LEU:O	1:51:A:VAL:H	18	0.26
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD11	7	0.26
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD12	7	0.26
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD13	7	0.26
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD21	7	0.26
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD22	7	0.26
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD23	7	0.26
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD11	7	0.26
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD12	7	0.26
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD13	7	0.26
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD21	7	0.26
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD22	7	0.26
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD23	7	0.26
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD11	7	0.26
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD12	7	0.26
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD13	7	0.26
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD21	7	0.26
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD22	7	0.26
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD23	7	0.26
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD11	7	0.26
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD12	7	0.26
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD13	7	0.26
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD21	7	0.26
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD22	7	0.26
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD23	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD11	7	0.26
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD12	7	0.26
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD13	7	0.26
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD21	7	0.26
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD22	7	0.26
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD23	7	0.26
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD11	7	0.26
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD12	7	0.26
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD13	7	0.26
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD21	7	0.26
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD22	7	0.26
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD23	7	0.26
(1,292)	1:47:A:PRO:HD2	1:74:A:TRP:HD1	7	0.26
(1,292)	1:47:A:PRO:HD3	1:74:A:TRP:HD1	7	0.26
(1,268)	1:5:A:VAL:H	1:28:A:GLU:H	10	0.26
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	15	0.26
(1,243)	1:88:A:GLU:H	1:89:A:GLU:H	6	0.26
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	15	0.26
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	9	0.26
(1,208)	1:17:A:ILE:H	1:18:A:VAL:H	19	0.26
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	18	0.26
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	14	0.26
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	18	0.26
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	1	0.26
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	11	0.26
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	11	0.26
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	6	0.26
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	14	0.26
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	11	0.26
(1,147)	1:37:A:ILE:HA	1:38:A:ALA:H	8	0.26
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	11	0.26
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	6	0.26
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	4	0.26
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	13	0.26
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	8	0.26
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	13	0.26
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	2	0.26
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	8	0.26
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	8	0.26
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	8	0.26
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	8	0.26
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	8	0.26
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	17	0.26
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	17	0.26
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	17	0.26
(1,15)	1:42:A:LEU:HD11	1:77:A:ILE:HD11	11	0.26
(1,15)	1:42:A:LEU:HD11	1:77:A:ILE:HD12	11	0.26
(1,15)	1:42:A:LEU:HD11	1:77:A:ILE:HD13	11	0.26
(1,15)	1:42:A:LEU:HD12	1:77:A:ILE:HD11	11	0.26
(1,15)	1:42:A:LEU:HD12	1:77:A:ILE:HD12	11	0.26
(1,15)	1:42:A:LEU:HD12	1:77:A:ILE:HD13	11	0.26
(1,15)	1:42:A:LEU:HD13	1:77:A:ILE:HD11	11	0.26
(1,15)	1:42:A:LEU:HD13	1:77:A:ILE:HD12	11	0.26
(1,15)	1:42:A:LEU:HD13	1:77:A:ILE:HD13	11	0.26
(1,15)	1:42:A:LEU:HD21	1:77:A:ILE:HD11	11	0.26
(1,15)	1:42:A:LEU:HD21	1:77:A:ILE:HD12	11	0.26
(1,15)	1:42:A:LEU:HD21	1:77:A:ILE:HD13	11	0.26
(1,15)	1:42:A:LEU:HD22	1:77:A:ILE:HD11	11	0.26
(1,15)	1:42:A:LEU:HD22	1:77:A:ILE:HD12	11	0.26
(1,15)	1:42:A:LEU:HD22	1:77:A:ILE:HD13	11	0.26
(1,15)	1:42:A:LEU:HD23	1:77:A:ILE:HD11	11	0.26
(1,15)	1:42:A:LEU:HD23	1:77:A:ILE:HD12	11	0.26
(1,15)	1:42:A:LEU:HD23	1:77:A:ILE:HD13	11	0.26
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	3	0.25
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	13	0.25
(2,107)	1:112:A:PHE:O	1:116:A:VAL:H	19	0.25
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	18	0.25
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	15	0.25
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	17	0.25
(2,86)	1:88:A:GLU:O	1:92:A:SER:N	7	0.25
(2,80)	1:64:A:VAL:O	1:68:A:LEU:N	13	0.25
(2,48)	1:16:A:LYS:O	1:20:A:PHE:N	13	0.25
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	20	0.25
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	16	0.25
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	11	0.25
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	1	0.25
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	1	0.25
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	1	0.25
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	1	0.25
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	19	0.25
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	19	0.25
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	19	0.25
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	19	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	3	0.25
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	1	0.25
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	8	0.25
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	11	0.25
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	3	0.25
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	9	0.25
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	12	0.25
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	3	0.25
(1,225)	1:43:A:SER:H	1:44:A:GLU:H	11	0.25
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	7	0.25
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	3	0.25
(1,212)	1:21:A:ASN:H	1:22:A:LEU:H	7	0.25
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	17	0.25
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	14	0.25
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	9	0.25
(1,200)	1:94:A:ALA:HA	1:97:A:LEU:H	17	0.25
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	9	0.25
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	6	0.25
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	11	0.25
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	4	0.25
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	4	0.25
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	10	0.25
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	1	0.25
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	11	0.25
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	6	0.25
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	17	0.25
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	12	0.25
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	8	0.25
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	5	0.25
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	12	0.25
(1,43)	1:34:A:ASN:HB2	1:59:A:MET:H	11	0.25
(1,43)	1:34:A:ASN:HB3	1:59:A:MET:H	11	0.25
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	11	0.25
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	11	0.25
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	11	0.25
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	11	0.25
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	11	0.25
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	11	0.25
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	1	0.25
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	1	0.25
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	1	0.25
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG21	8	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG22	8	0.25
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG23	8	0.25
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	5	0.24
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	10	0.24
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	16	0.24
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	1	0.24
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	10	0.24
(2,104)	1:110:A:SER:O	1:114:A:GLU:N	17	0.24
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	13	0.24
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	2	0.24
(2,81)	1:65:A:LEU:O	1:69:A:GLN:H	11	0.24
(2,75)	1:62:A:PHE:O	1:66:A:LYS:H	11	0.24
(2,67)	1:38:A:ALA:O	1:42:A:LEU:H	6	0.24
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	5	0.24
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	18	0.24
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	9	0.24
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	7	0.24
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	9	0.24
(2,53)	1:19:A:SER:O	1:23:A:LYS:H	3	0.24
(2,44)	1:14:A:LEU:O	1:18:A:VAL:N	11	0.24
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	1	0.24
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	11	0.24
(2,24)	1:50:A:ILE:N	1:78:A:PRO:O	7	0.24
(2,24)	1:50:A:ILE:N	1:78:A:PRO:O	16	0.24
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	19	0.24
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	15	0.24
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	6	0.24
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	6	0.24
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	6	0.24
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	6	0.24
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	6	0.24
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	6	0.24
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	6	0.24
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	6	0.24
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	6	0.24
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	6	0.24
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	6	0.24
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	6	0.24
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	6	0.24
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	6	0.24
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	6	0.24
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	6	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	6	0.24
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	6	0.24
(1,269)	1:5:A:VAL:H	1:30:A:ILE:H	17	0.24
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	9	0.24
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	5	0.24
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	10	0.24
(1,231)	1:62:A:PHE:H	1:63:A:THR:H	16	0.24
(1,223)	1:41:A:LYS:H	1:42:A:LEU:H	2	0.24
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	7	0.24
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	7	0.24
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	2	0.24
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	2	0.24
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	7	0.24
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	19	0.24
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	5	0.24
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	2	0.24
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	4	0.24
(1,173)	1:75:A:LYS:HA	1:76:A:ARG:H	13	0.24
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	5	0.24
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	7	0.24
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	3	0.24
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	6	0.24
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	10	0.24
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	12	0.24
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	18	0.24
(1,136)	1:19:A:SER:HA	1:20:A:PHE:H	20	0.24
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	1	0.24
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	4	0.24
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	17	0.24
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	12	0.24
(1,122)	1:52:A:LEU:H	1:81:A:VAL:HA	8	0.24
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	1	0.24
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	18	0.24
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	18	0.24
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	20	0.24
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	13	0.24
(1,71)	1:86:A:GLY:HA2	1:87:A:GLY:H	5	0.24
(1,71)	1:86:A:GLY:HA3	1:87:A:GLY:H	5	0.24
(1,71)	1:86:A:GLY:HA2	1:87:A:GLY:H	10	0.24
(1,71)	1:86:A:GLY:HA3	1:87:A:GLY:H	10	0.24
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	16	0.24
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	2	0.24
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	2	0.24
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	2	0.24
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	2	0.24
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	2	0.24
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	12	0.24
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	12	0.24
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	12	0.24
(1,19)	1:42:A:LEU:HB2	1:47:A:PRO:HD2	5	0.24
(1,19)	1:42:A:LEU:HB3	1:47:A:PRO:HD2	5	0.24
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	9	0.24
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	9	0.24
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	9	0.24
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	14	0.23
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	5	0.23
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	11	0.23
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	6	0.23
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	11	0.23
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	6	0.23
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	8	0.23
(2,96)	1:95:A:LEU:O	1:98:A:GLY:N	11	0.23
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	6	0.23
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	19	0.23
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	11	0.23
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	4	0.23
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	14	0.23
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	14	0.23
(2,43)	1:14:A:LEU:O	1:18:A:VAL:H	11	0.23
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	7	0.23
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	6	0.23
(2,34)	1:81:A:VAL:N	1:101:A:LYS:O	20	0.23
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	17	0.23
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	6	0.23
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	8	0.23
(2,13)	1:7:A:LEU:O	1:32:A:ALA:H	20	0.23
(2,7)	1:6:A:LEU:H	1:49:A:LEU:O	3	0.23
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	13	0.23
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	13	0.23
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	13	0.23
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	13	0.23
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	13	0.23
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	13	0.23
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	13	0.23
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	13	0.23
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	13	0.23
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	13	0.23
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	13	0.23
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	13	0.23
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	13	0.23
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	13	0.23
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	13	0.23
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	13	0.23
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	13	0.23
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD11	20	0.23
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD12	20	0.23
(1,281)	1:6:A:LEU:HD11	1:30:A:ILE:HD13	20	0.23
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD11	20	0.23
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD12	20	0.23
(1,281)	1:6:A:LEU:HD12	1:30:A:ILE:HD13	20	0.23
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD11	20	0.23
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD12	20	0.23
(1,281)	1:6:A:LEU:HD13	1:30:A:ILE:HD13	20	0.23
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD11	20	0.23
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD12	20	0.23
(1,281)	1:6:A:LEU:HD21	1:30:A:ILE:HD13	20	0.23
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD11	20	0.23
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD12	20	0.23
(1,281)	1:6:A:LEU:HD22	1:30:A:ILE:HD13	20	0.23
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD11	20	0.23
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD12	20	0.23
(1,281)	1:6:A:LEU:HD23	1:30:A:ILE:HD13	20	0.23
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB2	12	0.23
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB3	12	0.23
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB2	12	0.23
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB3	12	0.23
(1,268)	1:5:A:VAL:H	1:28:A:GLU:H	3	0.23
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	15	0.23
(1,258)	1:114:A:GLU:H	1:115:A:GLU:H	7	0.23
(1,256)	1:112:A:PHE:H	1:113:A:ILE:H	14	0.23
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	10	0.23
(1,244)	1:89:A:GLU:H	1:90:A:ASP:H	1	0.23
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	19	0.23
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	6	0.23
(1,225)	1:43:A:SER:H	1:44:A:GLU:H	4	0.23
(1,223)	1:41:A:LYS:H	1:42:A:LEU:H	6	0.23
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	3	0.23
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	4	0.23
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	18	0.23
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	5	0.23
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	20	0.23
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	12	0.23
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	18	0.23
(1,201)	1:95:A:LEU:HA	1:98:A:GLY:H	5	0.23
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	19	0.23
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	2	0.23
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	1	0.23
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	6	0.23
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	5	0.23
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	9	0.23
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	4	0.23
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	6	0.23
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	20	0.23
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	2	0.23
(1,154)	1:44:A:GLU:HA	1:45:A:PHE:H	4	0.23
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	14	0.23
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	9	0.23
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	16	0.23
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	1	0.23
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	19	0.23
(1,93)	1:50:A:ILE:HA	1:51:A:VAL:H	3	0.23
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG2	10	0.23
(1,69)	1:83:A:THR:H	1:105:A:LYS:HG3	10	0.23
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	18	0.23
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	18	0.23
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA2	1	0.23
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA2	1	0.23
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA2	1	0.23
(1,44)	1:56:A:MET:HE1	1:61:A:GLY:HA3	1	0.23
(1,44)	1:56:A:MET:HE2	1:61:A:GLY:HA3	1	0.23
(1,44)	1:56:A:MET:HE3	1:61:A:GLY:HA3	1	0.23
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	9	0.23
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	9	0.23
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	9	0.23
(2,112)	1:114:A:GLU:O	1:118:A:HIS:N	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	13	0.22
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	19	0.22
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	12	0.22
(2,94)	1:92:A:SER:O	1:96:A:SER:N	7	0.22
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	10	0.22
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	15	0.22
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	10	0.22
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	14	0.22
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	20	0.22
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	8	0.22
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	16	0.22
(2,26)	1:50:A:ILE:O	1:80:A:ILE:N	16	0.22
(2,5)	1:5:A:VAL:O	1:30:A:ILE:H	11	0.22
(1,308)	1:95:A:LEU:HD11	1:101:A:LYS:H	20	0.22
(1,308)	1:95:A:LEU:HD12	1:101:A:LYS:H	20	0.22
(1,308)	1:95:A:LEU:HD13	1:101:A:LYS:H	20	0.22
(1,308)	1:95:A:LEU:HD21	1:101:A:LYS:H	20	0.22
(1,308)	1:95:A:LEU:HD22	1:101:A:LYS:H	20	0.22
(1,308)	1:95:A:LEU:HD23	1:101:A:LYS:H	20	0.22
(1,297)	1:51:A:VAL:HG11	1:80:A:ILE:H	4	0.22
(1,297)	1:51:A:VAL:HG12	1:80:A:ILE:H	4	0.22
(1,297)	1:51:A:VAL:HG13	1:80:A:ILE:H	4	0.22
(1,297)	1:51:A:VAL:HG21	1:80:A:ILE:H	4	0.22
(1,297)	1:51:A:VAL:HG22	1:80:A:ILE:H	4	0.22
(1,297)	1:51:A:VAL:HG23	1:80:A:ILE:H	4	0.22
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB2	9	0.22
(1,278)	1:3:A:LYS:HB2	1:48:A:ASP:HB3	9	0.22
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB2	9	0.22
(1,278)	1:3:A:LYS:HB3	1:48:A:ASP:HB3	9	0.22
(1,267)	1:8:A:VAL:H	1:53:A:ASP:H	2	0.22
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	14	0.22
