



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:06 AM UTC

PDB ID : 5XO9 / pdb_00005xo9
BMRB ID : 36091
Title : Thanatin in presence of LPS
Authors : Sinha, S.; Bhattacharjya, S.
Deposited on : 2017-05-27

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

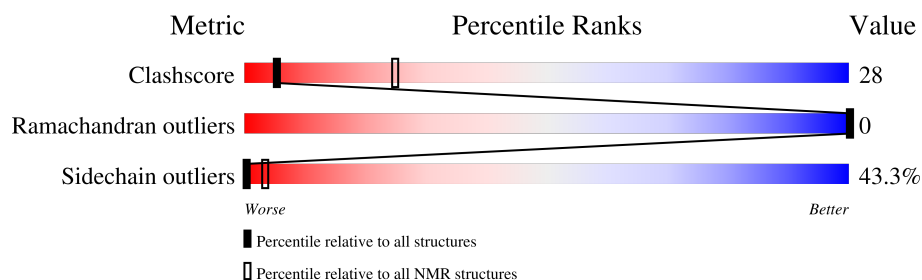
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 13%.

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	21	19% 33% 14% 33%
1	B	21	29% 24% 19% 29%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:21, B:39-B:53 (29)	0.48	10

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 696 atoms, of which 362 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thanatin.

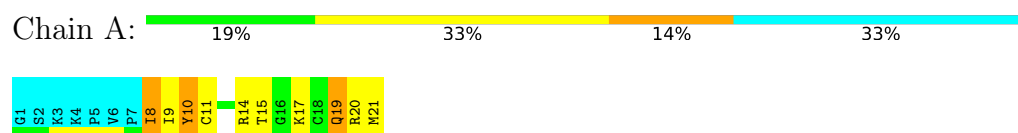
Mol	Chain	Residues	Atoms						Trace
1	A	21	Total	C	H	N	O	S	0
			348	103	181	35	26	3	
1	B	21	Total	C	H	N	O	S	0
			348	103	181	35	26	3	

4 Residue-property plots [i](#)

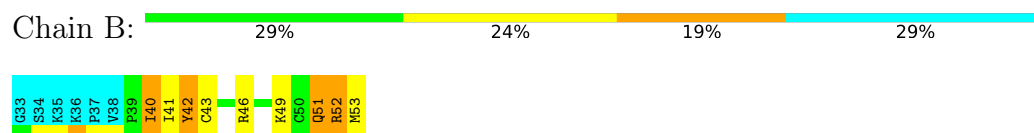
4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Thanatin



• Molecule 1: Thanatin

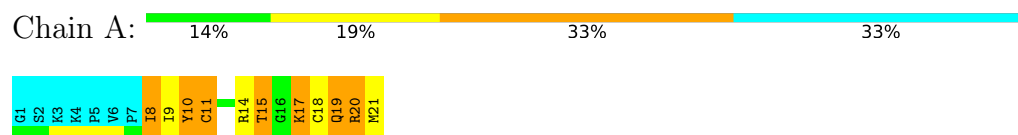


4.2 Scores per residue for each member of the ensemble

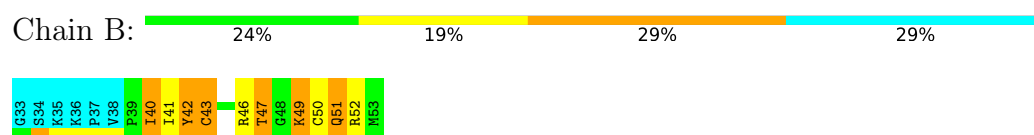
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Thanatin

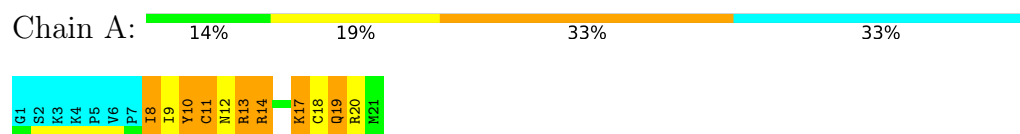


• Molecule 1: Thanatin



4.2.2 Score per residue for model 2

• Molecule 1: Thanatin

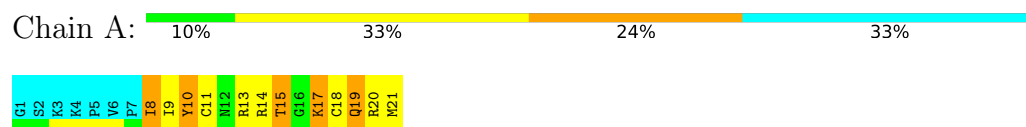


• Molecule 1: Thanatin

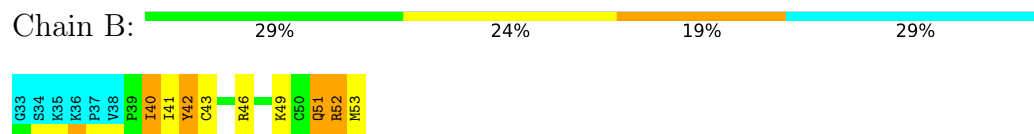


4.2.3 Score per residue for model 3

• Molecule 1: Thanatin

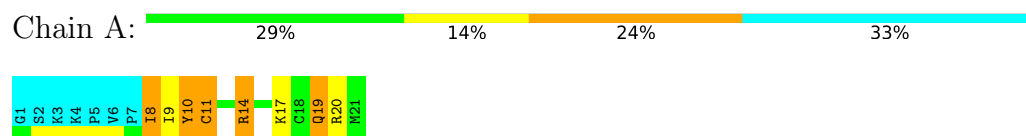


• Molecule 1: Thanatin

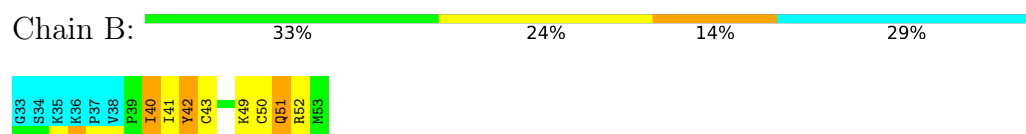


4.2.4 Score per residue for model 4

• Molecule 1: Thanatin

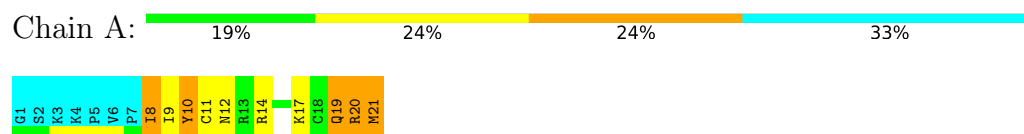


• Molecule 1: Thanatin

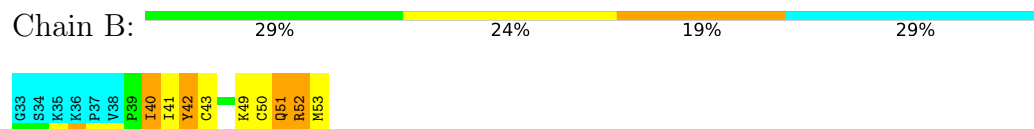


4.2.5 Score per residue for model 5

• Molecule 1: Thanatin



• Molecule 1: Thanatin

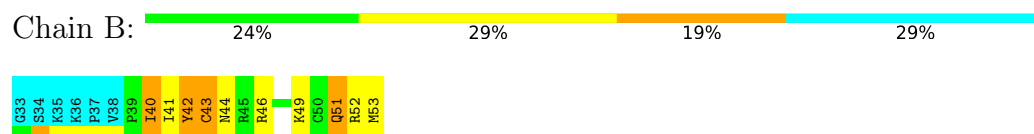


4.2.6 Score per residue for model 6

• Molecule 1: Thanatin



• Molecule 1: Thanatin

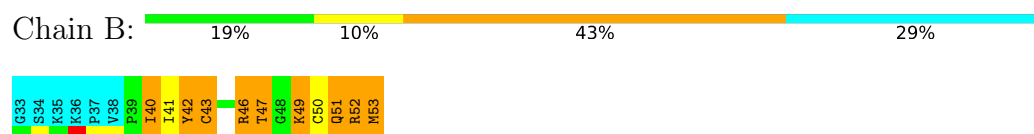


4.2.7 Score per residue for model 7

• Molecule 1: Thanatin



• Molecule 1: Thanatin

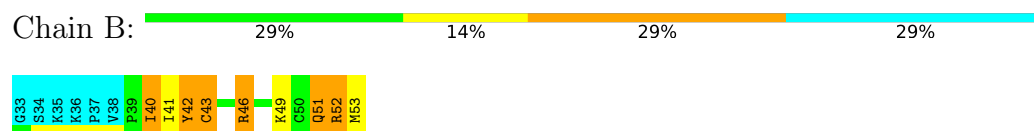


4.2.8 Score per residue for model 8

• Molecule 1: Thanatin

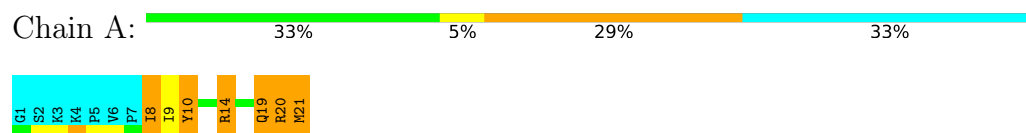


• Molecule 1: Thanatin

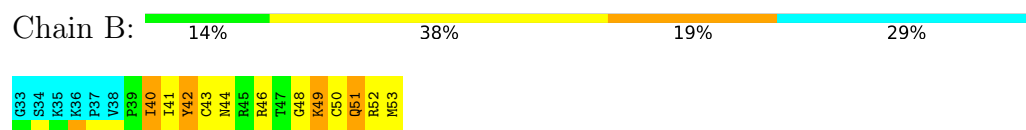


4.2.9 Score per residue for model 9

• Molecule 1: Thanatin

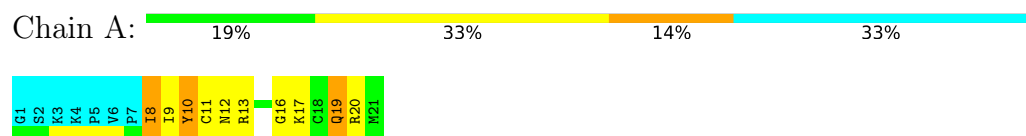


• Molecule 1: Thanatin



4.2.10 Score per residue for model 10 (medoid)

• Molecule 1: Thanatin

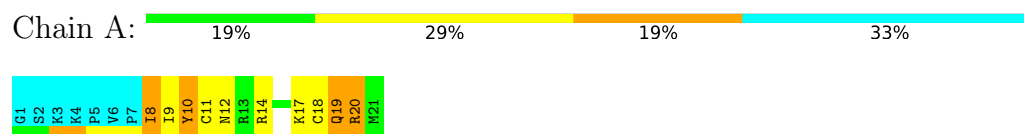


• Molecule 1: Thanatin

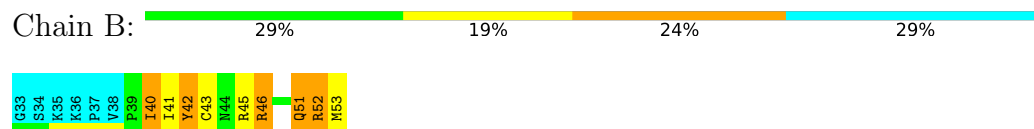


4.2.11 Score per residue for model 11

• Molecule 1: Thanatin

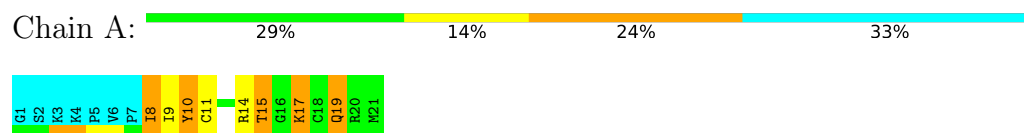


• Molecule 1: Thanatin

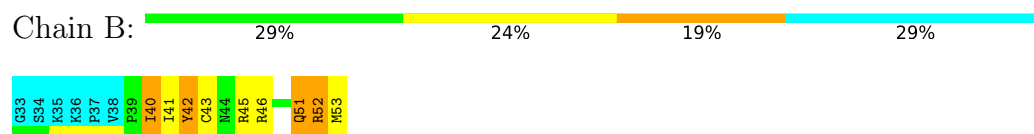


4.2.12 Score per residue for model 12

• Molecule 1: Thanatin

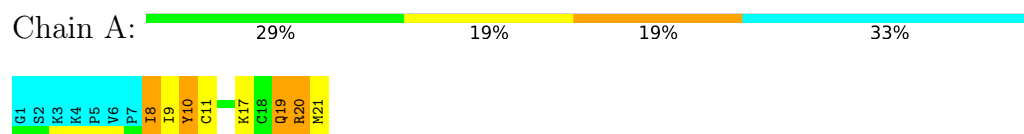


• Molecule 1: Thanatin

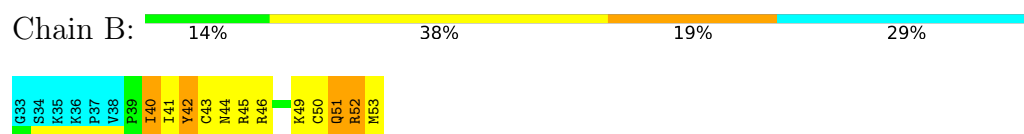


4.2.13 Score per residue for model 13

• Molecule 1: Thanatin

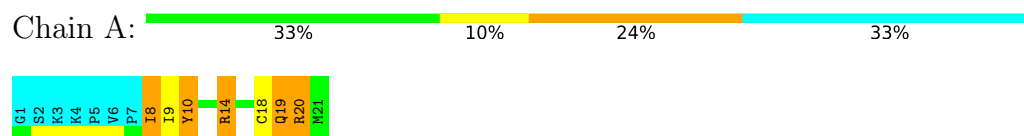


• Molecule 1: Thanatin

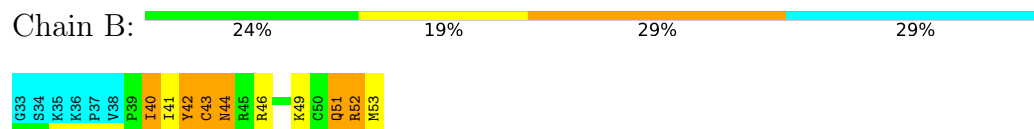


4.2.14 Score per residue for model 14

• Molecule 1: Thanatin



• Molecule 1: Thanatin

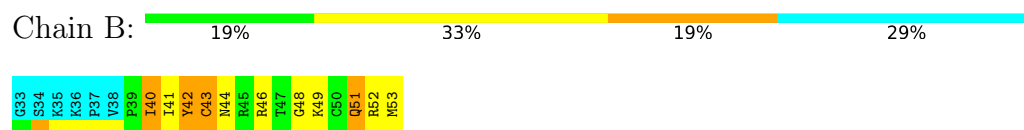


4.2.15 Score per residue for model 15

• Molecule 1: Thanatin

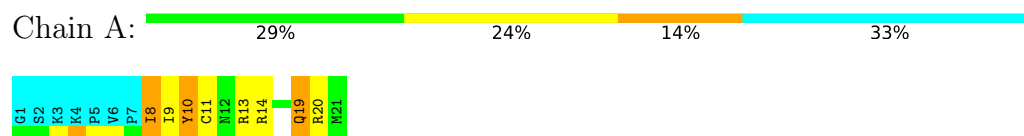


• Molecule 1: Thanatin

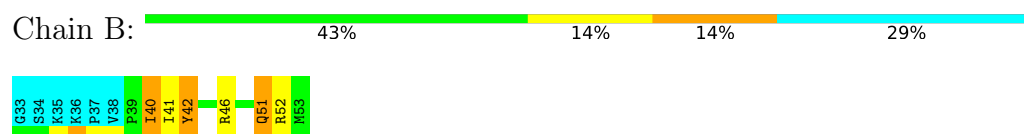


4.2.16 Score per residue for model 16

• Molecule 1: Thanatin



• Molecule 1: Thanatin



4.2.17 Score per residue for model 17

• Molecule 1: Thanatin

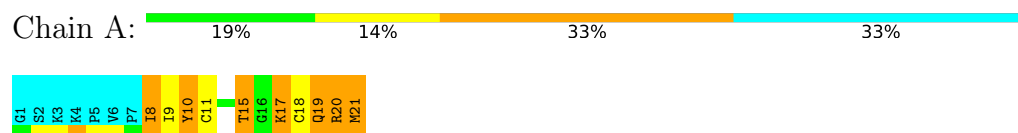


• Molecule 1: Thanatin

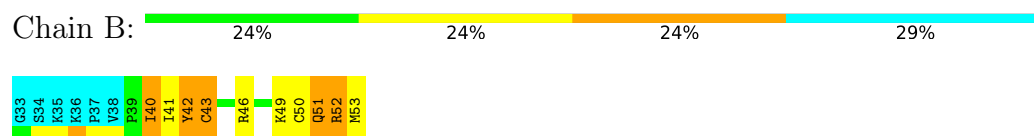


4.2.18 Score per residue for model 18

• Molecule 1: Thanatin

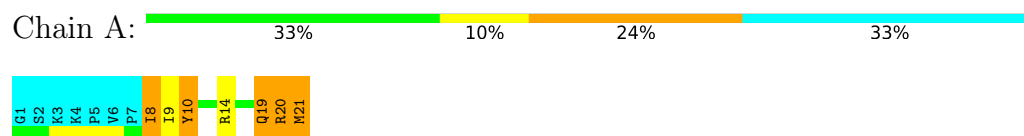


• Molecule 1: Thanatin

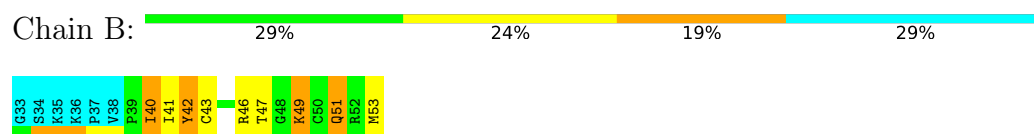


4.2.19 Score per residue for model 19

• Molecule 1: Thanatin

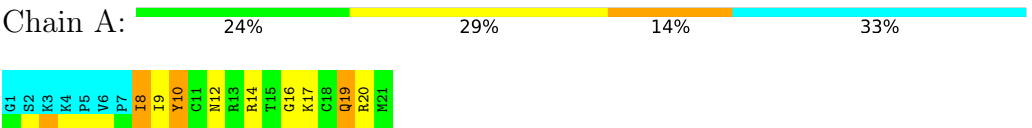


• Molecule 1: Thanatin

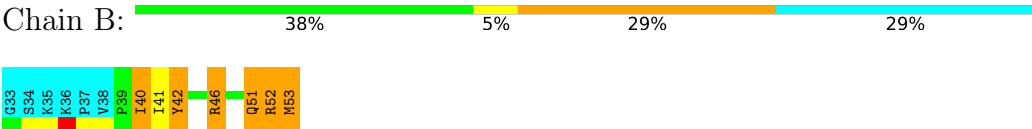


4.2.20 Score per residue for model 20

● Molecule 1: Thanatin



● Molecule 1: Thanatin



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

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

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

Software name	Classification	Version
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	76
Number of shifts mapped to atoms	76
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	13%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	118	124	124	8±2
1	B	125	131	131	7±2
All	All	4860	5100	5100	281