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	14	0.22
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	16	0.22
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	18	0.22
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	16	0.22
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	12	0.22
(1,238)	1:69:A:GLN:H	1:70:A:GLU:H	17	0.22
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	9	0.22
(1,222)	1:40:A:GLU:H	1:41:A:LYS:H	7	0.22
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	12	0.22
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	14	0.22
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	16	0.22
(1,203)	1:12:A:ALA:H	1:13:A:VAL:H	1	0.22
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	13	0.22
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	19	0.22
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	16	0.22
(1,175)	1:63:A:THR:HA	1:66:A:LYS:H	19	0.22
(1,172)	1:73:A:GLU:HA	1:74:A:TRP:H	8	0.22
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	7	0.22
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	17	0.22
(1,149)	1:39:A:LEU:HA	1:40:A:GLU:H	4	0.22
(1,146)	1:36:A:GLN:HA	1:37:A:ILE:H	15	0.22
(1,122)	1:52:A:LEU:H	1:81:A:VAL:HA	20	0.22
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	4	0.22
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	10	0.22
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	8	0.22
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	14	0.22
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	18	0.22
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	18	0.22
(1,63)	1:72:A:GLU:HA	1:75:A:LYS:H	10	0.22
(1,59)	1:71:A:LYS:HG2	1:73:A:GLU:H	19	0.22
(1,59)	1:71:A:LYS:HG3	1:73:A:GLU:H	19	0.22
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	20	0.22
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	20	0.22
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	20	0.22
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE1	18	0.22
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE2	18	0.22
(1,1)	1:35:A:GLY:HA2	1:56:A:MET:HE3	18	0.22
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	18	0.21
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	4	0.21
(2,103)	1:110:A:SER:O	1:114:A:GLU:H	3	0.21
(2,103)	1:110:A:SER:O	1:114:A:GLU:H	15	0.21
(2,82)	1:65:A:LEU:O	1:69:A:GLN:N	12	0.21
(2,76)	1:62:A:PHE:O	1:66:A:LYS:N	11	0.21
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	19	0.21
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	14	0.21
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	9	0.21
(2,52)	1:18:A:VAL:O	1:22:A:LEU:N	15	0.21
(2,50)	1:17:A:ILE:O	1:21:A:ASN:N	5	0.21
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	5	0.21
(2,38)	1:83:A:THR:N	1:103:A:MET:O	18	0.21
(2,37)	1:83:A:THR:H	1:103:A:MET:O	15	0.21
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	14	0.21
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	2	0.21
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	6	0.21
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	19	0.21
(1,272)	1:9:A:ASP:H	1:32:A:ALA:H	7	0.21
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	17	0.21
(1,266)	1:6:A:LEU:H	1:51:A:VAL:H	11	0.21
(1,266)	1:6:A:LEU:H	1:51:A:VAL:H	18	0.21
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	15	0.21
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	12	0.21
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	14	0.21
(1,252)	1:97:A:LEU:H	1:98:A:GLY:H	18	0.21
(1,245)	1:90:A:ASP:H	1:91:A:GLU:H	8	0.21
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	14	0.21
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	9	0.21
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	2	0.21
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	14	0.21
(1,225)	1:43:A:SER:H	1:44:A:GLU:H	16	0.21
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	10	0.21
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	18	0.21
(1,222)	1:40:A:GLU:H	1:41:A:LYS:H	9	0.21
(1,222)	1:40:A:GLU:H	1:41:A:LYS:H	12	0.21
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	9	0.21
(1,215)	1:33:A:GLU:H	1:34:A:ASN:H	20	0.21
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	10	0.21
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	19	0.21
(1,201)	1:95:A:LEU:HA	1:98:A:GLY:H	10	0.21
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	10	0.21
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	6	0.21
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	15	0.21
(1,167)	1:66:A:LYS:HA	1:67:A:LYS:H	4	0.21
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	20	0.21
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	15	0.21
(1,149)	1:39:A:LEU:HA	1:40:A:GLU:H	9	0.21
(1,149)	1:39:A:LEU:HA	1:40:A:GLU:H	12	0.21
(1,147)	1:37:A:ILE:HA	1:38:A:ALA:H	12	0.21
(1,146)	1:36:A:GLN:HA	1:37:A:ILE:H	16	0.21
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	4	0.21
(1,137)	1:20:A:PHE:HA	1:21:A:ASN:H	5	0.21
(1,135)	1:18:A:VAL:HA	1:19:A:SER:H	5	0.21
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	1	0.21
(1,128)	1:82:A:LEU:HA	1:103:A:MET:H	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	11	0.21
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	7	0.21
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	11	0.21
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	17	0.21
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	17	0.21
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	8	0.21
(1,60)	1:71:A:LYS:HB2	1:74:A:TRP:H	4	0.21
(1,60)	1:71:A:LYS:HB3	1:74:A:TRP:H	4	0.21
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	13	0.21
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	13	0.21
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	13	0.21
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	4	0.21
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	4	0.21
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	4	0.21
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG21	12	0.21
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG22	12	0.21
(1,2)	1:54:A:ILE:HG21	1:83:A:THR:HG23	12	0.21
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG21	12	0.21
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG22	12	0.21
(1,2)	1:54:A:ILE:HG22	1:83:A:THR:HG23	12	0.21
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG21	12	0.21
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG22	12	0.21
(1,2)	1:54:A:ILE:HG23	1:83:A:THR:HG23	12	0.21
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	3	0.2
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	11	0.2
(2,109)	1:113:A:ILE:O	1:117:A:LYS:H	8	0.2
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	5	0.2
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	20	0.2
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	16	0.2
(2,104)	1:110:A:SER:O	1:114:A:GLU:N	4	0.2
(2,103)	1:110:A:SER:O	1:114:A:GLU:H	4	0.2
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	12	0.2
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	3	0.2
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	20	0.2
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	20	0.2
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	17	0.2
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	2	0.2
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	16	0.2
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	14	0.2
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	3	0.2
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	2	0.2
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	20	0.2
(2,53)	1:19:A:SER:O	1:23:A:LYS:H	17	0.2
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	15	0.2
(2,32)	1:79:A:VAL:O	1:100:A:ARG:N	10	0.2
(2,24)	1:50:A:ILE:N	1:78:A:PRO:O	17	0.2
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	2	0.2
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	18	0.2
(2,14)	1:7:A:LEU:O	1:32:A:ALA:N	20	0.2
(2,8)	1:6:A:LEU:N	1:49:A:LEU:O	3	0.2
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	3	0.2
(1,308)	1:95:A:LEU:HD11	1:101:A:LYS:H	8	0.2
(1,308)	1:95:A:LEU:HD12	1:101:A:LYS:H	8	0.2
(1,308)	1:95:A:LEU:HD13	1:101:A:LYS:H	8	0.2
(1,308)	1:95:A:LEU:HD21	1:101:A:LYS:H	8	0.2
(1,308)	1:95:A:LEU:HD22	1:101:A:LYS:H	8	0.2
(1,308)	1:95:A:LEU:HD23	1:101:A:LYS:H	8	0.2
(1,272)	1:9:A:ASP:H	1:32:A:ALA:H	5	0.2
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	13	0.2
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	5	0.2
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	11	0.2
(1,251)	1:96:A:SER:H	1:97:A:LEU:H	11	0.2
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	12	0.2
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	14	0.2
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	2	0.2
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	11	0.2
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	1	0.2
(1,221)	1:39:A:LEU:H	1:40:A:GLU:H	9	0.2
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	6	0.2
(1,207)	1:16:A:LYS:H	1:17:A:ILE:H	1	0.2
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	4	0.2
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	6	0.2
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	6	0.2
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	4	0.2
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	11	0.2
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	2	0.2
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	2	0.2
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	8	0.2
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	5	0.2
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	2	0.2
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	12	0.2
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	2	0.2
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:68:A:LEU:HA	1:71:A:LYS:H	17	0.2
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	1	0.2
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	12	0.2
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	13	0.2
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	20	0.2
(1,167)	1:66:A:LYS:HA	1:67:A:LYS:H	17	0.2
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	10	0.2
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	14	0.2
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	16	0.2
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	6	0.2
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	16	0.2
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	19	0.2
(1,146)	1:36:A:GLN:HA	1:37:A:ILE:H	1	0.2
(1,142)	1:25:A:GLU:HA	1:26:A:GLY:H	12	0.2
(1,140)	1:23:A:LYS:HA	1:24:A:LYS:H	12	0.2
(1,136)	1:19:A:SER:HA	1:20:A:PHE:H	7	0.2
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	8	0.2
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	14	0.2
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	15	0.2
(1,92)	1:49:A:LEU:HA	1:50:A:ILE:H	12	0.2
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	5	0.2
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	5	0.2
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	6	0.2
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	6	0.2
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	20	0.2
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	20	0.2
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	20	0.2
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	5	0.2
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	5	0.2
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	5	0.2
(1,22)	1:42:A:LEU:HG	1:47:A:PRO:HD3	6	0.2
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	8	0.2
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	8	0.2
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	8	0.2
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	8	0.2
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	8	0.2
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	8	0.2
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	7	0.19
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	15	0.19
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	15	0.19
(2,112)	1:114:A:GLU:O	1:118:A:HIS:N	2	0.19
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,104)	1:110:A:SER:O	1:114:A:GLU:N	3	0.19
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	13	0.19
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	2	0.19
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	6	0.19
(2,94)	1:92:A:SER:O	1:96:A:SER:N	5	0.19
(2,93)	1:92:A:SER:O	1:96:A:SER:H	13	0.19
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	2	0.19
(2,79)	1:64:A:VAL:O	1:68:A:LEU:H	17	0.19
(2,78)	1:63:A:THR:O	1:67:A:LYS:N	2	0.19
(2,78)	1:63:A:THR:O	1:67:A:LYS:N	14	0.19
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	16	0.19
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	10	0.19
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	19	0.19
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	8	0.19
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	7	0.19
(2,11)	1:7:A:LEU:H	1:30:A:ILE:O	5	0.19
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	11	0.19
(1,297)	1:51:A:VAL:HG11	1:80:A:ILE:H	20	0.19
(1,297)	1:51:A:VAL:HG12	1:80:A:ILE:H	20	0.19
(1,297)	1:51:A:VAL:HG13	1:80:A:ILE:H	20	0.19
(1,297)	1:51:A:VAL:HG21	1:80:A:ILE:H	20	0.19
(1,297)	1:51:A:VAL:HG22	1:80:A:ILE:H	20	0.19
(1,297)	1:51:A:VAL:HG23	1:80:A:ILE:H	20	0.19
(1,274)	1:52:A:LEU:H	1:80:A:ILE:H	16	0.19
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	8	0.19
(1,258)	1:114:A:GLU:H	1:115:A:GLU:H	11	0.19
(1,257)	1:113:A:ILE:H	1:114:A:GLU:H	17	0.19
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	9	0.19
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	3	0.19
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	16	0.19
(1,238)	1:69:A:GLN:H	1:70:A:GLU:H	3	0.19
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	20	0.19
(1,215)	1:33:A:GLU:H	1:34:A:ASN:H	5	0.19
(1,213)	1:22:A:LEU:H	1:23:A:LYS:H	2	0.19
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	16	0.19
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	6	0.19
(1,209)	1:18:A:VAL:H	1:19:A:SER:H	6	0.19
(1,201)	1:95:A:LEU:HA	1:98:A:GLY:H	2	0.19
(1,201)	1:95:A:LEU:HA	1:98:A:GLY:H	8	0.19
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	13	0.19
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	3	0.19
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,194)	1:88:A:GLU:HA	1:91:A:GLU:H	17	0.19
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	13	0.19
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	15	0.19
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	17	0.19
(1,179)	1:67:A:LYS:HA	1:70:A:GLU:H	4	0.19
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	5	0.19
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	2	0.19
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	11	0.19
(1,151)	1:41:A:LYS:HA	1:42:A:LEU:H	15	0.19
(1,151)	1:41:A:LYS:HA	1:42:A:LEU:H	19	0.19
(1,149)	1:39:A:LEU:HA	1:40:A:GLU:H	13	0.19
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	13	0.19
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	9	0.19
(1,137)	1:20:A:PHE:HA	1:21:A:ASN:H	7	0.19
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	7	0.19
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	16	0.19
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	12	0.19
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	19	0.19
(1,121)	1:7:A:LEU:HA	1:51:A:VAL:H	8	0.19
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	5	0.19
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	1	0.19
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	14	0.19
(1,107)	1:83:A:THR:HA	1:84:A:ALA:H	5	0.19
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	1	0.19
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	1	0.19
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	19	0.19
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	19	0.19
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	12	0.19
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	12	0.19
(1,61)	1:71:A:LYS:HG2	1:74:A:TRP:H	19	0.19
(1,61)	1:71:A:LYS:HG3	1:74:A:TRP:H	19	0.19
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	20	0.19
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	20	0.19
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	20	0.19
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	20	0.19
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	20	0.19
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	20	0.19
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	15	0.19
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	15	0.19
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	15	0.19
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	13	0.19
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	13	0.19
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	14	0.19
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	14	0.19
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	14	0.19
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	18	0.18
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	6	0.18
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	4	0.18
(2,112)	1:114:A:GLU:O	1:118:A:HIS:N	10	0.18
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	8	0.18
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	19	0.18
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	6	0.18
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	3	0.18
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	15	0.18
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	5	0.18
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	16	0.18
(2,53)	1:19:A:SER:O	1:23:A:LYS:H	9	0.18
(2,37)	1:83:A:THR:H	1:103:A:MET:O	9	0.18
(2,34)	1:81:A:VAL:N	1:101:A:LYS:O	15	0.18
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	10	0.18
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	13	0.18
(2,32)	1:79:A:VAL:O	1:100:A:ARG:N	15	0.18
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	4	0.18
(2,30)	1:52:A:LEU:O	1:82:A:LEU:N	7	0.18
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	18	0.18
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	15	0.18
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	13	0.18
(2,9)	1:6:A:LEU:O	1:51:A:VAL:H	8	0.18
(2,3)	1:5:A:VAL:H	1:28:A:GLU:O	3	0.18
(1,268)	1:5:A:VAL:H	1:28:A:GLU:H	12	0.18
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	7	0.18
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	20	0.18
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	6	0.18
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	10	0.18
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	9	0.18
(1,221)	1:39:A:LEU:H	1:40:A:GLU:H	5	0.18
(1,218)	1:36:A:GLN:H	1:37:A:ILE:H	5	0.18
(1,212)	1:21:A:ASN:H	1:22:A:LEU:H	8	0.18
(1,208)	1:17:A:ILE:H	1:18:A:VAL:H	9	0.18
(1,207)	1:16:A:LYS:H	1:17:A:ILE:H	14	0.18
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	5	0.18
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	16	0.18
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	18	0.18
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	5	0.18
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	1	0.18
(1,179)	1:67:A:LYS:HA	1:70:A:GLU:H	13	0.18
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	3	0.18
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	17	0.18
(1,169)	1:68:A:LEU:HA	1:69:A:GLN:H	4	0.18
(1,162)	1:41:A:LYS:HA	1:44:A:GLU:H	20	0.18
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	2	0.18
(1,135)	1:18:A:VAL:HA	1:19:A:SER:H	18	0.18
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	14	0.18
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	13	0.18
(1,131)	1:14:A:LEU:HA	1:15:A:ARG:H	19	0.18
(1,129)	1:12:A:ALA:HA	1:13:A:VAL:H	17	0.18
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	1	0.18
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	11	0.18
(1,116)	1:9:A:ASP:H	1:33:A:GLU:HA	4	0.18
(1,100)	1:58:A:VAL:HA	1:59:A:MET:H	20	0.18
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	4	0.18
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	4	0.18
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	20	0.18
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	20	0.18
(1,84)	1:11:A:SER:HA	1:12:A:ALA:H	12	0.18
(1,71)	1:86:A:GLY:HA2	1:87:A:GLY:H	9	0.18
(1,71)	1:86:A:GLY:HA3	1:87:A:GLY:H	9	0.18
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG2	2	0.18
(1,67)	1:79:A:VAL:H	1:100:A:ARG:HG3	2	0.18
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG11	10	0.18
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG12	10	0.18
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG13	10	0.18
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG11	10	0.18
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG12	10	0.18
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG13	10	0.18
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG11	10	0.18
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG12	10	0.18
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG13	10	0.18
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG21	10	0.18
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG22	10	0.18
(1,40)	1:56:A:MET:HE1	1:64:A:VAL:HG23	10	0.18
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG21	10	0.18
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG22	10	0.18
(1,40)	1:56:A:MET:HE2	1:64:A:VAL:HG23	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG21	10	0.18
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG22	10	0.18
(1,40)	1:56:A:MET:HE3	1:64:A:VAL:HG23	10	0.18
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	18	0.17
(2,104)	1:110:A:SER:O	1:114:A:GLU:N	15	0.17
(2,93)	1:92:A:SER:O	1:96:A:SER:H	15	0.17
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	16	0.17
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	13	0.17
(2,78)	1:63:A:THR:O	1:67:A:LYS:N	12	0.17
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	14	0.17
(2,68)	1:38:A:ALA:O	1:42:A:LEU:N	6	0.17
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	15	0.17
(2,61)	1:35:A:GLY:O	1:39:A:LEU:H	15	0.17
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	1	0.17
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	13	0.17
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	16	0.17
(2,54)	1:19:A:SER:O	1:23:A:LYS:N	9	0.17
(2,52)	1:18:A:VAL:O	1:22:A:LEU:N	11	0.17
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	20	0.17
(2,40)	1:12:A:ALA:O	1:16:A:LYS:N	3	0.17
(2,39)	1:12:A:ALA:O	1:16:A:LYS:H	7	0.17
(2,34)	1:81:A:VAL:N	1:101:A:LYS:O	10	0.17