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:ILE:HG23	1:A:20:ARG:NE	0.70	2.01	11	17
1:B:42:TYR:N	1:B:42:TYR:CD1	0.68	2.61	11	14
1:A:10:TYR:CD1	1:A:10:TYR:N	0.68	2.62	1	11
1:A:10:TYR:N	1:A:10:TYR:CD2	0.67	2.61	4	9
1:B:42:TYR:CD1	1:B:42:TYR:N	0.67	2.62	4	2
1:B:41:ILE:HG23	1:B:52:ARG:NE	0.67	2.04	7	15
1:B:41:ILE:HG23	1:B:52:ARG:NH1	0.66	2.04	17	1
1:B:42:TYR:CD2	1:B:42:TYR:N	0.66	2.62	8	4
1:B:47:THR:HG23	1:B:49:LYS:HG3	0.63	1.69	7	4
1:B:46:ARG:N	1:B:46:ARG:HE	0.62	1.91	19	1
1:A:15:THR:HG23	1:A:17:LYS:HG3	0.61	1.71	18	7
1:B:42:TYR:CE2	1:B:53:MET:HE3	0.57	2.34	15	7
1:B:41:ILE:HG22	1:B:51:GLN:O	0.56	2.01	17	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:CYS:HA	1:A:17:LYS:O	0.55	2.02	8	15
1:A:21:MET:HE1	1:B:44:ASN:ND2	0.54	2.18	13	4
1:A:8:ILE:HG21	1:B:43:CYS:O	0.54	2.02	14	5
1:B:43:CYS:HA	1:B:49:LYS:O	0.54	2.03	1	16
1:A:14:ARG:NE	1:A:14:ARG:H	0.54	2.01	9	5
1:A:10:TYR:CE2	1:A:21:MET:HE3	0.53	2.38	8	2
1:A:9:ILE:HG23	1:A:20:ARG:CD	0.53	2.34	9	3
1:B:46:ARG:NE	1:B:46:ARG:H	0.52	2.02	7	4
1:A:8:ILE:HD12	1:A:21:MET:HG3	0.52	1.80	5	1
1:A:9:ILE:HG22	1:A:19:GLN:C	0.52	2.29	11	5
1:A:9:ILE:HG22	1:A:19:GLN:O	0.51	2.06	9	20
1:B:52:ARG:HB3	1:B:52:ARG:CZ	0.51	2.35	6	2
1:A:11:CYS:O	1:B:40:ILE:HG21	0.50	2.06	8	6
1:A:14:ARG:H	1:A:14:ARG:NE	0.50	2.05	4	1
1:A:21:MET:HE1	1:B:44:ASN:HD21	0.50	1.67	6	2
1:A:18:CYS:C	1:A:19:GLN:HG3	0.49	2.32	18	8
1:A:8:ILE:O	1:A:20:ARG:HD3	0.49	2.07	20	1
1:A:20:ARG:HB3	1:A:20:ARG:CZ	0.48	2.38	8	1
1:A:12:ASN:O	1:A:16:GLY:N	0.47	2.47	7	3
1:A:12:ASN:HD21	1:B:53:MET:HE1	0.47	1.70	5	1
1:A:12:ASN:ND2	1:B:53:MET:HE1	0.47	2.25	10	2
1:A:9:ILE:HG22	1:A:20:ARG:HA	0.46	1.85	5	3
1:A:10:TYR:CE1	1:A:21:MET:HE3	0.46	2.46	7	1
1:B:41:ILE:HG22	1:B:51:GLN:C	0.46	2.35	17	3
1:B:42:TYR:HE2	1:B:53:MET:HE3	0.46	1.71	12	7
1:B:44:ASN:O	1:B:48:GLY:N	0.45	2.49	17	3
1:A:10:TYR:CD2	1:A:19:GLN:O	0.45	2.70	11	2
1:A:9:ILE:C	1:A:9:ILE:HD12	0.45	2.37	12	6
1:A:8:ILE:N	1:A:8:ILE:HD13	0.45	2.26	19	1
1:B:50:CYS:C	1:B:51:GLN:HG3	0.44	2.37	18	8
1:A:10:TYR:HE1	1:A:21:MET:HE3	0.44	1.72	7	1
1:A:10:TYR:HE2	1:A:21:MET:HE3	0.43	1.72	8	2
1:B:44:ASN:ND2	1:B:44:ASN:H	0.43	2.11	14	1
1:A:21:MET:HE1	1:B:42:TYR:CA	0.43	2.43	1	1
1:A:12:ASN:HD22	1:B:53:MET:HE1	0.43	1.74	10	1
1:B:41:ILE:HG22	1:B:52:ARG:HA	0.43	1.90	1	1
1:B:41:ILE:HD12	1:B:41:ILE:C	0.43	2.39	19	3
1:A:9:ILE:HG23	1:A:20:ARG:HD2	0.42	1.91	8	1
1:A:9:ILE:HG23	1:A:20:ARG:CZ	0.42	2.44	14	1
1:A:9:ILE:HA	1:A:19:GLN:O	0.42	2.15	11	2
1:B:40:ILE:O	1:B:53:MET:N	0.42	2.53	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ILE:HD12	1:A:21:MET:CG	0.42	2.44	5	1
1:A:8:ILE:HD13	1:B:43:CYS:O	0.42	2.14	5	1
1:A:13:ARG:HD3	1:A:14:ARG:N	0.42	2.29	2	1
1:B:46:ARG:H	1:B:46:ARG:NE	0.41	2.13	8	1
1:B:46:ARG:NE	1:B:46:ARG:CA	0.41	2.84	19	1
1:A:12:ASN:C	1:A:14:ARG:N	0.41	2.78	2	1
1:A:15:THR:O	1:A:15:THR:OG1	0.41	2.39	18	1
1:A:9:ILE:HD12	1:A:9:ILE:C	0.41	2.41	6	1
1:A:8:ILE:HD12	1:B:46:ARG:NH2	0.41	2.31	11	1
1:A:8:ILE:O	1:A:20:ARG:HG3	0.40	2.16	14	1
1:A:15:THR:HG23	1:A:17:LYS:CG	0.40	2.45	18	1
1:B:47:THR:O	1:B:47:THR:OG1	0.40	2.38	10	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	13/21 (62%)	12±1 (88±5%)	2±1 (12±5%)	0±0 (0±0%)	100	100
1	B	14/21 (67%)	12±1 (83±4%)	2±1 (17±4%)	0±0 (0±0%)	100	100
All	All	540/840 (64%)	462 (86%)	78 (14%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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	13/19 (68%)	7±1 (55±9%)	6±1 (45±9%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	14/19 (74%)	8±1 (58±10%)	6±1 (42±10%)	0 4
All	All	540/760 (71%)	306 (57%)	234 (43%)	0 3

All 24 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	8	ILE	20
1	A	10	TYR	20
1	A	19	GLN	20
1	B	40	ILE	20
1	B	42	TYR	20
1	B	51	GLN	20
1	A	14	ARG	17
1	B	46	ARG	17
1	B	52	ARG	13
1	A	17	LYS	9
1	A	20	ARG	9
1	B	43	CYS	8
1	A	15	THR	7
1	A	11	CYS	6
1	B	49	LYS	6
1	B	47	THR	5
1	A	13	ARG	4
1	A	21	MET	4
1	B	53	MET	4
1	A	18	CYS	1
1	B	50	CYS	1
1	B	44	ASN	1
1	B	41	ILE	1
1	B	45	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 13% for the well-defined parts and 12% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Thanatin-LPS.NMR-STAR*

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	76
Number of shifts mapped to atoms	76
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

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 13%, i.e. 57 atoms were assigned a chemical shift out of a possible 442. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	57/145 (39%)	57/59 (97%)	0/58 (0%)	0/28 (0%)
Sidechain	0/279 (0%)	0/178 (0%)	0/77 (0%)	0/24 (0%)
Aromatic	0/18 (0%)	0/8 (0%)	0/10 (0%)	0/0 (—%)
Overall	57/442 (13%)	57/245 (23%)	0/145 (0%)	0/52 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 76 atoms were assigned a chemical shift out of a possible 608. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	76/206 (37%)	76/84 (90%)	0/84 (0%)	0/38 (0%)
Sidechain	0/384 (0%)	0/246 (0%)	0/110 (0%)	0/28 (0%)
Aromatic	0/18 (0%)	0/8 (0%)	0/10 (0%)	0/0 (—%)
Overall	76/608 (12%)	76/338 (22%)	0/204 (0%)	0/66 (0%)

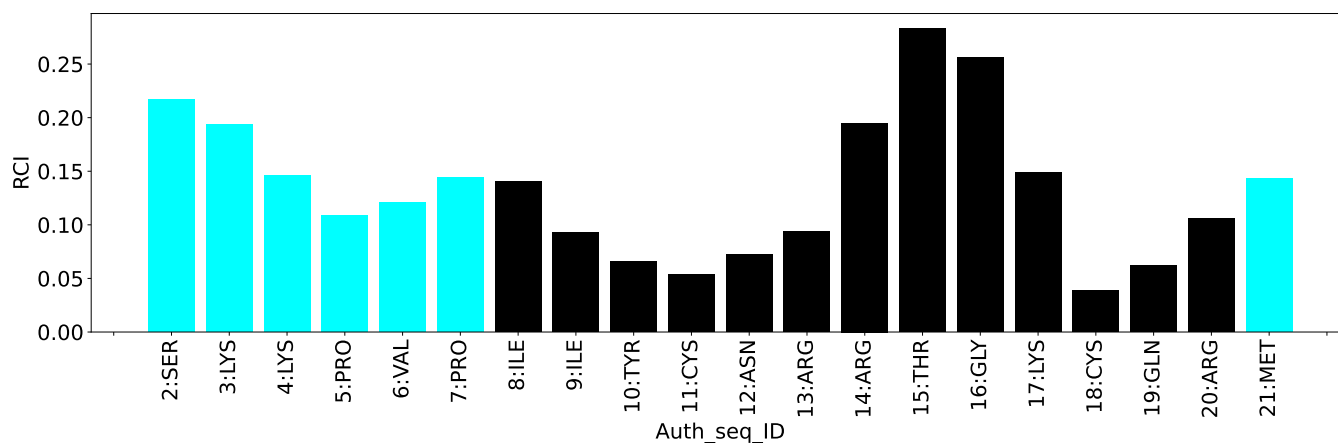
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

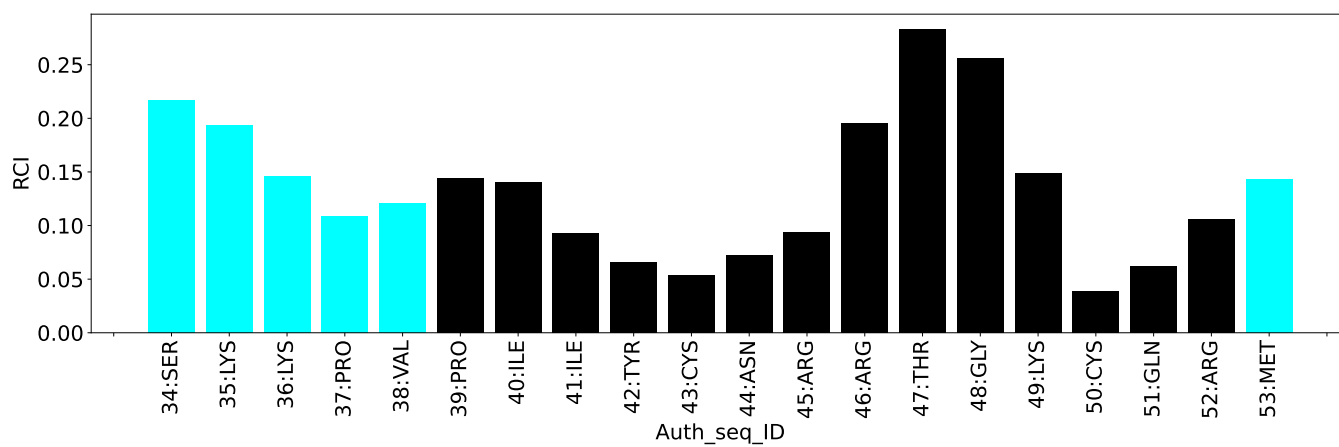
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis [i](#)

8.1 Conformationally restricting restraints [i](#)

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	382
Intra-residue ($ i-j =0$)	170
Sequential ($ i-j =1$)	118
Medium range ($ i-j >1$ and $ i-j <5$)	8
Long range ($ i-j \geq 5$)	80
Inter-chain	6
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	64
Number of unmapped restraints	0
Number of restraints per residue	10.6
Number of long range restraints per residue ¹	1.9

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 [i](#)

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 [i](#)

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)	53.6	0.2
0.2-0.5 (Medium)	30.7	0.5
>0.5 (Large)	2.6	0.77

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)	16.9	9.52
10.0-20.0 (Medium)	0.3	14.72
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

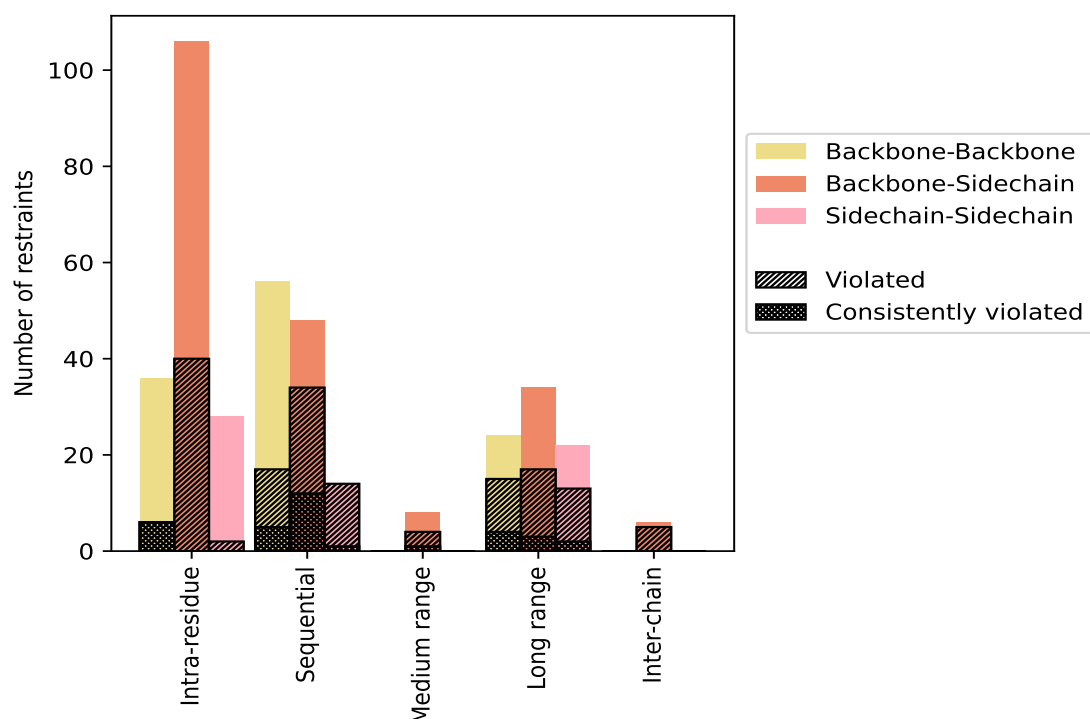
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	170	44.5	48	28.2	12.6	6	3.5	1.6
Backbone-Backbone	36	9.4	6	16.7	1.6	6	16.7	1.6
Backbone-Sidechain	106	27.7	40	37.7	10.5	0	0.0	0.0
Sidechain-Sidechain	28	7.3	2	7.1	0.5	0	0.0	0.0
Sequential (i-j =1)	118	30.9	65	55.1	17.0	18	15.3	4.7
Backbone-Backbone	56	14.7	17	30.4	4.5	5	8.9	1.3
Backbone-Sidechain	48	12.6	34	70.8	8.9	12	25.0	3.1
Sidechain-Sidechain	14	3.7	14	100.0	3.7	1	7.1	0.3
Medium range (i-j >1 & i-j <5)	8	2.1	4	50.0	1.0	1	12.5	0.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	2.1	4	50.0	1.0	1	12.5	0.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	80	20.9	45	56.2	11.8	9	11.2	2.4
Backbone-Backbone	24	6.3	15	62.5	3.9	4	16.7	1.0
Backbone-Sidechain	34	8.9	17	50.0	4.5	3	8.8	0.8
Sidechain-Sidechain	22	5.8	13	59.1	3.4	2	9.1	0.5
Inter-chain	6	1.6	5	83.3	1.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	1.6	5	83.3	1.3	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	382	100.0	167	43.7	43.7	34	8.9	8.9
Backbone-Backbone	116	30.4	38	32.8	9.9	15	12.9	3.9
Backbone-Sidechain	202	52.9	100	49.5	26.2	16	7.9	4.2
Sidechain-Sidechain	64	16.8	29	45.3	7.6	3	4.7	0.8