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	3	0.17
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	13	0.17
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	4	0.17
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	7	0.17
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	12	0.17
(2,13)	1:7:A:LEU:O	1:32:A:ALA:H	8	0.17
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	12	0.17
(1,294)	1:49:A:LEU:HD11	1:80:A:ILE:H	8	0.17
(1,294)	1:49:A:LEU:HD12	1:80:A:ILE:H	8	0.17
(1,294)	1:49:A:LEU:HD13	1:80:A:ILE:H	8	0.17
(1,294)	1:49:A:LEU:HD21	1:80:A:ILE:H	8	0.17
(1,294)	1:49:A:LEU:HD22	1:80:A:ILE:H	8	0.17
(1,294)	1:49:A:LEU:HD23	1:80:A:ILE:H	8	0.17
(1,263)	1:119:A:LEU:H	1:120:A:LEU:H	12	0.17
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	11	0.17
(1,246)	1:91:A:GLU:H	1:92:A:SER:H	19	0.17
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	4	0.17
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	5	0.17
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	19	0.17
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	1	0.17
(1,214)	1:23:A:LYS:H	1:24:A:LYS:H	16	0.17
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	12	0.17
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	13	0.17
(1,208)	1:17:A:ILE:H	1:18:A:VAL:H	7	0.17
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	20	0.17
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	1	0.17
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	1	0.17
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	3	0.17
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	9	0.17
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	9	0.17
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	7	0.17
(1,167)	1:66:A:LYS:HA	1:67:A:LYS:H	16	0.17
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	5	0.17
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	7	0.17
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	8	0.17
(1,160)	1:39:A:LEU:HA	1:42:A:LEU:H	12	0.17
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	9	0.17
(1,147)	1:37:A:ILE:HA	1:38:A:ALA:H	18	0.17
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	9	0.17
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	1	0.17
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	2	0.17
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	3	0.17
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	13	0.17
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	8	0.17
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	14	0.17
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	4	0.17
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	11	0.17
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	11	0.17
(1,84)	1:11:A:SER:HA	1:12:A:ALA:H	5	0.17
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	5	0.17
(1,70)	1:83:A:THR:H	1:105:A:LYS:H	7	0.17
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	11	0.17
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	11	0.17
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	11	0.17
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD11	18	0.17
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD12	18	0.17
(1,27)	1:22:A:LEU:HA	1:113:A:ILE:HD13	18	0.17
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	4	0.17
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	4	0.17
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	4	0.17
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	4	0.17
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	4	0.17
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	16	0.16
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	14	0.16
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	14	0.16
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	14	0.16
(2,110)	1:113:A:ILE:O	1:117:A:LYS:N	8	0.16
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	13	0.16
(2,101)	1:109:A:PRO:O	1:113:A:ILE:H	15	0.16
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	2	0.16
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	3	0.16
(2,83)	1:71:A:LYS:O	1:74:A:TRP:H	12	0.16
(2,81)	1:65:A:LEU:O	1:69:A:GLN:H	1	0.16
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	1	0.16
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	12	0.16
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	3	0.16
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	19	0.16
(2,62)	1:35:A:GLY:O	1:39:A:LEU:N	7	0.16
(2,58)	1:21:A:ASN:O	1:25:A:GLU:N	6	0.16
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	15	0.16
(2,55)	1:20:A:PHE:O	1:24:A:LYS:H	5	0.16
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	16	0.16
(2,34)	1:81:A:VAL:N	1:101:A:LYS:O	1	0.16
(2,34)	1:81:A:VAL:N	1:101:A:LYS:O	8	0.16
(2,21)	1:4:A:LYS:O	1:48:A:ASP:H	19	0.16
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	13	0.16
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	17	0.16
(2,10)	1:6:A:LEU:O	1:51:A:VAL:N	8	0.16
(2,4)	1:5:A:VAL:N	1:28:A:GLU:O	11	0.16
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	5	0.16
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD11	20	0.16
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD12	20	0.16
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD13	20	0.16
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD21	20	0.16
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD22	20	0.16
(1,303)	1:65:A:LEU:HD11	1:97:A:LEU:HD23	20	0.16
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD11	20	0.16
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD12	20	0.16
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD13	20	0.16
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD21	20	0.16
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD22	20	0.16
(1,303)	1:65:A:LEU:HD12	1:97:A:LEU:HD23	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD11	20	0.16
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD12	20	0.16
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD13	20	0.16
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD21	20	0.16
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD22	20	0.16
(1,303)	1:65:A:LEU:HD13	1:97:A:LEU:HD23	20	0.16
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD11	20	0.16
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD12	20	0.16
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD13	20	0.16
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD21	20	0.16
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD22	20	0.16
(1,303)	1:65:A:LEU:HD21	1:97:A:LEU:HD23	20	0.16
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD11	20	0.16
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD12	20	0.16
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD13	20	0.16
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD21	20	0.16
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD22	20	0.16
(1,303)	1:65:A:LEU:HD22	1:97:A:LEU:HD23	20	0.16
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD11	20	0.16
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD12	20	0.16
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD13	20	0.16
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD21	20	0.16
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD22	20	0.16
(1,303)	1:65:A:LEU:HD23	1:97:A:LEU:HD23	20	0.16
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE1	8	0.16
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE2	8	0.16
(1,298)	1:52:A:LEU:HD11	1:56:A:MET:HE3	8	0.16
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE1	8	0.16
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE2	8	0.16
(1,298)	1:52:A:LEU:HD12	1:56:A:MET:HE3	8	0.16
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE1	8	0.16
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE2	8	0.16
(1,298)	1:52:A:LEU:HD13	1:56:A:MET:HE3	8	0.16
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE1	8	0.16
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE2	8	0.16
(1,298)	1:52:A:LEU:HD21	1:56:A:MET:HE3	8	0.16
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE1	8	0.16
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE2	8	0.16
(1,298)	1:52:A:LEU:HD22	1:56:A:MET:HE3	8	0.16
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE1	8	0.16
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE2	8	0.16
(1,298)	1:52:A:LEU:HD23	1:56:A:MET:HE3	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:22:A:LEU:HD11	1:116:A:VAL:HB	1	0.16
(1,285)	1:22:A:LEU:HD12	1:116:A:VAL:HB	1	0.16
(1,285)	1:22:A:LEU:HD13	1:116:A:VAL:HB	1	0.16
(1,285)	1:22:A:LEU:HD21	1:116:A:VAL:HB	1	0.16
(1,285)	1:22:A:LEU:HD22	1:116:A:VAL:HB	1	0.16
(1,285)	1:22:A:LEU:HD23	1:116:A:VAL:HB	1	0.16
(1,266)	1:6:A:LEU:H	1:51:A:VAL:H	3	0.16
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	10	0.16
(1,259)	1:115:A:GLU:H	1:116:A:VAL:H	8	0.16
(1,257)	1:113:A:ILE:H	1:114:A:GLU:H	1	0.16
(1,256)	1:112:A:PHE:H	1:113:A:ILE:H	5	0.16
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	5	0.16
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	1	0.16
(1,249)	1:94:A:ALA:H	1:95:A:LEU:H	19	0.16
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	8	0.16
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	7	0.16
(1,244)	1:89:A:GLU:H	1:90:A:ASP:H	17	0.16
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	9	0.16
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	7	0.16
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	11	0.16
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	5	0.16
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	17	0.16
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	12	0.16
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	19	0.16
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	2	0.16
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	16	0.16
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	13	0.16
(1,193)	1:100:A:ARG:HA	1:101:A:LYS:H	16	0.16
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	14	0.16
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	3	0.16
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	1	0.16
(1,181)	1:88:A:GLU:HA	1:89:A:GLU:H	12	0.16
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	12	0.16
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	1	0.16
(1,162)	1:41:A:LYS:HA	1:44:A:GLU:H	1	0.16
(1,157)	1:36:A:GLN:HA	1:39:A:LEU:H	1	0.16
(1,154)	1:44:A:GLU:HA	1:45:A:PHE:H	11	0.16
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	7	0.16
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	13	0.16
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	3	0.16
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	2	0.16
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:20:A:PHE:HA	1:21:A:ASN:H	2	0.16
(1,136)	1:19:A:SER:HA	1:20:A:PHE:H	15	0.16
(1,136)	1:19:A:SER:HA	1:20:A:PHE:H	16	0.16
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	8	0.16
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	16	0.16
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	6	0.16
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	9	0.16
(1,112)	1:104:A:ARG:HA	1:105:A:LYS:H	5	0.16
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	4	0.16
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	5	0.16
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	19	0.16
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	8	0.16
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD11	5	0.16
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD12	5	0.16
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD13	5	0.16
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD21	5	0.16
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD22	5	0.16
(1,36)	1:116:A:VAL:HA	1:120:A:LEU:HD23	5	0.16
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	6	0.16
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	6	0.16
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	6	0.16
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD11	1	0.16
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD12	1	0.16
(1,16)	1:46:A:THR:HA	1:77:A:ILE:HD13	1	0.16
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG21	14	0.16
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG22	14	0.16
(1,7)	1:32:A:ALA:HA	1:37:A:ILE:HG23	14	0.16
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	9	0.15
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	7	0.15
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	8	0.15
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	3	0.15
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	12	0.15
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	3	0.15
(2,94)	1:92:A:SER:O	1:96:A:SER:N	13	0.15
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	5	0.15
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	17	0.15
(2,75)	1:62:A:PHE:O	1:66:A:LYS:H	1	0.15
(2,75)	1:62:A:PHE:O	1:66:A:LYS:H	19	0.15
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	12	0.15
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	15	0.15
(2,67)	1:38:A:ALA:O	1:42:A:LEU:H	17	0.15
(2,65)	1:37:A:ILE:O	1:41:A:LYS:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	10	0.15
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	13	0.15
(2,59)	1:22:A:LEU:O	1:26:A:GLY:H	10	0.15
(2,56)	1:20:A:PHE:O	1:24:A:LYS:N	15	0.15
(2,54)	1:19:A:SER:O	1:23:A:LYS:N	17	0.15
(2,52)	1:18:A:VAL:O	1:22:A:LEU:N	7	0.15
(2,36)	1:81:A:VAL:O	1:103:A:MET:N	1	0.15
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	1	0.15
(2,34)	1:81:A:VAL:N	1:101:A:LYS:O	13	0.15
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	4	0.15
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	2	0.15
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	19	0.15
(1,307)	1:95:A:LEU:HD11	1:100:A:ARG:H	12	0.15
(1,307)	1:95:A:LEU:HD12	1:100:A:ARG:H	12	0.15
(1,307)	1:95:A:LEU:HD13	1:100:A:ARG:H	12	0.15
(1,307)	1:95:A:LEU:HD21	1:100:A:ARG:H	12	0.15
(1,307)	1:95:A:LEU:HD22	1:100:A:ARG:H	12	0.15
(1,307)	1:95:A:LEU:HD23	1:100:A:ARG:H	12	0.15
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	18	0.15
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	1	0.15
(1,258)	1:114:A:GLU:H	1:115:A:GLU:H	8	0.15
(1,258)	1:114:A:GLU:H	1:115:A:GLU:H	9	0.15
(1,257)	1:113:A:ILE:H	1:114:A:GLU:H	4	0.15
(1,243)	1:88:A:GLU:H	1:89:A:GLU:H	12	0.15
(1,243)	1:88:A:GLU:H	1:89:A:GLU:H	20	0.15
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	14	0.15
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	2	0.15
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	7	0.15
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	16	0.15
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	6	0.15
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	4	0.15
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	18	0.15
(1,235)	1:66:A:LYS:H	1:67:A:LYS:H	20	0.15
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	2	0.15
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	20	0.15
(1,222)	1:40:A:GLU:H	1:41:A:LYS:H	1	0.15
(1,222)	1:40:A:GLU:H	1:41:A:LYS:H	13	0.15
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	19	0.15
(1,214)	1:23:A:LYS:H	1:24:A:LYS:H	2	0.15
(1,207)	1:16:A:LYS:H	1:17:A:ILE:H	19	0.15
(1,204)	1:13:A:VAL:H	1:14:A:LEU:H	12	0.15
(1,195)	1:89:A:GLU:HA	1:92:A:SER:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,192)	1:99:A:ALA:HA	1:100:A:ARG:H	3	0.15
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	17	0.15
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	2	0.15
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	18	0.15
(1,175)	1:63:A:THR:HA	1:66:A:LYS:H	16	0.15
(1,172)	1:73:A:GLU:HA	1:74:A:TRP:H	2	0.15
(1,172)	1:73:A:GLU:HA	1:74:A:TRP:H	10	0.15
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	10	0.15
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	12	0.15
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	16	0.15
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	20	0.15
(1,169)	1:68:A:LEU:HA	1:69:A:GLN:H	2	0.15
(1,169)	1:68:A:LEU:HA	1:69:A:GLN:H	3	0.15
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	7	0.15
(1,163)	1:62:A:PHE:HA	1:63:A:THR:H	10	0.15
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	15	0.15
(1,154)	1:44:A:GLU:HA	1:45:A:PHE:H	13	0.15
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	4	0.15
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	5	0.15
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	20	0.15
(1,146)	1:36:A:GLN:HA	1:37:A:ILE:H	11	0.15
(1,143)	1:33:A:GLU:HA	1:34:A:ASN:H	12	0.15
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	5	0.15
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	20	0.15
(1,137)	1:20:A:PHE:HA	1:21:A:ASN:H	16	0.15
(1,137)	1:20:A:PHE:HA	1:21:A:ASN:H	19	0.15
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	6	0.15
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	15	0.15
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	13	0.15
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	15	0.15
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	18	0.15
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	3	0.15
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	16	0.15
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	6	0.15
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	9	0.15
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	4	0.15
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	20	0.15
(1,47)	1:103:A:MET:HE1	1:112:A:PHE:HA	12	0.15
(1,47)	1:103:A:MET:HE2	1:112:A:PHE:HA	12	0.15
(1,47)	1:103:A:MET:HE3	1:112:A:PHE:HA	12	0.15
(1,6)	1:6:A:LEU:H	1:30:A:ILE:HB	9	0.15
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	14	0.15
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	14	0.15
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	14	0.15
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	14	0.15
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	14	0.15
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	12	0.14
(2,108)	1:112:A:PHE:O	1:116:A:VAL:N	19	0.14
(2,107)	1:112:A:PHE:O	1:116:A:VAL:H	9	0.14
(2,106)	1:111:A:GLN:O	1:115:A:GLU:N	4	0.14
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	6	0.14
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	6	0.14
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	18	0.14
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	1	0.14
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	4	0.14
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	4	0.14
(2,88)	1:89:A:GLU:O	1:93:A:LEU:N	13	0.14
(2,78)	1:63:A:THR:O	1:67:A:LYS:N	17	0.14
(2,72)	1:60:A:ASP:O	1:64:A:VAL:N	16	0.14
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	12	0.14
(2,66)	1:37:A:ILE:O	1:41:A:LYS:N	9	0.14
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	8	0.14
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	11	0.14
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	8	0.14
(2,56)	1:20:A:PHE:O	1:24:A:LYS:N	9	0.14
(2,52)	1:18:A:VAL:O	1:22:A:LEU:N	20	0.14
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	12	0.14
(2,23)	1:50:A:ILE:H	1:78:A:PRO:O	1	0.14
(2,21)	1:4:A:LYS:O	1:48:A:ASP:H	9	0.14
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	8	0.14
(2,7)	1:6:A:LEU:H	1:49:A:LEU:O	12	0.14
(1,276)	1:81:A:VAL:H	1:103:A:MET:H	18	0.14
(1,274)	1:52:A:LEU:H	1:80:A:ILE:H	14	0.14
(1,268)	1:5:A:VAL:H	1:28:A:GLU:H	17	0.14
(1,264)	1:120:A:LEU:H	1:121:A:ASN:H	1	0.14
(1,263)	1:119:A:LEU:H	1:120:A:LEU:H	15	0.14
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	16	0.14
(1,257)	1:113:A:ILE:H	1:114:A:GLU:H	7	0.14
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	1	0.14
(1,243)	1:88:A:GLU:H	1:89:A:GLU:H	17	0.14
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	11	0.14
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	13	0.14
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	6	0.14
(1,214)	1:23:A:LYS:H	1:24:A:LYS:H	13	0.14
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	5	0.14
(1,210)	1:19:A:SER:H	1:20:A:PHE:H	20	0.14
(1,206)	1:15:A:ARG:H	1:16:A:LYS:H	17	0.14
(1,198)	1:92:A:SER:HA	1:95:A:LEU:H	14	0.14
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	15	0.14
(1,193)	1:100:A:ARG:HA	1:101:A:LYS:H	3	0.14
(1,193)	1:100:A:ARG:HA	1:101:A:LYS:H	7	0.14
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	17	0.14
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	6	0.14
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	10	0.14
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	4	0.14
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	18	0.14
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	7	0.14
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	11	0.14
(1,174)	1:76:A:ARG:HA	1:77:A:ILE:H	16	0.14
(1,174)	1:76:A:ARG:HA	1:77:A:ILE:H	20	0.14
(1,173)	1:75:A:LYS:HA	1:76:A:ARG:H	15	0.14
(1,172)	1:73:A:GLU:HA	1:74:A:TRP:H	20	0.14
(1,169)	1:68:A:LEU:HA	1:69:A:GLN:H	10	0.14
(1,169)	1:68:A:LEU:HA	1:69:A:GLN:H	17	0.14
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	6	0.14
(1,158)	1:37:A:ILE:HA	1:40:A:GLU:H	12	0.14
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	9	0.14
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	15	0.14
(1,142)	1:25:A:GLU:HA	1:26:A:GLY:H	5	0.14
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	17	0.14
(1,136)	1:19:A:SER:HA	1:20:A:PHE:H	10	0.14
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	1	0.14
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	3	0.14
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	19	0.14
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	18	0.14
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	18	0.14
(1,131)	1:14:A:LEU:HA	1:15:A:ARG:H	7	0.14
(1,131)	1:14:A:LEU:HA	1:15:A:ARG:H	8	0.14
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	9	0.14
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	15	0.14
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	2	0.14
(1,118)	1:5:A:VAL:H	1:29:A:VAL:HA	18	0.14
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	7	0.14
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	13	0.14
(1,107)	1:83:A:THR:HA	1:84:A:ALA:H	15	0.14
(1,100)	1:58:A:VAL:HA	1:59:A:MET:H	12	0.14
(1,100)	1:58:A:VAL:HA	1:59:A:MET:H	13	0.14
(1,93)	1:50:A:ILE:HA	1:51:A:VAL:H	16	0.14
(1,89)	1:31:A:GLU:HA	1:32:A:ALA:H	10	0.14
(1,86)	1:28:A:GLU:HA	1:29:A:VAL:H	13	0.14
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	7	0.14
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	7	0.14
(1,84)	1:11:A:SER:HA	1:12:A:ALA:H	7	0.14
(1,84)	1:11:A:SER:HA	1:12:A:ALA:H	8	0.14
(1,74)	1:98:A:GLY:H	1:99:A:ALA:H	17	0.14
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	5	0.14
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	6	0.14
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	6	0.14
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	6	0.14
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	6	0.14
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	6	0.14
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	6	0.14
(2,112)	1:114:A:GLU:O	1:118:A:HIS:N	1	0.13
(2,103)	1:110:A:SER:O	1:114:A:GLU:H	1	0.13
(2,100)	1:108:A:SER:O	1:112:A:PHE:N	3	0.13
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	6	0.13
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	5	0.13
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	6	0.13
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	18	0.13
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	13	0.13
(2,80)	1:64:A:VAL:O	1:68:A:LEU:N	17	0.13
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	6	0.13
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	4	0.13
(2,58)	1:21:A:ASN:O	1:25:A:GLU:N	16	0.13
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	12	0.13
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	18	0.13
(2,56)	1:20:A:PHE:O	1:24:A:LYS:N	19	0.13
(2,52)	1:18:A:VAL:O	1:22:A:LEU:N	14	0.13
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	14	0.13
(2,49)	1:17:A:ILE:O	1:21:A:ASN:H	19	0.13
(2,43)	1:14:A:LEU:O	1:18:A:VAL:H	6	0.13
(2,39)	1:12:A:ALA:O	1:16:A:LYS:H	5	0.13
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	2	0.13
(2,31)	1:79:A:VAL:O	1:100:A:ARG:H	9	0.13
(2,28)	1:52:A:LEU:N	1:80:A:ILE:O	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,27)	1:52:A:LEU:H	1:80:A:ILE:O	5	0.13
(2,27)	1:52:A:LEU:H	1:80:A:ILE:O	6	0.13
(2,27)	1:52:A:LEU:H	1:80:A:ILE:O	8	0.13
(2,24)	1:50:A:ILE:N	1:78:A:PRO:O	2	0.13
(2,20)	1:9:A:ASP:N	1:32:A:ALA:O	15	0.13
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	16	0.13
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	15	0.13
(2,12)	1:7:A:LEU:N	1:30:A:ILE:O	5	0.13
(2,12)	1:7:A:LEU:N	1:30:A:ILE:O	9	0.13
(2,8)	1:6:A:LEU:N	1:49:A:LEU:O	12	0.13
(1,297)	1:51:A:VAL:HG11	1:80:A:ILE:H	14	0.13
(1,297)	1:51:A:VAL:HG12	1:80:A:ILE:H	14	0.13
(1,297)	1:51:A:VAL:HG13	1:80:A:ILE:H	14	0.13
(1,297)	1:51:A:VAL:HG21	1:80:A:ILE:H	14	0.13
(1,297)	1:51:A:VAL:HG22	1:80:A:ILE:H	14	0.13
(1,297)	1:51:A:VAL:HG23	1:80:A:ILE:H	14	0.13
(1,280)	1:5:A:VAL:HG11	1:48:A:ASP:H	1	0.13
(1,280)	1:5:A:VAL:HG12	1:48:A:ASP:H	1	0.13
(1,280)	1:5:A:VAL:HG13	1:48:A:ASP:H	1	0.13
(1,280)	1:5:A:VAL:HG21	1:48:A:ASP:H	1	0.13
(1,280)	1:5:A:VAL:HG22	1:48:A:ASP:H	1	0.13
(1,280)	1:5:A:VAL:HG23	1:48:A:ASP:H	1	0.13
(1,276)	1:81:A:VAL:H	1:103:A:MET:H	9	0.13
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	14	0.13
(1,261)	1:117:A:LYS:H	1:118:A:HIS:H	4	0.13
(1,244)	1:89:A:GLU:H	1:90:A:ASP:H	10	0.13
(1,244)	1:89:A:GLU:H	1:90:A:ASP:H	11	0.13
(1,238)	1:69:A:GLN:H	1:70:A:GLU:H	5	0.13
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	3	0.13
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	5	0.13
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	1	0.13
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	5	0.13
(1,234)	1:65:A:LEU:H	1:66:A:LYS:H	7	0.13
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	11	0.13
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	6	0.13
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	11	0.13
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	5	0.13
(1,213)	1:22:A:LEU:H	1:23:A:LYS:H	4	0.13
(1,213)	1:22:A:LEU:H	1:23:A:LYS:H	9	0.13
(1,207)	1:16:A:LYS:H	1:17:A:ILE:H	20	0.13
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	20	0.13
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	7	0.13
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	5	0.13
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	6	0.13
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	13	0.13
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	5	0.13
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	10	0.13
(1,179)	1:67:A:LYS:HA	1:70:A:GLU:H	20	0.13
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	14	0.13
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	15	0.13
(1,170)	1:69:A:GLN:HA	1:70:A:GLU:H	14	0.13
(1,167)	1:66:A:LYS:HA	1:67:A:LYS:H	11	0.13
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	8	0.13
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	20	0.13
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	4	0.13
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	14	0.13
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	19	0.13
(1,163)	1:62:A:PHE:HA	1:63:A:THR:H	7	0.13
(1,160)	1:39:A:LEU:HA	1:42:A:LEU:H	15	0.13
(1,154)	1:44:A:GLU:HA	1:45:A:PHE:H	10	0.13
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	3	0.13
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	16	0.13
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	18	0.13
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	8	0.13
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	11	0.13
(1,146)	1:36:A:GLN:HA	1:37:A:ILE:H	5	0.13
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	5	0.13
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	17	0.13
(1,140)	1:23:A:LYS:HA	1:24:A:LYS:H	2	0.13
(1,140)	1:23:A:LYS:HA	1:24:A:LYS:H	13	0.13
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	1	0.13
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	4	0.13
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	2	0.13
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	7	0.13
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	12	0.13
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	19	0.13
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	2	0.13
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	11	0.13
(1,130)	1:13:A:VAL:HA	1:14:A:LEU:H	20	0.13
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	16	0.13
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	9	0.13
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	11	0.13
(1,125)	1:53:A:ASP:HA	1:82:A:LEU:H	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	5	0.13
(1,103)	1:79:A:VAL:HA	1:80:A:ILE:H	11	0.13
(1,92)	1:49:A:LEU:HA	1:50:A:ILE:H	7	0.13
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	17	0.13
(1,71)	1:86:A:GLY:HA2	1:87:A:GLY:H	11	0.13
(1,71)	1:86:A:GLY:HA3	1:87:A:GLY:H	11	0.13
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	1	0.12
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	4	0.12
(2,108)	1:112:A:PHE:O	1:116:A:VAL:N	1	0.12
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	15	0.12
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	13	0.12
(2,99)	1:108:A:SER:O	1:112:A:PHE:H	18	0.12
(2,97)	1:94:A:ALA:O	1:99:A:ALA:H	15	0.12
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	9	0.12
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	6	0.12
(2,89)	1:90:A:ASP:O	1:94:A:ALA:H	9	0.12
(2,76)	1:62:A:PHE:O	1:66:A:LYS:N	1	0.12
(2,70)	1:39:A:LEU:O	1:43:A:SER:N	19	0.12
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	6	0.12
(2,64)	1:36:A:GLN:O	1:40:A:GLU:N	15	0.12
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	17	0.12
(2,57)	1:21:A:ASN:O	1:25:A:GLU:H	11	0.12
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	5	0.12
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	8	0.12
(2,51)	1:18:A:VAL:O	1:22:A:LEU:H	10	0.12
(2,40)	1:12:A:ALA:O	1:16:A:LYS:N	7	0.12
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	17	0.12
(2,24)	1:50:A:ILE:N	1:78:A:PRO:O	11	0.12
(2,19)	1:9:A:ASP:H	1:32:A:ALA:O	7	0.12
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	10	0.12
(2,11)	1:7:A:LEU:H	1:30:A:ILE:O	9	0.12
(2,10)	1:6:A:LEU:O	1:51:A:VAL:N	18	0.12
(2,4)	1:5:A:VAL:N	1:28:A:GLU:O	3	0.12
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	17	0.12
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	17	0.12
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	17	0.12
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	17	0.12
(1,297)	1:51:A:VAL:HG11	1:80:A:ILE:H	5	0.12
(1,297)	1:51:A:VAL:HG12	1:80:A:ILE:H	5	0.12
(1,297)	1:51:A:VAL:HG13	1:80:A:ILE:H	5	0.12
(1,297)	1:51:A:VAL:HG21	1:80:A:ILE:H	5	0.12
(1,297)	1:51:A:VAL:HG22	1:80:A:ILE:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:51:A:VAL:HG23	1:80:A:ILE:H	5	0.12
(1,276)	1:81:A:VAL:H	1:103:A:MET:H	14	0.12
(1,262)	1:118:A:HIS:H	1:119:A:LEU:H	11	0.12
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	10	0.12
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	10	0.12
(1,252)	1:97:A:LEU:H	1:98:A:GLY:H	15	0.12
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	5	0.12
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	9	0.12
(1,250)	1:95:A:LEU:H	1:96:A:SER:H	20	0.12
(1,247)	1:92:A:SER:H	1:93:A:LEU:H	14	0.12
(1,244)	1:89:A:GLU:H	1:90:A:ASP:H	6	0.12
(1,244)	1:89:A:GLU:H	1:90:A:ASP:H	8	0.12
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	2	0.12
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	7	0.12
(1,223)	1:41:A:LYS:H	1:42:A:LEU:H	13	0.12
(1,220)	1:38:A:ALA:H	1:39:A:LEU:H	7	0.12
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	4	0.12
(1,219)	1:37:A:ILE:H	1:38:A:ALA:H	5	0.12
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	20	0.12
(1,212)	1:21:A:ASN:H	1:22:A:LEU:H	14	0.12
(1,211)	1:20:A:PHE:H	1:21:A:ASN:H	1	0.12
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	11	0.12
(1,199)	1:93:A:LEU:HA	1:96:A:SER:H	8	0.12
(1,193)	1:100:A:ARG:HA	1:101:A:LYS:H	18	0.12
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	14	0.12
(1,186)	1:93:A:LEU:HA	1:94:A:ALA:H	11	0.12
(1,185)	1:92:A:SER:HA	1:93:A:LEU:H	18	0.12
(1,184)	1:91:A:GLU:HA	1:92:A:SER:H	12	0.12
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	12	0.12
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	16	0.12
(1,181)	1:88:A:GLU:HA	1:89:A:GLU:H	11	0.12
(1,177)	1:65:A:LEU:HA	1:68:A:LEU:H	3	0.12
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	4	0.12
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	12	0.12
(1,174)	1:76:A:ARG:HA	1:77:A:ILE:H	7	0.12
(1,174)	1:76:A:ARG:HA	1:77:A:ILE:H	9	0.12
(1,173)	1:75:A:LYS:HA	1:76:A:ARG:H	18	0.12
(1,171)	1:72:A:GLU:HA	1:73:A:GLU:H	8	0.12
(1,169)	1:68:A:LEU:HA	1:69:A:GLN:H	5	0.12
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	3	0.12
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	6	0.12
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:66:A:LYS:HA	1:67:A:LYS:H	12	0.12
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	5	0.12
(1,165)	1:64:A:VAL:HA	1:65:A:LEU:H	13	0.12
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	15	0.12
(1,163)	1:62:A:PHE:HA	1:63:A:THR:H	2	0.12
(1,161)	1:40:A:GLU:HA	1:43:A:SER:H	1	0.12
(1,158)	1:37:A:ILE:HA	1:40:A:GLU:H	3	0.12
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	1	0.12
(1,152)	1:42:A:LEU:HA	1:43:A:SER:H	4	0.12
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	6	0.12
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	8	0.12
(1,149)	1:39:A:LEU:HA	1:40:A:GLU:H	16	0.12
(1,147)	1:37:A:ILE:HA	1:38:A:ALA:H	13	0.12
(1,141)	1:24:A:LYS:HA	1:25:A:GLU:H	14	0.12
(1,140)	1:23:A:LYS:HA	1:24:A:LYS:H	3	0.12
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	13	0.12
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	14	0.12
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	15	0.12
(1,138)	1:21:A:ASN:HA	1:22:A:LEU:H	5	0.12
(1,136)	1:19:A:SER:HA	1:20:A:PHE:H	1	0.12
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	13	0.12
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	14	0.12
(1,127)	1:80:A:ILE:HA	1:101:A:LYS:H	3	0.12
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	1	0.12
(1,123)	1:51:A:VAL:HA	1:80:A:ILE:H	17	0.12
(1,122)	1:52:A:LEU:H	1:81:A:VAL:HA	19	0.12
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	3	0.12
(1,120)	1:50:A:ILE:H	1:79:A:VAL:HA	10	0.12
(1,119)	1:5:A:VAL:HA	1:49:A:LEU:H	5	0.12
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	12	0.12
(1,97)	1:54:A:ILE:HA	1:55:A:MET:H	15	0.12
(1,88)	1:30:A:ILE:HA	1:31:A:GLU:H	13	0.12
(1,88)	1:30:A:ILE:HA	1:31:A:GLU:H	14	0.12
(1,88)	1:30:A:ILE:HA	1:31:A:GLU:H	15	0.12
(1,86)	1:28:A:GLU:HA	1:29:A:VAL:H	12	0.12
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	8	0.12
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	8	0.12
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	9	0.12
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	9	0.12
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	14	0.12
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	14	0.12
(1,85)	1:26:A:GLY:HA2	1:27:A:TYR:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:26:A:GLY:HA3	1:27:A:TYR:H	15	0.12
(1,78)	1:3:A:LYS:HA	1:4:A:LYS:H	7	0.12
(1,71)	1:86:A:GLY:HA2	1:87:A:GLY:H	14	0.12
(1,71)	1:86:A:GLY:HA3	1:87:A:GLY:H	14	0.12
(1,68)	1:79:A:VAL:H	1:100:A:ARG:HD2	14	0.12
(1,68)	1:79:A:VAL:H	1:100:A:ARG:HD3	14	0.12
(1,61)	1:71:A:LYS:HG2	1:74:A:TRP:H	13	0.12
(1,61)	1:71:A:LYS:HG3	1:74:A:TRP:H	13	0.12
(1,58)	1:42:A:LEU:HA	1:45:A:PHE:H	15	0.12
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB2	20	0.12
(1,50)	1:13:A:VAL:HA	1:16:A:LYS:HB3	20	0.12
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	17	0.12
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	17	0.12
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	17	0.12
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	3	0.12
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	3	0.12
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	3	0.12
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD11	5	0.12
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD12	5	0.12
(1,18)	1:46:A:THR:HG21	1:77:A:ILE:HD13	5	0.12
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD11	5	0.12
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD12	5	0.12
(1,18)	1:46:A:THR:HG22	1:77:A:ILE:HD13	5	0.12
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD11	5	0.12
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD12	5	0.12
(1,18)	1:46:A:THR:HG23	1:77:A:ILE:HD13	5	0.12
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD11	7	0.12
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD12	7	0.12
(1,17)	1:46:A:THR:HB	1:77:A:ILE:HD13	7	0.12
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD1	13	0.12
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD1	13	0.12
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD1	13	0.12
(1,3)	1:30:A:ILE:HD11	1:45:A:PHE:HD2	13	0.12
(1,3)	1:30:A:ILE:HD12	1:45:A:PHE:HD2	13	0.12
(1,3)	1:30:A:ILE:HD13	1:45:A:PHE:HD2	13	0.12
(2,118)	1:117:A:LYS:O	1:121:A:ASN:N	15	0.11
(2,116)	1:116:A:VAL:O	1:120:A:LEU:N	14	0.11
(2,114)	1:115:A:GLU:O	1:119:A:LEU:N	10	0.11
(2,111)	1:114:A:GLU:O	1:118:A:HIS:H	5	0.11
(2,107)	1:112:A:PHE:O	1:116:A:VAL:H	1	0.11
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	12	0.11
(2,95)	1:95:A:LEU:O	1:98:A:GLY:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,93)	1:92:A:SER:O	1:96:A:SER:H	8	0.11
(2,90)	1:90:A:ASP:O	1:94:A:ALA:N	6	0.11
(2,87)	1:89:A:GLU:O	1:93:A:LEU:H	14	0.11
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	7	0.11
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	10	0.11
(2,77)	1:63:A:THR:O	1:67:A:LYS:H	19	0.11
(2,76)	1:62:A:PHE:O	1:66:A:LYS:N	19	0.11
(2,75)	1:62:A:PHE:O	1:66:A:LYS:H	16	0.11
(2,71)	1:60:A:ASP:O	1:64:A:VAL:H	8	0.11
(2,69)	1:39:A:LEU:O	1:43:A:SER:H	8	0.11
(2,65)	1:37:A:ILE:O	1:41:A:LYS:H	5	0.11
(2,54)	1:19:A:SER:O	1:23:A:LYS:N	13	0.11
(2,53)	1:19:A:SER:O	1:23:A:LYS:H	14	0.11
(2,52)	1:18:A:VAL:O	1:22:A:LEU:N	8	0.11
(2,43)	1:14:A:LEU:O	1:18:A:VAL:H	9	0.11
(2,39)	1:12:A:ALA:O	1:16:A:LYS:H	8	0.11
(2,38)	1:83:A:THR:N	1:103:A:MET:O	10	0.11
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	5	0.11
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	12	0.11
(2,35)	1:81:A:VAL:O	1:103:A:MET:H	20	0.11
(2,29)	1:52:A:LEU:O	1:82:A:LEU:H	19	0.11
(2,28)	1:52:A:LEU:N	1:80:A:ILE:O	6	0.11
(2,25)	1:50:A:ILE:O	1:80:A:ILE:H	2	0.11
(2,25)	1:50:A:ILE:O	1:80:A:ILE:H	3	0.11
(2,21)	1:4:A:LYS:O	1:48:A:ASP:H	10	0.11
(2,21)	1:4:A:LYS:O	1:48:A:ASP:H	20	0.11
(2,18)	1:8:A:VAL:O	1:53:A:ASP:N	3	0.11
(2,13)	1:7:A:LEU:O	1:32:A:ALA:H	10	0.11
(2,13)	1:7:A:LEU:O	1:32:A:ALA:H	19	0.11
(2,7)	1:6:A:LEU:H	1:49:A:LEU:O	18	0.11
(2,5)	1:5:A:VAL:O	1:30:A:ILE:H	7	0.11
(2,3)	1:5:A:VAL:H	1:28:A:GLU:O	6	0.11
(2,2)	1:3:A:LYS:O	1:28:A:GLU:N	11	0.11
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB2	20	0.11
(1,305)	1:78:A:PRO:HB2	1:119:A:LEU:HB3	20	0.11
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB2	20	0.11
(1,305)	1:78:A:PRO:HB3	1:119:A:LEU:HB3	20	0.11
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	10	0.11
(1,268)	1:5:A:VAL:H	1:28:A:GLU:H	5	0.11
(1,263)	1:119:A:LEU:H	1:120:A:LEU:H	20	0.11
(1,260)	1:116:A:VAL:H	1:117:A:LYS:H	4	0.11
(1,254)	1:110:A:SER:H	1:111:A:GLN:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,251)	1:96:A:SER:H	1:97:A:LEU:H	4	0.11
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	16	0.11
(1,242)	1:76:A:ARG:H	1:77:A:ILE:H	18	0.11
(1,241)	1:75:A:LYS:H	1:76:A:ARG:H	17	0.11
(1,240)	1:73:A:GLU:H	1:74:A:TRP:H	17	0.11
(1,236)	1:67:A:LYS:H	1:68:A:LEU:H	9	0.11
(1,230)	1:61:A:GLY:H	1:62:A:PHE:H	5	0.11
(1,221)	1:39:A:LEU:H	1:40:A:GLU:H	12	0.11
(1,214)	1:23:A:LYS:H	1:24:A:LYS:H	15	0.11
(1,209)	1:18:A:VAL:H	1:19:A:SER:H	4	0.11
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	7	0.11
(1,201)	1:95:A:LEU:HA	1:98:A:GLY:H	6	0.11
(1,197)	1:91:A:GLU:HA	1:94:A:ALA:H	12	0.11
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	4	0.11
(1,196)	1:90:A:ASP:HA	1:93:A:LEU:H	14	0.11
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	8	0.11
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	12	0.11
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	16	0.11
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	8	0.11
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	15	0.11
(1,181)	1:88:A:GLU:HA	1:89:A:GLU:H	6	0.11
(1,181)	1:88:A:GLU:HA	1:89:A:GLU:H	17	0.11
(1,176)	1:64:A:VAL:HA	1:67:A:LYS:H	6	0.11
(1,172)	1:73:A:GLU:HA	1:74:A:TRP:H	3	0.11
(1,168)	1:67:A:LYS:HA	1:68:A:LEU:H	10	0.11
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	2	0.11
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	13	0.11
(1,166)	1:65:A:LEU:HA	1:66:A:LYS:H	15	0.11
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	5	0.11
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	8	0.11
(1,164)	1:63:A:THR:HA	1:64:A:VAL:H	16	0.11
(1,163)	1:62:A:PHE:HA	1:63:A:THR:H	1	0.11
(1,163)	1:62:A:PHE:HA	1:63:A:THR:H	5	0.11
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	5	0.11
(1,154)	1:44:A:GLU:HA	1:45:A:PHE:H	8	0.11
(1,154)	1:44:A:GLU:HA	1:45:A:PHE:H	15	0.11
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	5	0.11
(1,153)	1:43:A:SER:HA	1:44:A:GLU:H	14	0.11
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	1	0.11
(1,150)	1:40:A:GLU:HA	1:41:A:LYS:H	19	0.11
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	9	0.11
(1,140)	1:23:A:LYS:HA	1:24:A:LYS:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	9	0.11
(1,135)	1:18:A:VAL:HA	1:19:A:SER:H	10	0.11
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	4	0.11
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	5	0.11
(1,132)	1:15:A:ARG:HA	1:16:A:LYS:H	20	0.11
(1,131)	1:14:A:LEU:HA	1:15:A:ARG:H	13	0.11
(1,126)	1:83:A:THR:H	1:104:A:ARG:HA	19	0.11
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	10	0.11
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	12	0.11
(1,117)	1:7:A:LEU:H	1:31:A:GLU:HA	14	0.11
(1,105)	1:81:A:VAL:HA	1:82:A:LEU:H	11	0.11
(1,100)	1:58:A:VAL:HA	1:59:A:MET:H	7	0.11
(1,86)	1:28:A:GLU:HA	1:29:A:VAL:H	15	0.11
(1,84)	1:11:A:SER:HA	1:12:A:ALA:H	18	0.11
(1,80)	1:5:A:VAL:HA	1:6:A:LEU:H	15	0.11
(1,77)	1:2:A:SER:HA	1:3:A:LYS:H	19	0.11
(1,70)	1:83:A:THR:H	1:105:A:LYS:H	8	0.11
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG21	7	0.11
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG22	7	0.11
(1,37)	1:50:A:ILE:HB	1:77:A:ILE:HG23	7	0.11
(1,34)	1:80:A:ILE:HD11	1:116:A:VAL:HA	12	0.11
(1,34)	1:80:A:ILE:HD12	1:116:A:VAL:HA	12	0.11
(1,34)	1:80:A:ILE:HD13	1:116:A:VAL:HA	12	0.11
(1,23)	1:42:A:LEU:HB2	1:47:A:PRO:HD3	5	0.11
(1,23)	1:42:A:LEU:HB3	1:47:A:PRO:HD3	5	0.11
(2,117)	1:117:A:LYS:O	1:121:A:ASN:H	2	0.1
(2,115)	1:116:A:VAL:O	1:120:A:LEU:H	3	0.1
(2,113)	1:115:A:GLU:O	1:119:A:LEU:H	10	0.1
(2,108)	1:112:A:PHE:O	1:116:A:VAL:N	18	0.1
(2,105)	1:111:A:GLN:O	1:115:A:GLU:H	18	0.1
(2,98)	1:94:A:ALA:O	1:99:A:ALA:N	2	0.1
(2,93)	1:92:A:SER:O	1:96:A:SER:H	18	0.1
(2,84)	1:71:A:LYS:O	1:74:A:TRP:N	8	0.1
(2,81)	1:65:A:LEU:O	1:69:A:GLN:H	9	0.1
(2,63)	1:36:A:GLN:O	1:40:A:GLU:H	9	0.1
(2,60)	1:22:A:LEU:O	1:26:A:GLY:N	18	0.1
(2,44)	1:14:A:LEU:O	1:18:A:VAL:N	9	0.1
(2,33)	1:81:A:VAL:H	1:101:A:LYS:O	14	0.1
(2,26)	1:50:A:ILE:O	1:80:A:ILE:N	3	0.1
(2,17)	1:8:A:VAL:O	1:53:A:ASP:H	3	0.1
(2,8)	1:6:A:LEU:N	1:49:A:LEU:O	13	0.1
(2,7)	1:6:A:LEU:H	1:49:A:LEU:O	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:3:A:LYS:O	1:28:A:GLU:H	18	0.1
(1,271)	1:7:A:LEU:H	1:32:A:ALA:H	15	0.1
(1,256)	1:112:A:PHE:H	1:113:A:ILE:H	8	0.1
(1,248)	1:93:A:LEU:H	1:94:A:ALA:H	15	0.1
(1,239)	1:72:A:GLU:H	1:73:A:GLU:H	2	0.1
(1,237)	1:68:A:LEU:H	1:69:A:GLN:H	14	0.1
(1,233)	1:64:A:VAL:H	1:65:A:LEU:H	6	0.1
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	15	0.1
(1,224)	1:42:A:LEU:H	1:43:A:SER:H	16	0.1
(1,218)	1:36:A:GLN:H	1:37:A:ILE:H	3	0.1
(1,217)	1:35:A:GLY:H	1:36:A:GLN:H	8	0.1
(1,208)	1:17:A:ILE:H	1:18:A:VAL:H	16	0.1
(1,202)	1:95:A:LEU:HA	1:99:A:ALA:H	6	0.1
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	4	0.1
(1,188)	1:95:A:LEU:HA	1:96:A:SER:H	15	0.1
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	13	0.1
(1,187)	1:94:A:ALA:HA	1:95:A:LEU:H	19	0.1
(1,183)	1:90:A:ASP:HA	1:91:A:GLU:H	15	0.1
(1,182)	1:89:A:GLU:HA	1:90:A:ASP:H	17	0.1
(1,178)	1:66:A:LYS:HA	1:69:A:GLN:H	13	0.1
(1,170)	1:69:A:GLN:HA	1:70:A:GLU:H	10	0.1
(1,163)	1:62:A:PHE:HA	1:63:A:THR:H	16	0.1
(1,159)	1:38:A:ALA:HA	1:41:A:LYS:H	18	0.1
(1,148)	1:38:A:ALA:HA	1:39:A:LEU:H	3	0.1
(1,147)	1:37:A:ILE:HA	1:38:A:ALA:H	6	0.1
(1,139)	1:22:A:LEU:HA	1:23:A:LYS:H	16	0.1
(1,137)	1:20:A:PHE:HA	1:21:A:ASN:H	8	0.1
(1,135)	1:18:A:VAL:HA	1:19:A:SER:H	11	0.1
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	9	0.1
(1,134)	1:17:A:ILE:HA	1:18:A:VAL:H	20	0.1
(1,133)	1:16:A:LYS:HA	1:17:A:ILE:H	13	0.1
(1,115)	1:8:A:VAL:H	1:52:A:LEU:HA	9	0.1
(1,114)	1:6:A:LEU:H	1:50:A:ILE:HA	6	0.1
(1,113)	1:106:A:PRO:HA	1:107:A:PHE:H	18	0.1
(1,111)	1:103:A:MET:HA	1:104:A:ARG:H	15	0.1
(1,109)	1:101:A:LYS:HA	1:102:A:VAL:H	4	0.1
(1,71)	1:86:A:GLY:HA2	1:87:A:GLY:H	18	0.1
(1,71)	1:86:A:GLY:HA3	1:87:A:GLY:H	18	0.1
(1,32)	1:99:A:ALA:HB1	1:100:A:ARG:HA	2	0.1
(1,32)	1:99:A:ALA:HB2	1:100:A:ARG:HA	2	0.1
(1,32)	1:99:A:ALA:HB3	1:100:A:ARG:HA	2	0.1