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	20	44	1	23	4	92	0.2	0.64	0.1	0.18
2	18	41	1	23	3	86	0.2	0.7	0.1	0.18
3	21	39	1	23	2	86	0.21	0.68	0.1	0.18
4	18	39	2	24	2	85	0.21	0.73	0.11	0.18
5	15	43	1	21	3	83	0.21	0.77	0.12	0.18
6	21	42	3	25	3	94	0.2	0.69	0.11	0.17
7	22	40	3	23	2	90	0.2	0.67	0.1	0.17
8	23	43	2	22	3	93	0.21	0.72	0.11	0.16
9	20	42	2	22	3	89	0.21	0.68	0.1	0.18
10	22	36	1	21	3	83	0.22	0.69	0.12	0.18

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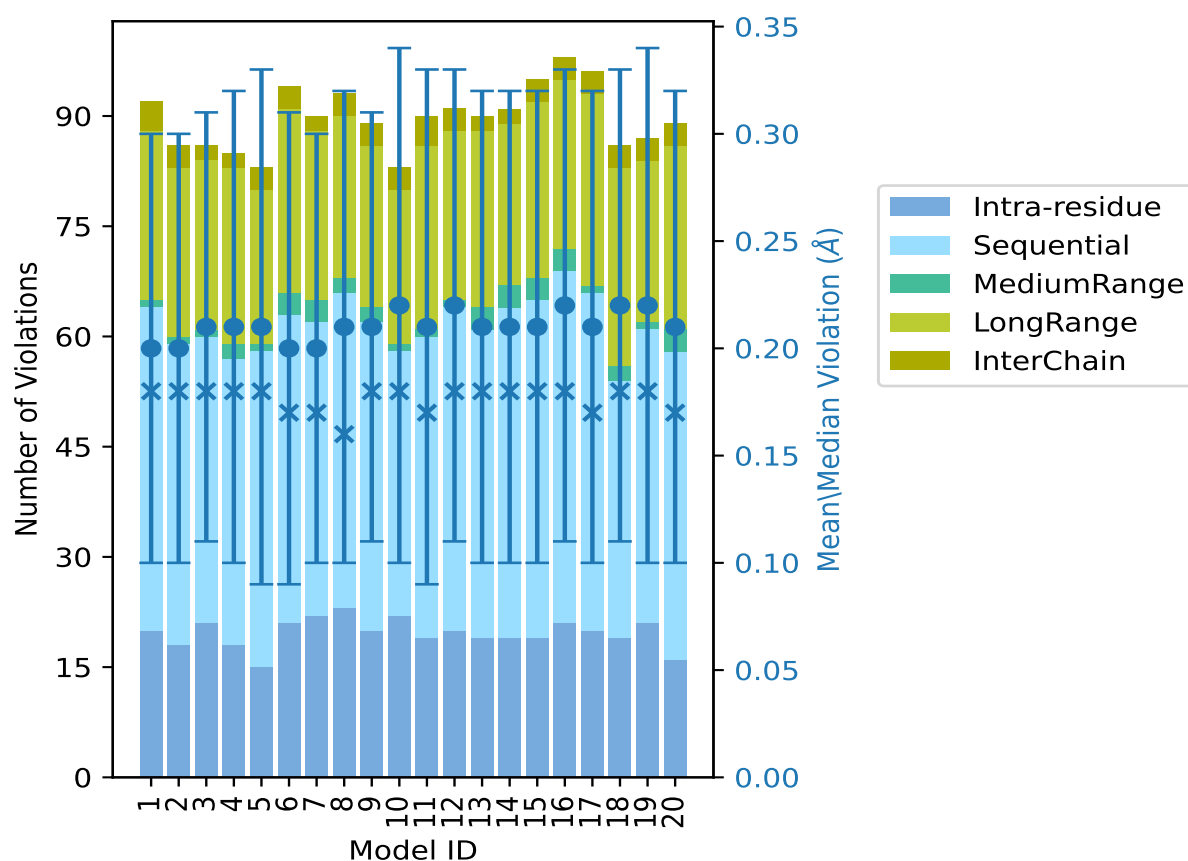
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	19	41	1	25	4	90	0.21	0.7	0.12	0.17
12	20	44	1	23	3	91	0.22	0.7	0.11	0.18
13	19	42	3	24	2	90	0.21	0.68	0.11	0.18
14	19	45	3	22	2	91	0.21	0.72	0.11	0.18
15	19	46	3	24	3	95	0.21	0.69	0.11	0.18
16	21	48	3	23	3	98	0.22	0.7	0.11	0.18
17	20	46	1	26	3	96	0.21	0.73	0.11	0.17
18	19	35	2	27	3	86	0.22	0.74	0.11	0.18
19	21	40	1	22	3	87	0.22	0.7	0.12	0.18
20	16	42	3	25	3	89	0.21	0.64	0.11	0.17

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

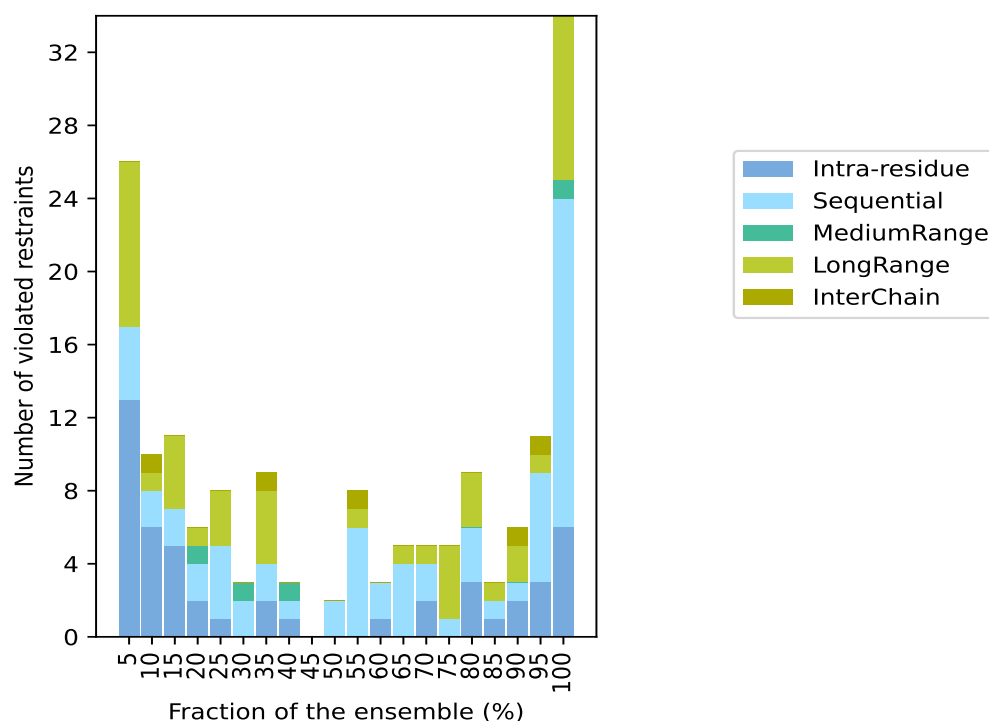
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 215(IR:122, SQ:53, MR:4, LR:35, IC:1) restraints are not 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	%
13	4	0	9	0	26	1	5.0
6	2	0	1	1	10	2	10.0
5	2	0	4	0	11	3	15.0
2	2	1	1	0	6	4	20.0
1	4	0	3	0	8	5	25.0
0	2	1	0	0	3	6	30.0
2	2	0	4	1	9	7	35.0
1	1	1	0	0	3	8	40.0
0	0	0	0	0	0	9	45.0
0	2	0	0	0	2	10	50.0
0	6	0	1	1	8	11	55.0
1	2	0	0	0	3	12	60.0
0	4	0	1	0	5	13	65.0
2	2	0	1	0	5	14	70.0
0	1	0	4	0	5	15	75.0
3	3	0	3	0	9	16	80.0
1	1	0	1	0	3	17	85.0
2	1	0	2	1	6	18	90.0
3	6	0	1	1	11	19	95.0
6	18	1	9	0	34	20	100.0