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

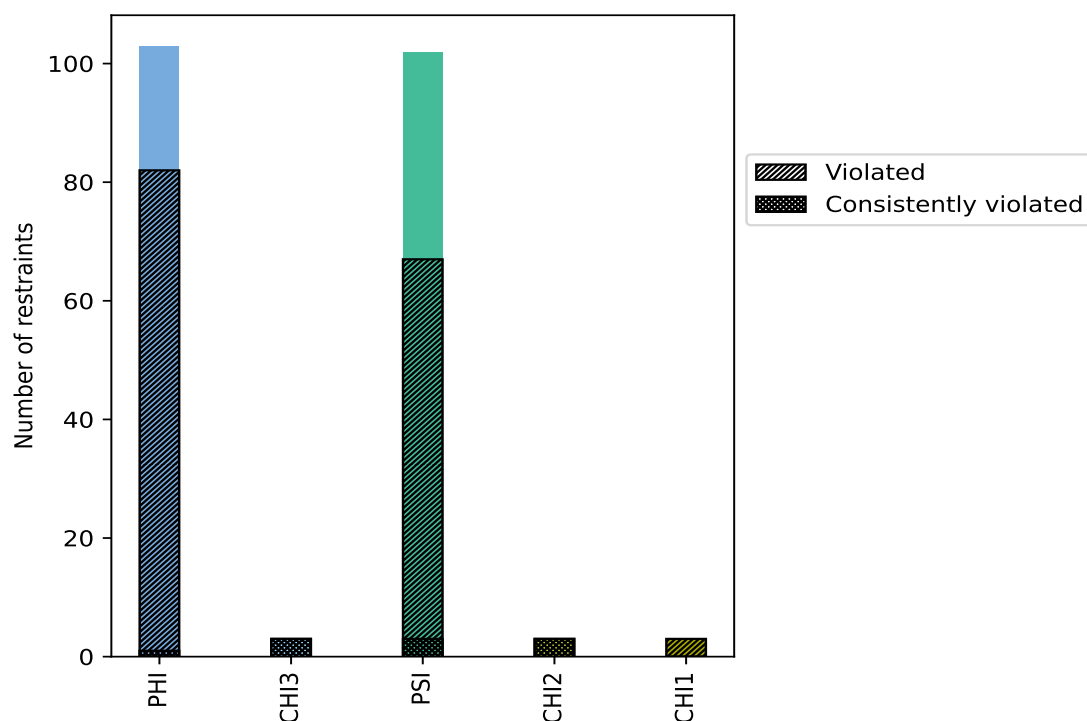
10.1 Summary of dihedral-angle violations [i](#)

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	103	48.1	82	79.6	38.3	1	1.0	0.5
CHI3	3	1.4	3	100.0	1.4	3	100.0	1.4
PSI	102	47.7	67	65.7	31.3	3	2.9	1.4
CHI2	3	1.4	3	100.0	1.4	3	100.0	1.4
CHI1	3	1.4	3	100.0	1.4	0	0.0	0.0
Total	214	100.0	158	73.8	73.8	10	4.7	4.7

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](#)



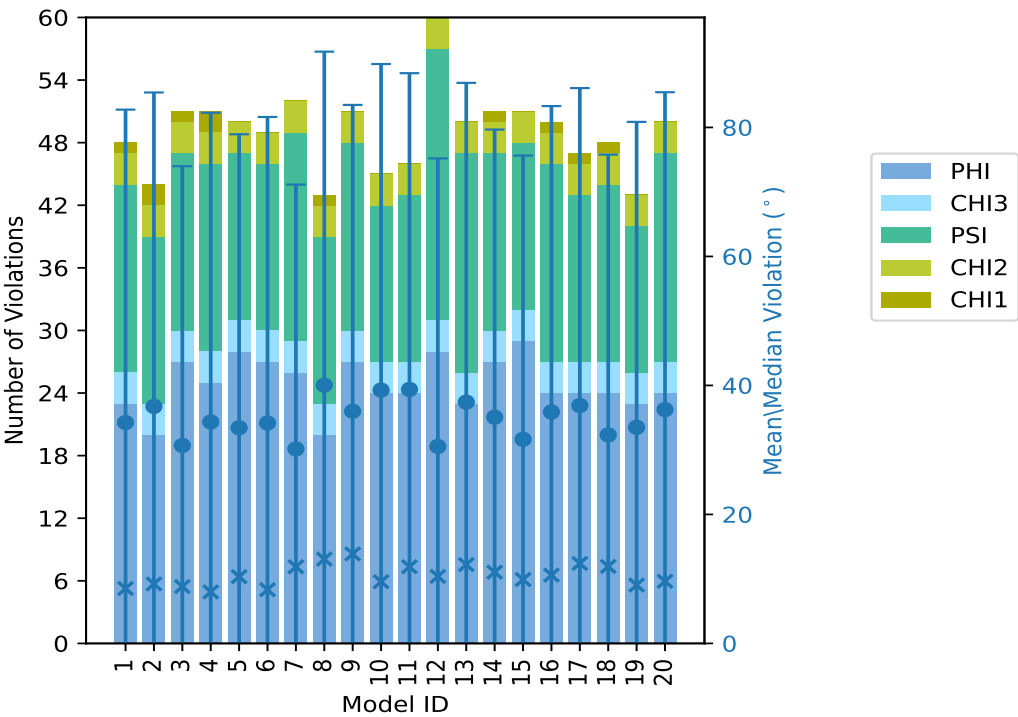
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	CHI3	PSI	CHI2	CHI1	Total				
1	23	3	18	3	1	48	34.25	156.6	48.51	8.52
2	20	3	16	3	2	44	36.74	155.5	48.68	9.23
3	27	3	17	3	1	51	30.68	152.03	43.31	8.82
4	25	3	18	3	2	51	34.34	149.93	47.93	7.99
5	28	3	16	3	0	50	33.43	160.12	45.51	10.35
6	27	3	16	3	0	49	34.17	151.5	47.45	8.33
7	26	3	20	3	0	52	30.16	140.47	40.98	11.89
8	20	3	16	3	1	43	40.04	146.32	51.71	13.07
9	27	3	18	3	0	51	36.0	159.7	47.49	13.88
10	24	3	15	3	0	45	39.28	154.89	50.55	9.57
11	24	3	16	3	0	46	39.38	158.24	49.03	11.89
12	28	3	26	3	0	60	30.54	155.35	44.66	10.39
13	23	3	21	3	0	50	37.41	155.85	49.5	12.22
14	27	3	17	3	1	51	35.07	147.75	44.6	11.05
15	29	3	16	3	0	51	31.64	154.87	44.0	9.91
16	24	3	19	3	1	50	35.88	149.9	47.43	10.59
17	24	3	16	3	1	47	36.88	157.07	49.22	12.4
18	24	3	17	3	1	48	32.33	141.28	43.46	11.93
19	23	3	14	3	0	43	33.51	147.39	47.35	9.05
20	24	3	20	3	0	50	36.25	158.32	49.21	9.64

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 ⓘ

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	CHI3	PSI	CHI2	CHI1	Total	Count ¹	%
15	0	19	0	0	34	1	5.0
3	0	10	0	1	14	2	10.0
9	0	3	0	1	13	3	15.0
15	0	6	0	0	21	4	20.0
5	0	6	0	0	11	5	25.0
8	0	6	0	1	15	6	30.0
3	0	2	0	0	5	7	35.0
6	0	1	0	0	7	8	40.0
2	0	1	0	0	3	9	45.0
2	0	2	0	0	4	10	50.0
3	0	4	0	0	7	11	55.0

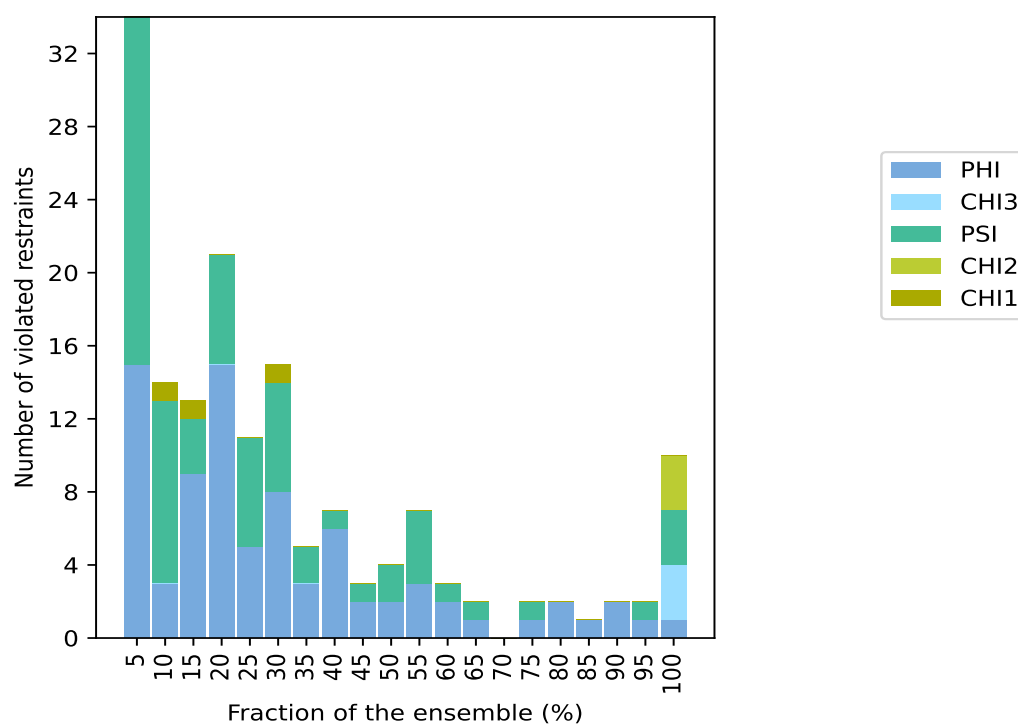
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Number of violated restraints						Fraction of the ensemble	
PHI	CHI3	PSI	CHI2	CHI1	Total	Count ¹	%
2	0	1	0	0	3	12	60.0
1	0	1	0	0	2	13	65.0
0	0	0	0	0	0	14	70.0
1	0	1	0	0	2	15	75.0
2	0	0	0	0	2	16	80.0
1	0	0	0	0	1	17	85.0
2	0	0	0	0	2	18	90.0
1	0	1	0	0	2	19	95.0
1	3	3	3	0	10	20	100.0

¹ Number of models with violations

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

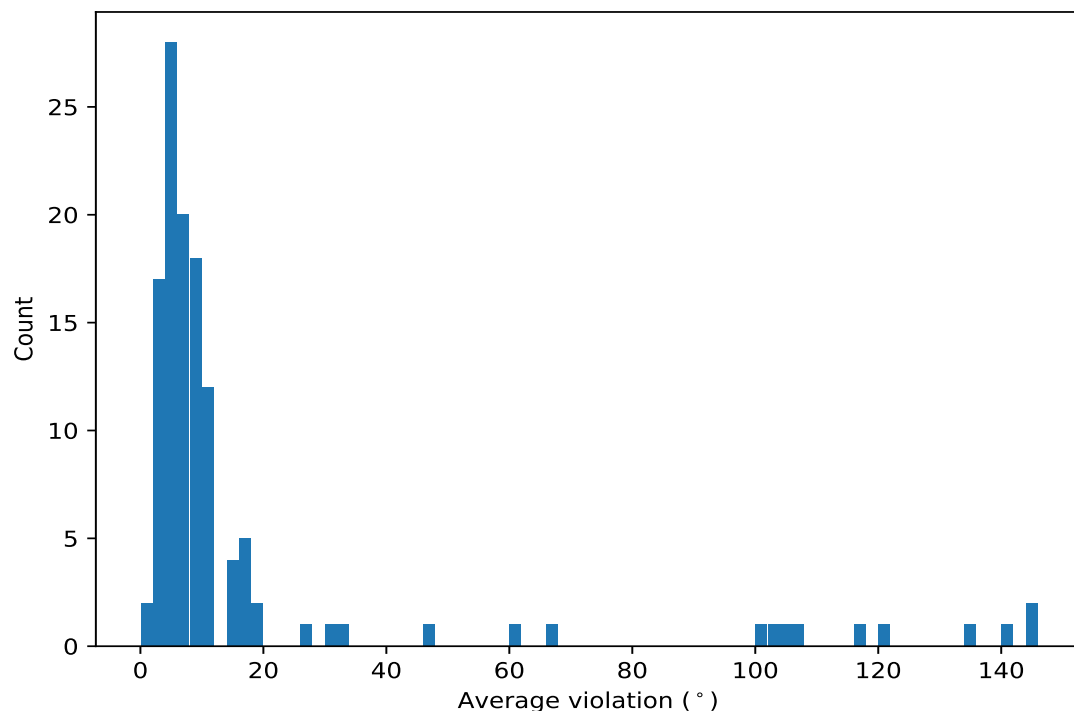


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [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	Media
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	20	145.39	8.23	147.1
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	20	144.3	12.6	145.7
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	20	134.14	5.29	133.2
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	20	107.23	18.96	112.9
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	20	103.52	15.54	100.0
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	20	101.59	28.79	116.8
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	20	67.1	25.86	78.74
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	20	61.7	27.8	48.96
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	20	33.34	26.94	20.34
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	20	26.67	17.74	21.58
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	19	141.75	6.26	141.2
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	19	105.2	6.73	105.0
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	18	47.78	7.82	48.0
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	18	30.63	15.38	31.36
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	17	117.31	36.38	130.9
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	16	19.9	13.11	17.4
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	16	16.43	8.67	15.1
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	15	121.35	10.39	120.1
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	15	6.07	3.48	5.19
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	13	14.26	10.05	11.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Media
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	13	8.24	4.86	9.05
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	12	18.0	12.05	13.5
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	12	8.77	5.3	7.12
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	12	6.53	4.97	4.24
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	11	16.74	9.68	14.4
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	11	16.66	9.47	12.1
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	11	11.74	11.37	6.79
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	11	8.44	7.09	8.53
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	11	7.32	5.53	6.42
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	11	6.97	6.29	4.02
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	11	5.64	3.07	5.59
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	10	11.58	6.35	12.1
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	10	10.04	6.75	7.31
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	10	6.51	3.21	5.86
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	10	5.97	4.97	3.9
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	9	16.27	12.43	11.0
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	9	7.28	4.32	5.39
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	9	6.77	5.16	4.54
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	8	11.73	5.66	11.8
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	8	9.61	9.32	6.26
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	8	8.14	5.73	7.29
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	8	6.49	4.18	4.68
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	8	5.96	2.88	5.63
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	8	5.14	3.01	4.31
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	8	3.58	1.84	3.6
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	7	14.01	6.14	13.5
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	7	11.94	4.44	11.0
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	7	9.99	3.28	9.78
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	7	8.75	4.77	8.22
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	7	3.29	1.98	2.89
(1,52)	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1:31:A:GLU:N	6	15.48	7.21	14.9
(1,140)	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1:83:A:THR:N	6	10.52	7.23	9.59
(1,137)	1:80:A:ILE:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	6	9.5	10.07	3.44
(1,3)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	6	9.38	8.9	5.01
(1,175)	1:104:A:ARG:C	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	6	8.03	4.43	8.52
(1,143)	1:87:A:GLY:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	6	6.8	5.15	5.44
(1,25)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	6	6.29	1.94	6.78
(1,67)	1:39:A:LEU:C	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	6	6.12	4.96	3.78
(1,118)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:GLU:N	6	5.78	5.39	2.83
(1,186)	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	1:112:A:PHE:N	6	5.67	3.44	5.49
(1,116)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLN:N	6	5.45	3.12	5.11
(1,153)	1:92:A:SER:C	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	6	5.44	3.64	5.26
(1,206)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	6	4.73	2.33	5.16
(1,151)	1:91:A:GLU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	6	4.62	1.83	5.01
(1,196)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:LYS:N	6	3.78	2.62	2.7
(1,155)	1:93:A:LEU:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	5	10.16	5.88	11.9
(1,145)	1:88:A:GLU:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	5	10.13	6.08	9.62
(1,146)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:ASP:N	5	9.65	3.09	9.08
(1,88)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:LEU:N	5	8.26	3.94	7.43
(1,76)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:PHE:N	5	7.66	4.81	9.84
(1,71)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	5	6.81	5.26	4.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Media
(1,105)	1:62:A:PHE:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	5	6.62	4.57	5.61
(1,7)	1:5:A:VAL:C	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	5	5.77	4.32	3.1
(1,60)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:ILE:N	5	5.48	3.86	3.7
(1,106)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:VAL:N	5	4.09	1.91	3.63
(1,24)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:ILE:N	5	3.18	1.41	2.77
(1,179)	1:107:A:PHE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	4	10.52	2.28	10.3
(1,127)	1:75:A:LYS:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	4	10.01	4.57	9.62
(1,149)	1:90:A:ASP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	4	8.74	4.48	8.1
(1,152)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:LEU:N	4	6.94	3.28	6.44
(1,147)	1:89:A:GLU:C	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	4	6.31	3.12	6.47
(1,205)	1:46:A:THR:C	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	4	6.13	3.66	6.56
(1,189)	1:112:A:PHE:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	4	6.11	3.72	5.81
(1,33)	1:20:A:PHE:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	4	5.92	4.58	3.76
(1,110)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:LYS:N	4	5.53	2.81	5.27
(1,111)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	4	5.44	3.02	5.51
(1,185)	1:110:A:SER:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	4	4.91	2.61	5.22
(1,29)	1:18:A:VAL:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	4	4.88	1.57	5.18
(1,119)	1:69:A:GLN:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	4	4.78	3.74	2.88
(1,21)	1:14:A:LEU:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	4	4.68	1.44	4.86
(1,164)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ALA:N	4	4.35	2.76	3.56
(1,22)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LYS:N	4	4.34	1.96	4.68
(1,193)	1:114:A:GLU:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	4	4.1	2.82	3.1
(1,187)	1:111:A:GLN:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	4	3.38	1.51	2.7
(1,134)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:ILE:N	4	3.26	2.67	1.88
(1,38)	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	1:24:A:LYS:N	4	2.8	0.91	2.46
(1,197)	1:116:A:VAL:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	4	2.25	0.46	2.16
(1,55)	1:32:A:ALA:C	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	3	16.45	5.54	16.7
(1,123)	1:72:A:GLU:C	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	3	10.94	9.99	5.9
(1,141)	1:82:A:LEU:C	1:83:A:THR:N	1:83:A:THR:CA	1:83:A:THR:C	3	9.05	9.6	2.9
(1,136)	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	1:81:A:VAL:N	3	8.22	4.95	9.76
(1,35)	1:21:A:ASN:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	3	7.88	5.69	6.2
(1,128)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ILE:N	3	7.24	3.25	8.66
(1,182)	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:C	1:110:A:SER:N	3	4.76	2.95	3.11
(1,209)	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	3	4.51	0.6	4.85
(1,37)	1:22:A:LEU:C	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	3	4.35	1.4	4.72
(1,23)	1:15:A:ARG:C	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	3	4.31	2.87	3.82
(1,191)	1:113:A:ILE:C	1:114:A:GLU:N	1:114:A:GLU:CA	1:114:A:GLU:C	3	3.11	0.75	3.35
(1,27)	1:17:A:ILE:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	3	2.5	1.7	1.5
(1,159)	1:95:A:LEU:C	1:96:A:SER:N	1:96:A:SER:CA	1:96:A:SER:C	3	2.11	0.47	1.8
(1,144)	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	1:89:A:GLU:N	2	14.61	4.5	14.6
(1,113)	1:66:A:LYS:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	2	11.87	4.53	11.8
(1,172)	1:103:A:MET:N	1:103:A:MET:CA	1:103:A:MET:C	1:104:A:ARG:N	2	9.35	4.3	9.35
(1,53)	1:30:A:ILE:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	2	9.14	1.75	9.14
(1,184)	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	1:111:A:GLN:N	2	8.61	0.49	8.61
(1,112)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	2	5.73	3.45	5.73
(1,28)	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1:19:A:SER:N	2	3.92	1.06	3.92
(1,138)	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	1:82:A:LEU:N	2	3.73	0.45	3.73
(1,32)	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	1:21:A:ASN:N	2	3.66	2.57	3.66
(1,109)	1:64:A:VAL:C	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	2	3.61	0.14	3.61
(1,64)	1:38:A:ALA:N	1:38:A:ALA:CA	1:38:A:ALA:C	1:39:A:LEU:N	2	3.43	1.73	3.43
(1,212)	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	2	3.38	2.02	3.38

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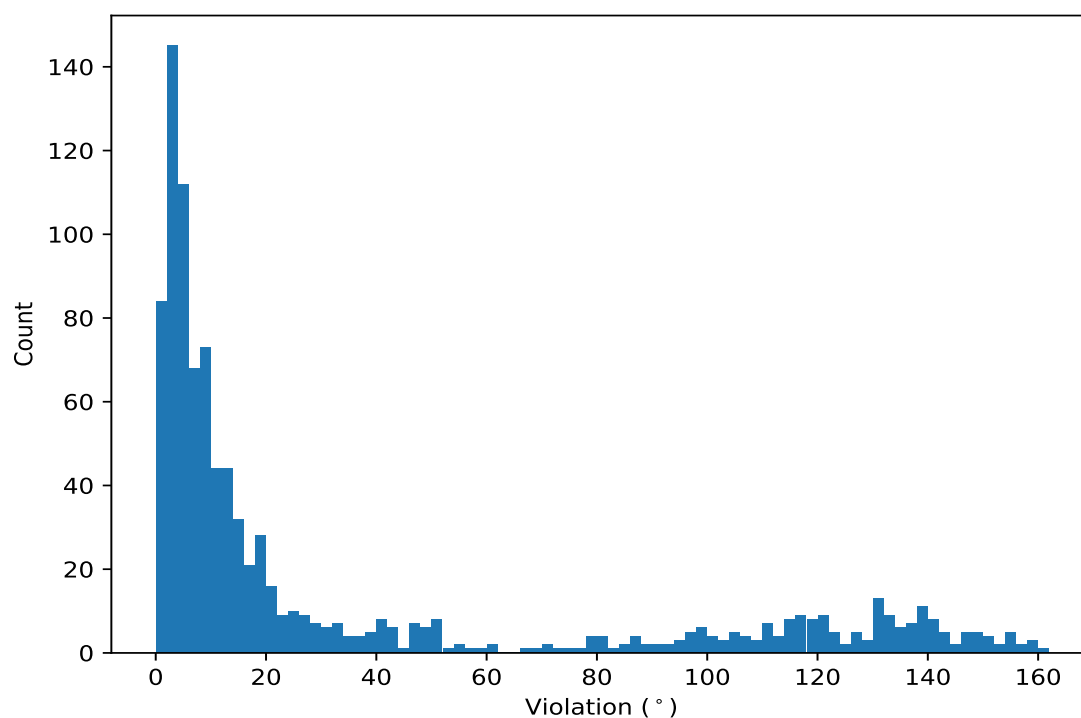
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Media
(1,26)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	2	1.37	0.11	1.37
(1,198)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:HIS:N	2	1.27	0.26	1.27

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	5	160.12
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	9	159.7
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	20	158.32
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	11	158.24
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	17	157.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	1	156.6
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	13	155.85
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	2	155.5
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	12	155.35
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	10	154.89
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	15	154.87
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	20	152.14
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	3	152.03
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	5	151.53
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	6	151.5
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	9	150.68
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	12	150.28
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	4	149.93
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	16	149.9
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	9	149.8
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	2	148.86
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	13	148.02
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	14	147.75
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	4	147.62
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	19	147.39
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	6	147.35
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	8	146.32
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	10	145.98
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	10	144.16
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	9	143.06
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	1	142.8
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	20	142.67
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	13	142.57
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	20	142.13
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	5	141.51
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	18	141.28
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	3	141.03
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	2	140.84
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	8	140.79
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	11	140.59
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	7	140.47
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	12	140.39
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	10	139.76
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	8	139.5
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	7	139.45
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	11	139.32
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	19	139.26
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	15	138.89
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	16	138.72
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	20	138.36
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	13	138.35
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	16	138.28
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	5	138.05
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	8	137.67
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	18	137.31
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	4	136.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	1	136.65
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	13	136.31
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	11	136.28
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	15	136.26
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	12	135.86
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	17	135.78
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	16	135.52
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	8	135.51
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	7	135.3
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	3	135.2
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	17	133.83
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	10	133.71
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	14	133.68
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	18	133.48
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	4	133.4
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	10	132.89
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	3	132.84
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	18	132.42
(1,178)	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	1:108:A:SER:N	12	132.04
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	14	131.94
(1,94)	1:54:A:ILE:N	1:54:A:ILE:CA	1:54:A:ILE:C	1:55:A:MET:N	19	131.84
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	1	131.66
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	17	131.19
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1	131.18
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	11	130.94
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	6	130.88
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	17	130.87
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	2	130.63
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	15	130.41
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	7	130.27
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	13	130.25
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	19	130.11
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	20	129.37
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	6	129.28
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	9	128.24
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	17	127.18
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	8	126.92
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	14	126.72
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	4	126.44
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	10	126.28
(1,99)	1:57:A:PRO:C	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	18	125.3
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	4	124.11
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	15	123.82
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	13	122.81
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	16	122.77
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	14	122.53
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	2	122.07
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	17	121.87
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	19	121.8
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	11	121.35
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	16	121.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	8	120.52
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	3	120.36
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	1	120.23
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	4	120.17
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	4	120.15
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	6	119.56
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	14	119.41
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	2	119.15
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	11	118.9
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	8	118.62
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	9	118.62
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	9	118.51
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	13	118.04
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	8	117.47
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	5	117.29
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	17	117.24
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	20	117.15
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	15	117.09
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	14	116.88
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	11	116.47
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	13	116.41
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	7	116.12
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	12	115.79
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	19	115.74
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	6	115.47
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	6	114.79
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	5	114.65
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	12	114.62
(1,58)	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	1:35:A:GLY:N	6	114.27
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	11	114.16
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	5	113.69
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	16	113.33
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	20	112.6
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	16	112.6
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	1	111.6
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	19	111.21
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	18	111.16
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1	111.13
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	3	110.81
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	15	110.55
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	8	110.39
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1	109.43
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	16	108.87
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	18	108.7
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	4	107.42
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	2	107.4
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	12	107.04
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	6	106.32
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	13	105.04
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	19	104.75
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	17	104.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	16	104.12
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	19	104.09
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	17	103.93
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	3	103.64
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	7	102.61
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	14	101.14
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	6	100.64
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	7	100.36
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	12	100.26
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	10	99.9
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	20	99.18
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	10	99.12
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	9	98.88
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	14	98.21
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	18	98.1
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	9	97.94
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	2	97.54
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	12	97.41
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	8	97.21
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	3	96.82
(1,78)	1:45:A:PHE:N	1:45:A:PHE:CA	1:45:A:PHE:C	1:46:A:THR:N	2	94.73
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	9	94.57
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	17	94.29
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	2	92.21
(1,95)	1:54:A:ILE:C	1:55:A:MET:N	1:55:A:MET:CA	1:55:A:MET:C	10	92.13
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	14	91.44
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	11	91.29
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	15	89.92
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	4	89.84
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	1	87.62
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	16	87.11
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	14	86.67
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	13	86.51
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	5	85.87
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	15	85.18
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	1	82.63
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	7	81.95
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	3	81.51
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	20	81.45
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	5	80.4
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	20	79.44
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	10	79.42
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	4	78.8
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	7	78.05
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	12	76.72
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	11	75.24
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	6	72.28
(1,102)	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	1:60:A:ASP:N	2	71.55
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	18	71.34
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	9	68.5
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	5	67.87