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

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

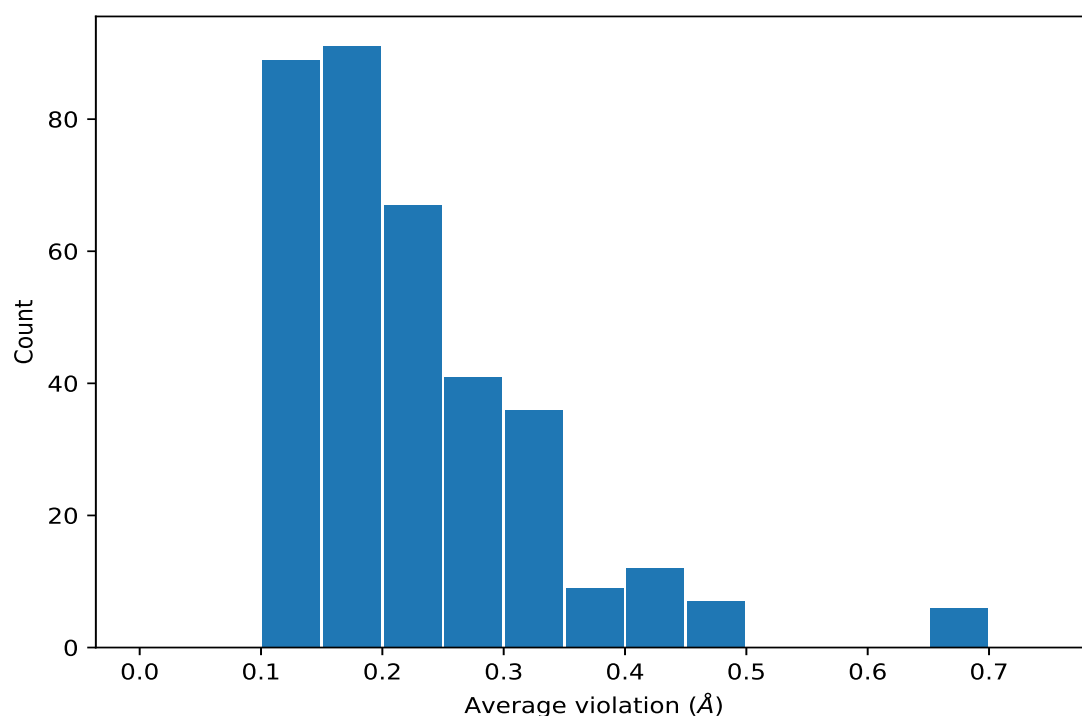
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	20	0.36	0.08	0.33
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	20	0.36	0.08	0.33
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	20	0.36	0.08	0.33
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	20	0.36	0.08	0.33
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	20	0.36	0.08	0.33
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	20	0.36	0.08	0.33
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	20	0.29	0.01	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	20	0.29	0.01	0.29
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	20	0.29	0.07	0.32
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	20	0.29	0.07	0.32
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	20	0.26	0.09	0.24
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	20	0.26	0.07	0.29
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	20	0.26	0.07	0.29
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	20	0.23	0.08	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	20	0.22	0.03	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	20	0.22	0.03	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	20	0.22	0.04	0.22
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	20	0.22	0.08	0.22
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	20	0.22	0.08	0.22
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	20	0.22	0.04	0.23
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	20	0.22	0.03	0.22
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	20	0.22	0.03	0.22
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	20	0.2	0.04	0.2
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	20	0.2	0.05	0.2
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	20	0.2	0.03	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	20	0.2	0.03	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	20	0.2	0.03	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	20	0.2	0.03	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	20	0.19	0.04	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	20	0.19	0.04	0.18
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	20	0.19	0.02	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	20	0.19	0.02	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	20	0.19	0.02	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	20	0.19	0.02	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	20	0.19	0.02	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	20	0.19	0.02	0.19
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	20	0.19	0.03	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	20	0.19	0.03	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	20	0.19	0.03	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	20	0.19	0.03	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	20	0.18	0.01	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	20	0.18	0.01	0.18
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	20	0.18	0.02	0.18
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	20	0.18	0.02	0.18
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	20	0.17	0.05	0.16
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	20	0.17	0.02	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	20	0.17	0.02	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	20	0.17	0.02	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	20	0.17	0.02	0.17
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	20	0.16	0.03	0.15
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	20	0.16	0.03	0.15
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	20	0.16	0.02	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	20	0.16	0.02	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	20	0.16	0.02	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	20	0.16	0.02	0.16
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	20	0.16	0.02	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	20	0.16	0.02	0.16
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	20	0.15	0.0	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	20	0.15	0.0	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	20	0.14	0.01	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	20	0.14	0.01	0.15
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	20	0.14	0.02	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	20	0.13	0.01	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	20	0.12	0.01	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	20	0.12	0.0	0.12
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	19	0.34	0.05	0.33
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	19	0.34	0.05	0.33
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	19	0.24	0.05	0.26
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	19	0.24	0.05	0.26
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	19	0.22	0.07	0.26
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	19	0.22	0.07	0.26
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	19	0.22	0.11	0.2
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	19	0.22	0.11	0.2
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	19	0.22	0.11	0.2
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	19	0.21	0.06	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	19	0.21	0.06	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	19	0.21	0.06	0.19
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	19	0.2	0.1	0.17
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	19	0.2	0.05	0.2
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	19	0.2	0.02	0.19
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	19	0.2	0.02	0.19
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	19	0.19	0.08	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	19	0.18	0.02	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	19	0.18	0.02	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	19	0.18	0.02	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	19	0.18	0.02	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	19	0.18	0.02	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	19	0.18	0.02	0.18
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	19	0.18	0.03	0.18
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	19	0.18	0.03	0.18
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	18	0.69	0.03	0.68
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	18	0.69	0.03	0.68
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	18	0.69	0.03	0.68
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	18	0.42	0.08	0.42
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	18	0.42	0.08	0.42
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	18	0.42	0.08	0.42
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	18	0.42	0.08	0.42
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	18	0.42	0.08	0.42
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	18	0.42	0.08	0.42
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	18	0.3	0.08	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	18	0.28	0.12	0.24
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	18	0.28	0.12	0.24
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	18	0.23	0.04	0.25
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	18	0.22	0.07	0.21
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	18	0.22	0.07	0.21
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	18	0.22	0.07	0.21
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	17	0.67	0.04	0.68
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	17	0.67	0.04	0.68
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	17	0.67	0.04	0.68
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	17	0.21	0.07	0.23
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	17	0.2	0.04	0.21
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	16	0.41	0.06	0.42
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	16	0.41	0.06	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	16	0.41	0.06	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	16	0.41	0.06	0.42
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	16	0.41	0.06	0.42
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	16	0.41	0.06	0.42
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	16	0.34	0.07	0.34
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	16	0.34	0.07	0.34
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	16	0.29	0.07	0.32
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	16	0.29	0.07	0.32
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	16	0.29	0.07	0.32
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	16	0.29	0.07	0.32
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	16	0.29	0.07	0.32
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	16	0.29	0.07	0.32
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	16	0.25	0.05	0.26
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	16	0.21	0.06	0.2
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	16	0.21	0.06	0.2
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	16	0.19	0.06	0.18
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	16	0.19	0.06	0.18
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	16	0.19	0.06	0.18
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	16	0.16	0.02	0.16
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	16	0.16	0.02	0.16
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	16	0.15	0.03	0.15
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	16	0.13	0.01	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	16	0.13	0.01	0.12
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	15	0.33	0.02	0.33
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	15	0.33	0.02	0.33
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	15	0.33	0.02	0.33
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	15	0.33	0.02	0.33
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	15	0.33	0.02	0.33
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	15	0.33	0.02	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	15	0.24	0.05	0.25
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	15	0.24	0.05	0.25
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	15	0.22	0.05	0.23
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	15	0.2	0.12	0.14
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	15	0.2	0.12	0.14
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	15	0.13	0.01	0.13
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	15	0.13	0.01	0.13
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	14	0.18	0.09	0.14
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	14	0.18	0.09	0.14
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	14	0.17	0.02	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	14	0.17	0.02	0.16
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	14	0.14	0.04	0.12
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	14	0.14	0.04	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	14	0.12	0.02	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	14	0.12	0.02	0.12
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	14	0.11	0.01	0.11
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	14	0.11	0.01	0.11
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	13	0.27	0.02	0.27
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	13	0.27	0.02	0.27
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	13	0.17	0.02	0.17
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	13	0.17	0.02	0.17
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	13	0.16	0.05	0.14
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	13	0.16	0.06	0.14
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	13	0.16	0.06	0.14
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	13	0.11	0.01	0.11
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	12	0.2	0.08	0.18
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	12	0.2	0.08	0.18
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	12	0.15	0.02	0.16
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	12	0.15	0.02	0.15
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	11	0.27	0.02	0.27
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	11	0.27	0.02	0.27
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	11	0.23	0.01	0.22
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	11	0.23	0.01	0.22
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	11	0.18	0.11	0.14
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	11	0.18	0.11	0.14
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	11	0.18	0.11	0.14
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	11	0.18	0.11	0.14
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	11	0.18	0.11	0.14
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	11	0.18	0.11	0.14
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	11	0.18	0.06	0.17
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	11	0.17	0.02	0.16
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	11	0.17	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	11	0.12	0.01	0.12
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	11	0.12	0.01	0.12
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	11	0.11	0.01	0.11
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	10	0.14	0.05	0.12
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	10	0.14	0.05	0.12
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	10	0.14	0.05	0.12
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	10	0.13	0.03	0.12
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	10	0.13	0.03	0.12
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	8	0.22	0.12	0.18
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	8	0.22	0.12	0.18
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	8	0.22	0.12	0.18
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	8	0.22	0.12	0.18
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	8	0.22	0.12	0.18
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	8	0.22	0.12	0.18
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	8	0.22	0.09	0.2
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	8	0.22	0.09	0.2
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	8	0.12	0.01	0.12
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	8	0.12	0.01	0.12
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	8	0.12	0.01	0.12
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	8	0.12	0.01	0.12
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	7	0.3	0.22	0.12
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	7	0.3	0.22	0.12
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	7	0.3	0.22	0.12
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	7	0.3	0.22	0.12
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	7	0.3	0.22	0.12
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	7	0.3	0.22	0.12
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	7	0.27	0.02	0.27
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	7	0.27	0.02	0.27
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	7	0.26	0.12	0.21
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	7	0.26	0.12	0.21
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	7	0.26	0.12	0.21
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	7	0.26	0.12	0.21
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	7	0.26	0.12	0.21
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	7	0.26	0.12	0.21
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	7	0.24	0.19	0.18
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	7	0.24	0.19	0.18
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	7	0.24	0.19	0.18
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	7	0.22	0.13	0.19
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	7	0.22	0.13	0.19
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	7	0.22	0.13	0.19
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	7	0.22	0.13	0.19
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	7	0.22	0.13	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	7	0.22	0.13	0.19
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	7	0.2	0.08	0.17
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	7	0.2	0.08	0.17
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	7	0.13	0.03	0.13
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	7	0.13	0.03	0.13
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	7	0.12	0.01	0.12
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	7	0.12	0.01	0.12
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	7	0.12	0.01	0.12
(1,368)	1:38:B:VAL:HG11	1:35:B:LYS:H	6	0.19	0.07	0.15
(1,368)	1:38:B:VAL:HG12	1:35:B:LYS:H	6	0.19	0.07	0.15
(1,368)	1:38:B:VAL:HG13	1:35:B:LYS:H	6	0.19	0.07	0.15
(1,368)	1:38:B:VAL:HG21	1:35:B:LYS:H	6	0.19	0.07	0.15
(1,368)	1:38:B:VAL:HG22	1:35:B:LYS:H	6	0.19	0.07	0.15
(1,368)	1:38:B:VAL:HG23	1:35:B:LYS:H	6	0.19	0.07	0.15
(1,178)	1:15:A:THR:HG21	1:14:A:ARG:HE	6	0.17	0.04	0.16
(1,178)	1:15:A:THR:HG22	1:14:A:ARG:HE	6	0.17	0.04	0.16
(1,178)	1:15:A:THR:HG23	1:14:A:ARG:HE	6	0.17	0.04	0.16
(1,174)	1:10:A:TYR:HA	1:9:A:ILE:H	6	0.16	0.02	0.16
(1,341)	1:40:B:ILE:HD11	1:53:B:MET:H	5	0.37	0.17	0.3
(1,341)	1:40:B:ILE:HD12	1:53:B:MET:H	5	0.37	0.17	0.3
(1,341)	1:40:B:ILE:HD13	1:53:B:MET:H	5	0.37	0.17	0.3
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD2	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD3	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD2	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD3	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD2	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD3	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD2	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD3	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD2	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD3	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD2	5	0.35	0.12	0.4
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD3	5	0.35	0.12	0.4
(1,300)	1:49:B:LYS:HB2	1:49:B:LYS:H	5	0.26	0.01	0.26
(1,300)	1:49:B:LYS:HB3	1:49:B:LYS:H	5	0.26	0.01	0.26
(1,16)	1:2:A:SER:HB2	1:3:A:LYS:H	5	0.14	0.05	0.12
(1,16)	1:2:A:SER:HB3	1:3:A:LYS:H	5	0.14	0.05	0.12
(1,360)	1:41:B:ILE:HG21	1:40:B:ILE:H	5	0.12	0.01	0.12
(1,360)	1:41:B:ILE:HG22	1:40:B:ILE:H	5	0.12	0.01	0.12
(1,360)	1:41:B:ILE:HG23	1:40:B:ILE:H	5	0.12	0.01	0.12
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	5	0.11	0.01	0.11
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	5	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	5	0.11	0.01	0.11
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	5	0.11	0.01	0.11
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE1	5	0.11	0.01	0.1
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE2	5	0.11	0.01	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE1	5	0.11	0.01	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE2	5	0.11	0.01	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE1	5	0.11	0.01	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE2	5	0.11	0.01	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD1	5	0.1	0.0	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD2	5	0.1	0.0	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD1	5	0.1	0.0	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD2	5	0.1	0.0	0.1
(1,337)	1:41:B:ILE:HG12	1:52:B:ARG:HE	4	0.35	0.12	0.3
(1,337)	1:41:B:ILE:HG13	1:52:B:ARG:HE	4	0.35	0.12	0.3
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD2	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD3	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD2	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD3	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD2	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD3	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD2	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD3	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD2	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD3	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD2	4	0.31	0.14	0.34
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD3	4	0.31	0.14	0.34
(1,181)	1:6:A:VAL:HG11	1:3:A:LYS:H	4	0.19	0.09	0.15
(1,181)	1:6:A:VAL:HG12	1:3:A:LYS:H	4	0.19	0.09	0.15
(1,181)	1:6:A:VAL:HG13	1:3:A:LYS:H	4	0.19	0.09	0.15
(1,181)	1:6:A:VAL:HG21	1:3:A:LYS:H	4	0.19	0.09	0.15
(1,181)	1:6:A:VAL:HG22	1:3:A:LYS:H	4	0.19	0.09	0.15
(1,181)	1:6:A:VAL:HG23	1:3:A:LYS:H	4	0.19	0.09	0.15
(1,52)	1:3:A:LYS:HB2	1:3:A:LYS:H	4	0.18	0.03	0.18
(1,52)	1:3:A:LYS:HB3	1:3:A:LYS:H	4	0.18	0.03	0.18
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	4	0.12	0.01	0.12
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	4	0.12	0.01	0.12
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	4	0.12	0.01	0.12
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	4	0.12	0.01	0.12
(1,100)	1:14:A:ARG:HA	1:14:A:ARG:HE	4	0.12	0.01	0.12
(1,106)	1:14:A:ARG:HG2	1:14:A:ARG:H	3	0.49	0.01	0.5
(1,106)	1:14:A:ARG:HG3	1:14:A:ARG:H	3	0.49	0.01	0.5
(1,154)	1:8:A:ILE:HD11	1:21:A:MET:H	3	0.47	0.01	0.47