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	10	60.47
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	15	60.03
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	11	58.2
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	4	56.87
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	2	55.87
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	9	54.15
(1,210)	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	20	53.03
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	18	51.95
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	19	51.93
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	20	51.52
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	5	51.48
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	12	51.44
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	16	51.18
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	11	50.62
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	11	50.12
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	7	49.7
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	5	49.42
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	15	49.11
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	3	48.99
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	6	48.93
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	20	48.17
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	9	47.82
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	16	47.54
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	10	47.36
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	18	47.16
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	17	46.8
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	10	46.27
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	13	46.22
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	3	44.58
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	7	43.28
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	5	43.01
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	14	42.86
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	5	42.78
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	4	42.24
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	16	42.11
(1,207)	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	4	41.7
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	14	41.33
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	15	41.29
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	14	41.2
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	7	41.02
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	13	40.81
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	18	40.53
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	15	40.14
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	16	39.9
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	2	39.4
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	10	38.71
(1,213)	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1	38.46
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	12	38.1
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	3	37.23
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	14	36.64
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	13	36.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	20	36.34
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	4	35.68
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	10	34.56
(1,57)	1:33:A:GLU:C	1:34:A:ASN:N	1:34:A:ASN:CA	1:34:A:ASN:C	6	34.2
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	7	34.15
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	8	33.84
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	9	33.68
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	9	32.88
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	7	32.77
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	17	32.54
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	16	32.38
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	14	32.19
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	15	31.94
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	5	31.79
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	7	30.69
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	20	30.63
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	6	30.54
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	7	30.5
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	3	29.93
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	1	29.22
(1,137)	1:80:A:ILE:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	18	28.92
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	6	28.92
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	8	28.89
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	9	28.81
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	17	28.72
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	11	27.51
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	12	26.97
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	6	26.79
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	13	26.74
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	14	26.7
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	18	26.68
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	5	26.66
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	19	26.66
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	8	26.05
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	1	25.85
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	6	25.65
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	14	25.5
(1,3)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	19	25.35
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	19	25.04
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	2	24.95
(1,123)	1:72:A:GLU:C	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	14	24.9
(1,52)	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1:31:A:GLU:N	5	24.64
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	13	24.54
(1,163)	1:97:A:LEU:C	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	12	24.14
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	15	23.41
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	3	23.19
(1,55)	1:32:A:ALA:C	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	8	23.09
(1,140)	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1:83:A:THR:N	3	22.72
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	5	22.71
(1,141)	1:82:A:LEU:C	1:83:A:THR:N	1:83:A:THR:CA	1:83:A:THR:C	3	22.61
(1,52)	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1:31:A:GLU:N	7	22.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	20	22.24
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	3	22.02
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	12	21.94
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	15	21.82
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	13	21.56
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	12	21.49
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	3	21.31
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	16	21.31
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	9	21.29
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	15	21.15
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	10	20.91
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	8	20.73
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	6	20.69
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	14	20.62
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	9	20.4
(1,145)	1:88:A:GLU:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	18	20.36
(1,70)	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	1:42:A:LEU:N	20	20.2
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	9	20.0
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	11	19.99
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	9	19.96
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	17	19.92
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	16	19.88
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	13	19.71
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	15	19.52
(1,79)	1:45:A:PHE:C	1:46:A:THR:N	1:46:A:THR:CA	1:46:A:THR:C	18	19.43
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	14	19.39
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	20	19.33
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	19	19.28
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	13	19.24
(1,144)	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	1:89:A:GLU:N	18	19.11
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	19	19.05
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	15	19.03
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	18	19.01
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	15	19.0
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	4	18.9
(1,155)	1:93:A:LEU:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	2	18.82
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	12	18.81
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	12	18.77
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	12	18.76
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	11	18.75
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	2	18.75
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	3	18.61
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	13	18.5
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	13	18.35
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1	18.27
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	8	18.0
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	1	17.94
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	18	17.72
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	11	17.41
(1,3)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	3	17.35
(1,143)	1:87:A:GLY:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	18	16.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	9	16.95
(1,127)	1:75:A:LYS:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	16	16.76
(1,55)	1:32:A:ALA:C	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	10	16.74
(1,137)	1:80:A:ILE:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	4	16.67
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	18	16.64
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	9	16.58
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	7	16.46
(1,113)	1:66:A:LYS:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1	16.4
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	18	16.35
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1	16.34
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	20	16.23
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	19	16.23
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	14	16.18
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	11	16.07
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	8	16.06
(1,67)	1:39:A:LEU:C	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	10	16.01
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	11	15.94
(1,214)	1:109:A:PRO:CB	1:109:A:PRO:CG	1:109:A:PRO:CD	1:109:A:PRO:N	17	15.91
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	2	15.83
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	9	15.82
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	2	15.79
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	7	15.71
(1,35)	1:21:A:ASN:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	13	15.54
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	6	15.54
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	13	15.47
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	9	15.44
(1,140)	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1:83:A:THR:N	4	15.33
(1,118)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:GLU:N	16	15.29
(1,149)	1:90:A:ASP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	11	15.23
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	14	15.17
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	18	15.17
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	8	15.16
(1,52)	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1:31:A:GLU:N	14	15.1
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	17	15.08
(1,105)	1:62:A:PHE:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	9	15.06
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	5	14.99
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	7	14.87
(1,52)	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1:31:A:GLU:N	17	14.85
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	20	14.68
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	12	14.63
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	4	14.62
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	12	14.49
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	2	14.32
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	2	14.2
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	6	14.19
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	20	14.13
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	6	14.08
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	1	14.0
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	5	13.99
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	7	13.95
(1,179)	1:107:A:PHE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	3	13.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,175)	1:104:A:ARG:C	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	16	13.89
(1,88)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:LEU:N	20	13.88
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	9	13.88
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	12	13.85
(1,52)	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1:31:A:GLU:N	12	13.85
(1,33)	1:20:A:PHE:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	17	13.68
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	17	13.67
(1,172)	1:103:A:MET:N	1:103:A:MET:CA	1:103:A:MET:C	1:104:A:ARG:N	11	13.65
(1,146)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:ASP:N	3	13.64
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	8	13.59
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	7	13.54
(1,76)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:PHE:N	16	13.41
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	8	13.4
(1,136)	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	1:81:A:VAL:N	4	13.36
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	12	13.34
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	17	13.34
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	13	13.26
(1,140)	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1:83:A:THR:N	17	13.17
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	9	13.09
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	15	13.08
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	8	13.07
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	17	12.83
(1,155)	1:93:A:LEU:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	7	12.78
(1,146)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:ASP:N	11	12.78
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	7	12.76
(1,168)	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	1:102:A:VAL:N	8	12.65
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	6	12.65
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	13	12.59
(1,145)	1:88:A:GLU:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	7	12.55
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	4	12.51
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	20	12.46
(1,8)	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	1:7:A:LEU:N	7	12.43
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	17	12.4
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	18	12.35
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	16	12.29
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	5	12.24
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	12	12.21
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	5	12.12
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	3	12.11
(1,7)	1:5:A:VAL:C	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	6	12.09
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	19	12.08
(1,175)	1:104:A:ARG:C	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	12	11.97
(1,155)	1:93:A:LEU:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	15	11.95
(1,152)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:LEU:N	9	11.94
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	19	11.93
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	5	11.9
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	13	11.86
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	10	11.82
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	16	11.61
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	14	11.55
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	18	11.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	10	11.52
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	12	11.5
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	18	11.48
(1,88)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:LEU:N	9	11.41
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	7	11.35
(1,60)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:ILE:N	8	11.27
(1,119)	1:69:A:GLN:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	12	11.19
(1,76)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:PHE:N	4	11.18
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	5	11.12
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	16	11.07
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	18	11.06
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	17	11.06
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	14	11.05
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1	11.02
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	11	11.0
(1,118)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:GLU:N	14	10.96
(1,116)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLN:N	19	10.96
(1,179)	1:107:A:PHE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	12	10.94
(1,53)	1:30:A:ILE:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	5	10.88
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	11	10.77
(1,161)	1:96:A:SER:C	1:97:A:LEU:N	1:97:A:LEU:CA	1:97:A:LEU:C	13	10.75
(1,127)	1:75:A:LYS:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	15	10.68
(1,189)	1:112:A:PHE:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	17	10.66
(1,153)	1:92:A:SER:C	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	15	10.55
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	10	10.46
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	19	10.42
(1,186)	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	1:112:A:PHE:N	1	10.39
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	13	10.39
(1,149)	1:90:A:ASP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	14	10.31
(1,128)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ILE:N	15	10.31
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	2	10.22
(1,175)	1:104:A:ARG:C	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	20	10.2
(1,205)	1:46:A:THR:C	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	16	10.11
(1,144)	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	1:89:A:GLU:N	1	10.11
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	15	9.91
(1,7)	1:5:A:VAL:C	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	11	9.85
(1,76)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:PHE:N	12	9.84
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	5	9.82
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	11	9.78
(1,147)	1:89:A:GLU:C	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	4	9.77
(1,136)	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	1:81:A:VAL:N	18	9.76
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	5	9.72
(1,110)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:LYS:N	14	9.7
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	14	9.68
(1,179)	1:107:A:PHE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	11	9.65
(1,145)	1:88:A:GLU:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	19	9.62
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	6	9.6
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	10	9.57
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	17	9.55
(1,55)	1:32:A:ALA:C	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	15	9.53
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	18	9.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	14	9.44
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	16	9.41
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	7	9.41
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	2	9.39
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	14	9.38
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	3	9.37
(1,196)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:LYS:N	1	9.32
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	9	9.27
(1,205)	1:46:A:THR:C	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	18	9.18
(1,112)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	12	9.18
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	3	9.17
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	10	9.11
(1,184)	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	1:111:A:GLN:N	7	9.1
(1,146)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:ASP:N	20	9.08
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	2	9.07
(1,34)	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	1:22:A:LEU:N	13	9.06
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	19	9.05
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	19	9.05
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	10	9.04
(1,147)	1:89:A:GLU:C	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	15	8.98
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	4	8.97
(1,186)	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	1:112:A:PHE:N	17	8.95
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	15	8.94
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	5	8.91
(1,189)	1:112:A:PHE:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	5	8.9
(1,182)	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:C	1:110:A:SER:N	11	8.9
(1,143)	1:87:A:GLY:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	4	8.89
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	13	8.83
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	3	8.82
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	9	8.82
(1,60)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:ILE:N	2	8.77
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	16	8.76
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	9	8.74
(1,164)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ALA:N	12	8.73
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	13	8.68
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	1	8.68
(1,67)	1:39:A:LEU:C	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	13	8.67
(1,128)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ILE:N	16	8.66
(1,193)	1:114:A:GLU:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	9	8.63
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	12	8.61
(1,127)	1:75:A:LYS:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	7	8.55
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	20	8.53
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	12	8.49
(1,201)	1:118:A:HIS:C	1:119:A:LEU:N	1:119:A:LEU:CA	1:119:A:LEU:C	11	8.45
(1,115)	1:67:A:LYS:C	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	17	8.44
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	2	8.42
(1,153)	1:92:A:SER:C	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1	8.35
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	8	8.35
(1,25)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	6	8.33
(1,177)	1:106:A:PRO:C	1:107:A:PHE:N	1:107:A:PHE:CA	1:107:A:PHE:C	3	8.28
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	20	8.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	1:111:A:GLN:N	11	8.12
(1,25)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	5	8.12
(1,23)	1:15:A:ARG:C	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	3	8.05
(1,153)	1:92:A:SER:C	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	13	8.04
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	8	8.04
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	4	7.99
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	5	7.94
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	14	7.9
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	19	7.88
(1,134)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:ILE:N	11	7.85
(1,185)	1:110:A:SER:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	4	7.82
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	10	7.77
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	19	7.71
(1,179)	1:107:A:PHE:C	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1	7.61
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	11	7.53
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	18	7.45
(1,186)	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	1:112:A:PHE:N	4	7.44
(1,88)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:LEU:N	12	7.43
(1,106)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:VAL:N	7	7.41
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	11	7.39
(1,53)	1:30:A:ILE:C	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	7	7.39
(1,113)	1:66:A:LYS:C	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	2	7.34
(1,152)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:LEU:N	15	7.31
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	6	7.31
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	10	7.29
(1,206)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	3	7.28
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	5	7.28
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	3	7.25
(1,206)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	8	7.24
(1,116)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLN:N	5	7.24
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	3	7.24
(1,101)	1:58:A:VAL:C	1:59:A:MET:N	1:59:A:MET:CA	1:59:A:MET:C	7	7.21
(1,151)	1:91:A:GLU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	11	7.2
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	17	7.2
(1,105)	1:62:A:PHE:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	2	7.17
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	10	7.09
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	14	7.04
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	15	7.03
(1,14)	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	1:12:A:ALA:N	8	7.01
(1,185)	1:110:A:SER:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	20	6.98
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	10	6.92
(1,25)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	8	6.91
(1,75)	1:43:A:SER:C	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	18	6.9
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	4	6.89
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	7	6.89
(1,175)	1:104:A:ARG:C	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	3	6.84
(1,111)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	12	6.79
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	11	6.79
(1,146)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:ASP:N	12	6.73
(1,43)	1:25:A:GLU:C	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	4	6.73
(1,22)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LYS:N	2	6.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	3	6.67
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	19	6.66
(1,25)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	19	6.65
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	15	6.57
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	14	6.55
(1,29)	1:18:A:VAL:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	19	6.55
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	15	6.53
(1,71)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	13	6.52
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	17	6.42
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	12	6.37
(1,21)	1:14:A:LEU:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1	6.37
(1,3)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	4	6.25
(1,32)	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	1:21:A:ASN:N	8	6.23
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	1	6.22
(1,35)	1:21:A:ASN:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	7	6.2
(1,206)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	16	6.13
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	13	6.12
(1,29)	1:18:A:VAL:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	3	6.12
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	2	6.11
(1,146)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:ASP:N	17	6.04
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1	6.0
(1,140)	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1:83:A:THR:N	7	6.0
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	15	5.96
(1,187)	1:111:A:GLN:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	17	5.95
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	9	5.95
(1,143)	1:87:A:GLY:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	5	5.94
(1,149)	1:90:A:ASP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	2	5.9
(1,123)	1:72:A:GLU:C	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	18	5.9
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	6	5.9
(1,110)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:LYS:N	17	5.89
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	11	5.88
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	4	5.87
(1,37)	1:22:A:LEU:C	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	15	5.86
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	20	5.84
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	12	5.84
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	6	5.82
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	7	5.76
(1,87)	1:50:A:ILE:C	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	16	5.72
(1,88)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:LEU:N	13	5.63
(1,105)	1:62:A:PHE:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	10	5.61
(1,21)	1:14:A:LEU:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	9	5.61
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	1	5.6
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	13	5.59
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	10	5.59
(1,1)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	12	5.58
(1,152)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:LEU:N	13	5.56
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	16	5.5
(1,116)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLN:N	17	5.48
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	8	5.41
(1,212)	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	1	5.4
(1,151)	1:91:A:GLU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	9	5.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	4	5.39
(1,151)	1:91:A:GLU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	17	5.38
(1,211)	1:78:A:PRO:CB	1:78:A:PRO:CG	1:78:A:PRO:CD	1:78:A:PRO:N	11	5.36
(1,97)	1:55:A:MET:C	1:56:A:MET:N	1:56:A:MET:CA	1:56:A:MET:C	3	5.35
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	18	5.31
(1,165)	1:99:A:ALA:C	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	8	5.27
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	17	5.21
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	13	5.21
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	5	5.2
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	15	5.19
(1,64)	1:38:A:ALA:N	1:38:A:ALA:CA	1:38:A:ALA:C	1:39:A:LEU:N	15	5.16
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	12	5.13
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	16	5.06
(1,172)	1:103:A:MET:N	1:103:A:MET:CA	1:103:A:MET:C	1:104:A:ARG:N	7	5.05
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	14	5.05
(1,22)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LYS:N	9	5.05
(1,25)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	7	5.04
(1,209)	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	4	5.02
(1,28)	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1:19:A:SER:N	3	4.97
(1,24)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:ILE:N	6	4.97
(1,143)	1:87:A:GLY:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	20	4.93
(1,44)	1:26:A:GLY:N	1:26:A:GLY:CA	1:26:A:GLY:C	1:27:A:TYR:N	19	4.92
(1,33)	1:20:A:PHE:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	6	4.9
(1,27)	1:17:A:ILE:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	2	4.9
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	5	4.88
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	7	4.87
(1,209)	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	2	4.85
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	16	4.8
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	2	4.8
(1,167)	1:100:A:ARG:C	1:101:A:LYS:N	1:101:A:LYS:CA	1:101:A:LYS:C	9	4.79
(1,116)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLN:N	3	4.73
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	8	4.72
(1,37)	1:22:A:LEU:C	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	8	4.72
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	1	4.72
(1,155)	1:93:A:LEU:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	1	4.71
(1,106)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:VAL:N	16	4.69
(1,24)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:ILE:N	5	4.66
(1,110)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:LYS:N	4	4.65
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	4	4.65
(1,151)	1:91:A:GLU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	12	4.64
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	2	4.64
(1,164)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ALA:N	18	4.62
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	19	4.56
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	17	4.56
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	3	4.55
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	14	4.54
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	8	4.5
(1,190)	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	1:114:A:GLU:N	11	4.48
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	7	4.48
(1,114)	1:67:A:LYS:N	1:67:A:LYS:CA	1:67:A:LYS:C	1:68:A:LEU:N	16	4.48
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	20	4.38