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,154)	1:8:A:ILE:HD12	1:21:A:MET:H	3	0.47	0.01	0.47
(1,154)	1:8:A:ILE:HD13	1:21:A:MET:H	3	0.47	0.01	0.47
(1,239)	1:35:B:LYS:HB2	1:35:B:LYS:H	3	0.2	0.03	0.21
(1,239)	1:35:B:LYS:HB3	1:35:B:LYS:H	3	0.2	0.03	0.21
(1,219)	1:42:B:TYR:HD1	1:43:B:CYS:H	3	0.17	0.05	0.2
(1,219)	1:42:B:TYR:HD2	1:43:B:CYS:H	3	0.17	0.05	0.2
(1,336)	1:40:B:ILE:HG12	1:52:B:ARG:HE	3	0.17	0.04	0.15
(1,336)	1:40:B:ILE:HG13	1:52:B:ARG:HE	3	0.17	0.04	0.15
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB2	3	0.16	0.04	0.14
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB3	3	0.16	0.04	0.14
(1,126)	1:20:A:ARG:HA	1:20:A:ARG:HE	3	0.15	0.04	0.12
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB2	3	0.14	0.02	0.14
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB3	3	0.14	0.02	0.14
(1,287)	1:46:B:ARG:HA	1:46:B:ARG:HE	3	0.14	0.0	0.14
(1,94)	1:13:A:ARG:HA	1:13:A:ARG:HE	3	0.12	0.01	0.13
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE1	3	0.11	0.0	0.11
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE2	3	0.11	0.0	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE1	3	0.11	0.0	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE2	3	0.11	0.0	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE1	3	0.11	0.0	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE2	3	0.11	0.0	0.11
(1,293)	1:46:B:ARG:HG2	1:46:B:ARG:H	2	0.49	0.01	0.49
(1,293)	1:46:B:ARG:HG3	1:46:B:ARG:H	2	0.49	0.01	0.49
(1,330)	1:53:B:MET:HG2	1:42:B:TYR:HD1	2	0.3	0.06	0.3
(1,330)	1:53:B:MET:HG2	1:42:B:TYR:HD2	2	0.3	0.06	0.3
(1,330)	1:53:B:MET:HG3	1:42:B:TYR:HD1	2	0.3	0.06	0.3
(1,330)	1:53:B:MET:HG3	1:42:B:TYR:HD2	2	0.3	0.06	0.3
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG11	2	0.18	0.04	0.18
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG12	2	0.18	0.04	0.18
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG13	2	0.18	0.04	0.18
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG21	2	0.18	0.04	0.18
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG22	2	0.18	0.04	0.18
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG23	2	0.18	0.04	0.18
(1,265)	1:41:B:ILE:HG21	1:41:B:ILE:H	2	0.15	0.0	0.15
(1,265)	1:41:B:ILE:HG22	1:41:B:ILE:H	2	0.15	0.0	0.15
(1,265)	1:41:B:ILE:HG23	1:41:B:ILE:H	2	0.15	0.0	0.15
(1,245)	1:36:B:LYS:HD2	1:36:B:LYS:H	2	0.15	0.03	0.15
(1,245)	1:36:B:LYS:HD3	1:36:B:LYS:H	2	0.15	0.03	0.15
(1,228)	1:47:B:THR:HG21	1:48:B:GLY:H	2	0.14	0.03	0.14
(1,228)	1:47:B:THR:HG22	1:48:B:GLY:H	2	0.14	0.03	0.14
(1,228)	1:47:B:THR:HG23	1:48:B:GLY:H	2	0.14	0.03	0.14
(1,59)	1:4:A:LYS:HG2	1:4:A:LYS:H	2	0.14	0.01	0.14