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	1	4.37
(1,194)	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	1:116:A:VAL:N	13	4.35
(1,38)	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	1:24:A:LYS:N	13	4.34
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	16	4.34
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	13	4.32
(1,193)	1:114:A:GLU:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	11	4.31
(1,71)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	14	4.31
(1,145)	1:88:A:GLU:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	3	4.3
(1,22)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LYS:N	1	4.3
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	20	4.29
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	3	4.25
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	15	4.25
(1,196)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:LYS:N	14	4.24
(1,111)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	17	4.23
(1,29)	1:18:A:VAL:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	11	4.23
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	15	4.23
(1,206)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	4	4.19
(1,71)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	7	4.19
(1,138)	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	1:82:A:LEU:N	7	4.18
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	17	4.14
(1,21)	1:14:A:LEU:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	5	4.11
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	12	4.1
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	14	4.1
(1,90)	1:52:A:LEU:N	1:52:A:LEU:CA	1:52:A:LEU:C	1:53:A:ASP:N	16	4.09
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	4	4.08
(1,127)	1:75:A:LYS:C	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	20	4.05
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	9	4.03
(1,67)	1:39:A:LEU:C	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	5	4.03
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	10	4.03
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	3	4.02
(1,175)	1:104:A:ARG:C	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	6	4.01
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	6	4.01
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	20	3.99
(1,180)	1:108:A:SER:N	1:108:A:SER:CA	1:108:A:SER:C	1:109:A:PRO:N	14	3.97
(1,147)	1:89:A:GLU:C	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	12	3.96
(1,205)	1:46:A:THR:C	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	3	3.95
(1,191)	1:113:A:ILE:C	1:114:A:GLU:N	1:114:A:GLU:CA	1:114:A:GLU:C	1	3.88
(1,151)	1:91:A:GLU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	6	3.88
(1,18)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:LEU:N	16	3.85
(1,41)	1:24:A:LYS:C	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1	3.84
(1,23)	1:15:A:ARG:C	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	19	3.82
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	9	3.81
(1,145)	1:88:A:GLU:C	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	12	3.8
(1,137)	1:80:A:ILE:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	19	3.79
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	9	3.79
(1,3)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1	3.78
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	7	3.77
(1,109)	1:64:A:VAL:C	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	4	3.74
(1,45)	1:26:A:GLY:C	1:27:A:TYR:N	1:27:A:TYR:CA	1:27:A:TYR:C	16	3.73
(1,60)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:ILE:N	3	3.7
(1,209)	1:78:A:PRO:N	1:78:A:PRO:CA	1:78:A:PRO:CB	1:78:A:PRO:CG	14	3.67

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	11	3.66
(1,208)	1:47:A:PRO:CB	1:47:A:PRO:CG	1:47:A:PRO:CD	1:47:A:PRO:N	10	3.65
(1,106)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:VAL:N	19	3.63
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	4	3.62
(1,118)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:GLU:N	12	3.58
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	10	3.57
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	15	3.57
(1,119)	1:69:A:GLN:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1	3.56
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	9	3.55
(1,200)	1:118:A:HIS:N	1:118:A:HIS:CA	1:118:A:HIS:C	1:119:A:LEU:N	18	3.54
(1,186)	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	1:112:A:PHE:N	18	3.54
(1,67)	1:39:A:LEU:C	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	20	3.53
(1,36)	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	1:23:A:LYS:N	7	3.53
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	8	3.51
(1,149)	1:90:A:ASP:C	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	3	3.5
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	14	3.48
(1,109)	1:64:A:VAL:C	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	14	3.47
(1,185)	1:110:A:SER:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	18	3.45
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	4	3.45
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	16	3.43
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	20	3.41
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	5	3.4
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	4	3.4
(1,124)	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	1:74:A:TRP:N	1	3.39
(1,191)	1:113:A:ILE:C	1:114:A:GLU:N	1:114:A:GLU:CA	1:114:A:GLU:C	2	3.35
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	20	3.3
(1,67)	1:39:A:LEU:C	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	18	3.29
(1,138)	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	1:82:A:LEU:N	9	3.28
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	17	3.24
(1,116)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLN:N	16	3.23
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	12	3.21
(1,139)	1:81:A:VAL:C	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	20	3.19
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	5	3.19
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	2	3.16
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	20	3.13
(1,140)	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1:83:A:THR:N	19	3.12
(1,182)	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:C	1:110:A:SER:N	3	3.11
(1,7)	1:5:A:VAL:C	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	15	3.1
(1,137)	1:80:A:ILE:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	11	3.08
(1,199)	1:117:A:LYS:C	1:118:A:HIS:N	1:118:A:HIS:CA	1:118:A:HIS:C	18	3.05
(1,48)	1:28:A:GLU:N	1:28:A:GLU:CA	1:28:A:GLU:C	1:29:A:VAL:N	6	3.05
(1,108)	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	1:65:A:LEU:N	14	3.04
(1,42)	1:25:A:GLU:N	1:25:A:GLU:CA	1:25:A:GLU:C	1:26:A:GLY:N	4	3.01
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	10	3.01
(1,137)	1:80:A:ILE:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	10	3.0
(1,143)	1:87:A:GLY:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	1	2.98
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	15	2.98
(1,197)	1:116:A:VAL:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	9	2.97
(1,187)	1:111:A:GLN:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	5	2.96
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	12	2.96
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	6	2.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,106)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:VAL:N	4	2.94
(1,152)	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	1:93:A:LEU:N	7	2.93
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	12	2.93
(1,88)	1:51:A:VAL:N	1:51:A:VAL:CA	1:51:A:VAL:C	1:52:A:LEU:N	11	2.93
(1,141)	1:82:A:LEU:C	1:83:A:THR:N	1:83:A:THR:CA	1:83:A:THR:C	7	2.9
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	5	2.89
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	13	2.89
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:PHE:N	19	2.89
(1,28)	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	1:19:A:SER:N	20	2.86
(1,105)	1:62:A:PHE:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	14	2.84
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	11	2.84
(1,140)	1:82:A:LEU:N	1:82:A:LEU:CA	1:82:A:LEU:C	1:83:A:THR:N	8	2.81
(1,196)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:LYS:N	10	2.78
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	20	2.77
(1,159)	1:95:A:LEU:C	1:96:A:SER:N	1:96:A:SER:CA	1:96:A:SER:C	16	2.77
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	5	2.77
(1,24)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:ILE:N	3	2.77
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	18	2.75
(1,128)	1:76:A:ARG:N	1:76:A:ARG:CA	1:76:A:ARG:C	1:77:A:ILE:N	20	2.74
(1,189)	1:112:A:PHE:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	10	2.72
(1,25)	1:16:A:LYS:C	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	9	2.67
(1,196)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:LYS:N	18	2.63
(1,33)	1:20:A:PHE:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	15	2.62
(1,29)	1:18:A:VAL:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	4	2.62
(1,21)	1:14:A:LEU:C	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	20	2.61
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	7	2.58
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	9	2.58
(1,155)	1:93:A:LEU:C	1:94:A:ALA:N	1:94:A:ALA:CA	1:94:A:ALA:C	10	2.55
(1,147)	1:89:A:GLU:C	1:90:A:ASP:N	1:90:A:ASP:CA	1:90:A:ASP:C	3	2.54
(1,164)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ALA:N	13	2.5
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	16	2.5
(1,153)	1:92:A:SER:C	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	19	2.49
(1,33)	1:20:A:PHE:C	1:21:A:ASN:N	1:21:A:ASN:CA	1:21:A:ASN:C	2	2.49
(1,38)	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	1:24:A:LYS:N	12	2.48
(1,37)	1:22:A:LEU:C	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	19	2.48
(1,186)	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	1:112:A:PHE:N	12	2.47
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	6	2.45
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	15	2.44
(1,187)	1:111:A:GLN:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	1	2.44
(1,38)	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	1:24:A:LYS:N	15	2.44
(1,51)	1:29:A:VAL:C	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	11	2.43
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	2	2.42
(1,105)	1:62:A:PHE:C	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	15	2.4
(1,162)	1:97:A:LEU:N	1:97:A:LEU:CA	1:97:A:LEU:C	1:98:A:GLY:N	12	2.39
(1,56)	1:33:A:GLU:N	1:33:A:GLU:CA	1:33:A:GLU:C	1:34:A:ASN:N	10	2.38
(1,196)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:LYS:N	13	2.33
(1,134)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:ILE:N	8	2.28
(1,112)	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1:67:A:LYS:N	19	2.28
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	12	2.28
(1,182)	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:C	1:110:A:SER:N	4	2.27
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	16	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:50:A:ILE:N	1:50:A:ILE:CA	1:50:A:ILE:C	1:51:A:VAL:N	12	2.25
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	16	2.23
(1,100)	1:58:A:VAL:N	1:58:A:VAL:CA	1:58:A:VAL:C	1:59:A:MET:N	6	2.23
(1,197)	1:116:A:VAL:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	20	2.2
(1,119)	1:69:A:GLN:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	5	2.19
(1,119)	1:69:A:GLN:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	19	2.18
(1,15)	1:11:A:SER:C	1:12:A:ALA:N	1:12:A:ALA:CA	1:12:A:ALA:C	13	2.18
(1,189)	1:112:A:PHE:C	1:113:A:ILE:N	1:113:A:ILE:CA	1:113:A:ILE:C	9	2.17
(1,107)	1:63:A:THR:C	1:64:A:VAL:N	1:64:A:VAL:CA	1:64:A:VAL:C	4	2.17
(1,187)	1:111:A:GLN:C	1:112:A:PHE:N	1:112:A:PHE:CA	1:112:A:PHE:C	8	2.15
(1,24)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:ILE:N	18	2.14
(1,122)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLU:N	9	2.13
(1,72)	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	1:43:A:SER:N	14	2.13
(1,52)	1:30:A:ILE:N	1:30:A:ILE:CA	1:30:A:ILE:C	1:31:A:GLU:N	6	2.13
(1,3)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	15	2.13
(1,197)	1:116:A:VAL:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	15	2.12
(1,191)	1:113:A:ILE:C	1:114:A:GLU:N	1:114:A:GLU:CA	1:114:A:GLU:C	17	2.09
(1,118)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:GLU:N	19	2.08
(1,171)	1:102:A:VAL:C	1:103:A:MET:N	1:103:A:MET:CA	1:103:A:MET:C	6	2.07
(1,71)	1:41:A:LYS:C	1:42:A:LEU:N	1:42:A:LEU:CA	1:42:A:LEU:C	12	2.06
(1,10)	1:7:A:LEU:N	1:7:A:LEU:CA	1:7:A:LEU:C	1:8:A:VAL:N	13	2.04
(1,123)	1:72:A:GLU:C	1:73:A:GLU:N	1:73:A:GLU:CA	1:73:A:GLU:C	16	2.03
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	1	2.03
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	16	2.02
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	12	1.97
(1,7)	1:5:A:VAL:C	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	7	1.97
(1,76)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:PHE:N	10	1.96
(1,39)	1:23:A:LYS:C	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	13	1.94
(1,38)	1:23:A:LYS:N	1:23:A:LYS:CA	1:23:A:LYS:C	1:24:A:LYS:N	6	1.94
(1,76)	1:44:A:GLU:N	1:44:A:GLU:CA	1:44:A:GLU:C	1:45:A:PHE:N	20	1.93
(1,60)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:ILE:N	13	1.9
(1,35)	1:21:A:ASN:C	1:22:A:LEU:N	1:22:A:LEU:CA	1:22:A:LEU:C	14	1.9
(1,173)	1:103:A:MET:C	1:104:A:ARG:N	1:104:A:ARG:CA	1:104:A:ARG:C	10	1.89
(1,195)	1:115:A:GLU:C	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	9	1.88
(1,193)	1:114:A:GLU:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	13	1.88
(1,110)	1:65:A:LEU:N	1:65:A:LEU:CA	1:65:A:LEU:C	1:66:A:LYS:N	9	1.87
(1,7)	1:5:A:VAL:C	1:6:A:LEU:N	1:6:A:LEU:CA	1:6:A:LEU:C	10	1.85
(1,159)	1:95:A:LEU:C	1:96:A:SER:N	1:96:A:SER:CA	1:96:A:SER:C	15	1.8
(1,206)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	17	1.79
(1,106)	1:63:A:THR:N	1:63:A:THR:CA	1:63:A:THR:C	1:64:A:VAL:N	14	1.79
(1,13)	1:10:A:ASP:C	1:11:A:SER:N	1:11:A:SER:CA	1:11:A:SER:C	18	1.79
(1,206)	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:CB	1:47:A:PRO:CG	2	1.76
(1,159)	1:95:A:LEU:C	1:96:A:SER:N	1:96:A:SER:CA	1:96:A:SER:C	5	1.75
(1,154)	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	1:94:A:ALA:N	17	1.75
(1,60)	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	1:37:A:ILE:N	17	1.74
(1,197)	1:116:A:VAL:C	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	6	1.71
(1,64)	1:38:A:ALA:N	1:38:A:ALA:CA	1:38:A:ALA:C	1:39:A:LEU:N	16	1.7
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	4	1.7
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	18	1.66
(1,153)	1:92:A:SER:C	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	6	1.65
(1,141)	1:82:A:LEU:C	1:83:A:THR:N	1:83:A:THR:CA	1:83:A:THR:C	17	1.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:35:A:GLY:C	1:36:A:GLN:N	1:36:A:GLN:CA	1:36:A:GLN:C	2	1.64
(1,118)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:GLU:N	10	1.61
(1,61)	1:36:A:GLN:C	1:37:A:ILE:N	1:37:A:ILE:CA	1:37:A:ILE:C	12	1.61
(1,193)	1:114:A:GLU:C	1:115:A:GLU:N	1:115:A:GLU:CA	1:115:A:GLU:C	6	1.6
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	19	1.59
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	3	1.57
(1,153)	1:92:A:SER:C	1:93:A:LEU:N	1:93:A:LEU:CA	1:93:A:LEU:C	18	1.56
(1,164)	1:98:A:GLY:N	1:98:A:GLY:CA	1:98:A:GLY:C	1:99:A:ALA:N	1	1.55
(1,136)	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	1:81:A:VAL:N	8	1.54
(1,198)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:HIS:N	4	1.53
(1,137)	1:80:A:ILE:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	12	1.53
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	12	1.51
(1,27)	1:17:A:ILE:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	16	1.5
(1,26)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	2	1.48
(1,134)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:ILE:N	5	1.47
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	3	1.46
(1,3)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	8	1.45
(1,134)	1:79:A:VAL:N	1:79:A:VAL:CA	1:79:A:VAL:C	1:80:A:ILE:N	6	1.44
(1,68)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:LYS:N	1	1.41
(1,196)	1:116:A:VAL:N	1:116:A:VAL:CA	1:116:A:VAL:C	1:117:A:LYS:N	7	1.39
(1,185)	1:110:A:SER:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	19	1.38
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	17	1.38
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	1	1.38
(1,212)	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:CB	1:109:A:PRO:CG	18	1.37
(1,125)	1:74:A:TRP:C	1:75:A:LYS:N	1:75:A:LYS:CA	1:75:A:LYS:C	15	1.36
(1,49)	1:28:A:GLU:C	1:29:A:VAL:N	1:29:A:VAL:CA	1:29:A:VAL:C	3	1.36
(1,24)	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	1:17:A:ILE:N	8	1.36
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	10	1.36
(1,63)	1:37:A:ILE:C	1:38:A:ALA:N	1:38:A:ALA:CA	1:38:A:ALA:C	8	1.34
(1,22)	1:15:A:ARG:N	1:15:A:ARG:CA	1:15:A:ARG:C	1:16:A:LYS:N	20	1.3
(1,111)	1:65:A:LEU:C	1:66:A:LYS:N	1:66:A:LYS:CA	1:66:A:LYS:C	1	1.29
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	2	1.29
(1,205)	1:46:A:THR:C	1:47:A:PRO:N	1:47:A:PRO:CA	1:47:A:PRO:C	19	1.27
(1,175)	1:104:A:ARG:C	1:105:A:LYS:N	1:105:A:LYS:CA	1:105:A:LYS:C	2	1.26
(1,121)	1:71:A:LYS:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	14	1.26
(1,26)	1:17:A:ILE:N	1:17:A:ILE:CA	1:17:A:ILE:C	1:18:A:VAL:N	6	1.26
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	15	1.24
(1,186)	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	1:112:A:PHE:N	20	1.21
(1,69)	1:40:A:GLU:C	1:41:A:LYS:N	1:41:A:LYS:CA	1:41:A:LYS:C	4	1.21
(1,151)	1:91:A:GLU:C	1:92:A:SER:N	1:92:A:SER:CA	1:92:A:SER:C	5	1.19
(1,181)	1:108:A:SER:C	1:109:A:PRO:N	1:109:A:PRO:CA	1:109:A:PRO:C	6	1.18
(1,118)	1:69:A:GLN:N	1:69:A:GLN:CA	1:69:A:GLN:C	1:70:A:GLU:N	5	1.17
(1,67)	1:39:A:LEU:C	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	7	1.17
(1,19)	1:13:A:VAL:C	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	5	1.17
(1,183)	1:109:A:PRO:C	1:110:A:SER:N	1:110:A:SER:CA	1:110:A:SER:C	20	1.15
(1,135)	1:79:A:VAL:C	1:80:A:ILE:N	1:80:A:ILE:CA	1:80:A:ILE:C	3	1.14
(1,54)	1:31:A:GLU:N	1:31:A:GLU:CA	1:31:A:GLU:C	1:32:A:ALA:N	6	1.14
(1,31)	1:19:A:SER:C	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	9	1.14
(1,40)	1:24:A:LYS:N	1:24:A:LYS:CA	1:24:A:LYS:C	1:25:A:GLU:N	1	1.13
(1,32)	1:20:A:PHE:N	1:20:A:PHE:CA	1:20:A:PHE:C	1:21:A:ASN:N	14	1.1
(1,27)	1:17:A:ILE:C	1:18:A:VAL:N	1:18:A:VAL:CA	1:18:A:VAL:C	6	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,143)	1:87:A:GLY:C	1:88:A:GLU:N	1:88:A:GLU:CA	1:88:A:GLU:C	6	1.08
(1,23)	1:15:A:ARG:C	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	4	1.07
(1,150)	1:91:A:GLU:N	1:91:A:GLU:CA	1:91:A:GLU:C	1:92:A:SER:N	20	1.06
(1,116)	1:68:A:LEU:N	1:68:A:LEU:CA	1:68:A:LEU:C	1:69:A:GLN:N	18	1.06
(1,198)	1:117:A:LYS:N	1:117:A:LYS:CA	1:117:A:LYS:C	1:118:A:HIS:N	2	1.02
(1,17)	1:12:A:ALA:C	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	7	1.01