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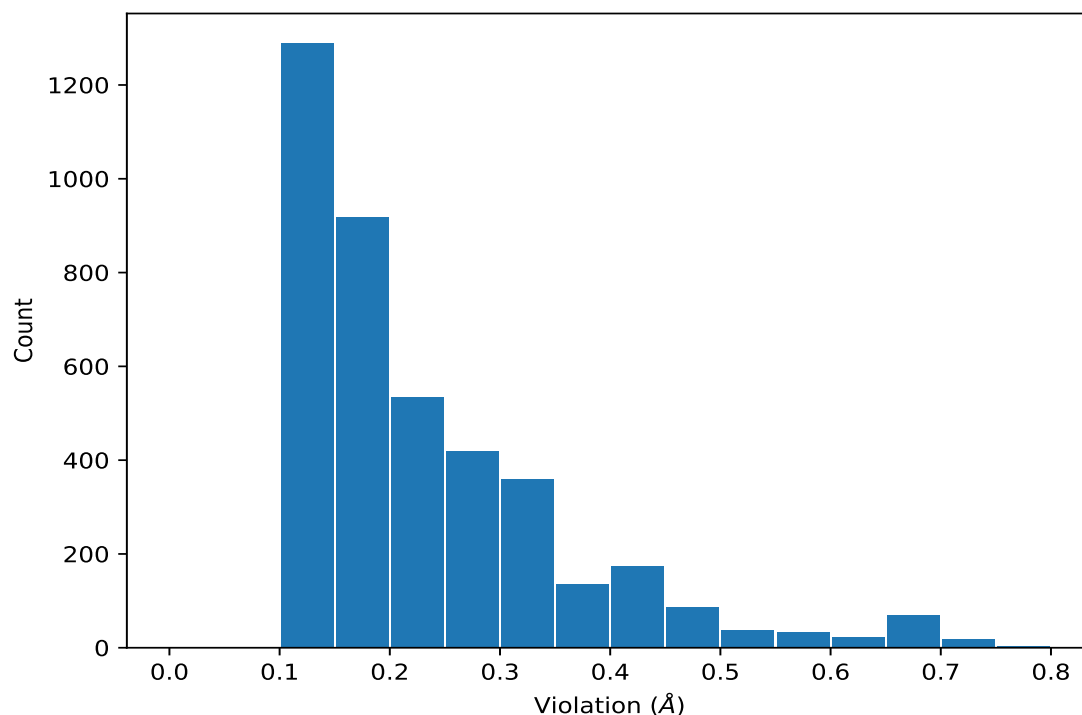
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,59)	1:4:A:LYS:HG3	1:4:A:LYS:H	2	0.14	0.01	0.14
(1,270)	1:42:B:TYR:HA	1:42:B:TYR:HD1	2	0.13	0.0	0.13
(1,270)	1:42:B:TYR:HA	1:42:B:TYR:HD2	2	0.13	0.0	0.13
(1,83)	1:10:A:TYR:HA	1:10:A:TYR:HD1	2	0.12	0.01	0.12
(1,83)	1:10:A:TYR:HA	1:10:A:TYR:HD2	2	0.12	0.01	0.12
(1,361)	1:42:B:TYR:HA	1:41:B:ILE:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	5	0.77
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	5	0.77
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	5	0.77
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	18	0.74
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	18	0.74
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	18	0.74
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	4	0.73
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	4	0.73
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	4	0.73
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	17	0.73
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	17	0.73
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	17	0.73
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	8	0.72
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	8	0.72
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	8	0.72
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	14	0.72
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	14	0.72
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	14	0.72
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	14	0.71
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	14	0.71
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	14	0.71
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	19	0.7
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	19	0.7
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	19	0.7
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	11	0.7
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	11	0.7
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	11	0.7
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	12	0.7
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	12	0.7
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	12	0.7
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	16	0.7
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	16	0.7
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	16	0.7
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	2	0.7
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	2	0.7
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	2	0.7
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	10	0.69
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	10	0.69
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	10	0.69
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	6	0.69
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	6	0.69
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	6	0.69
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	11	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	11	0.69
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	11	0.69
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	15	0.69
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	15	0.69
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	15	0.69
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	16	0.69
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	16	0.69
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	16	0.69
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	2	0.68
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	2	0.68
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	2	0.68
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	3	0.68
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	3	0.68
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	3	0.68
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	5	0.68
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	5	0.68
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	5	0.68
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	9	0.68
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	9	0.68
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	9	0.68
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	4	0.68
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	4	0.68
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	4	0.68
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	13	0.68
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	13	0.68
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	13	0.68
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	15	0.67
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	15	0.67
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	15	0.67
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	19	0.67
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	19	0.67
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	19	0.67
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	3	0.67
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	3	0.67
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	3	0.67
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	7	0.67
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	7	0.67
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	7	0.67
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	10	0.67
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	10	0.67
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	10	0.67
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	6	0.66
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	6	0.66
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	8	0.65
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	8	0.65
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	8	0.65
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	13	0.64
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	13	0.64
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	13	0.64
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	20	0.64
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	20	0.64
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	20	0.64
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	20	0.64
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	20	0.64
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	20	0.64
(1,98)	1:13:A:ARG:HD2	1:13:A:ARG:H	10	0.64
(1,98)	1:13:A:ARG:HD3	1:13:A:ARG:H	10	0.64
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	1	0.64
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	1	0.64
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	1	0.64
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	12	0.64
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	12	0.64
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	12	0.64
(1,258)	1:40:B:ILE:HD11	1:40:B:ILE:H	1	0.63
(1,258)	1:40:B:ILE:HD12	1:40:B:ILE:H	1	0.63
(1,258)	1:40:B:ILE:HD13	1:40:B:ILE:H	1	0.63
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	17	0.63
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	17	0.63
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	17	0.63
(1,341)	1:40:B:ILE:HD11	1:53:B:MET:H	7	0.59
(1,341)	1:40:B:ILE:HD12	1:53:B:MET:H	7	0.59
(1,341)	1:40:B:ILE:HD13	1:53:B:MET:H	7	0.59
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	8	0.59
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	8	0.59
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	8	0.59
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	8	0.59
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	8	0.59
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	8	0.59
(1,313)	1:52:B:ARG:HA	1:52:B:ARG:HE	17	0.57
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	12	0.57
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	12	0.57
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	16	0.56
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	16	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	16	0.56
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	16	0.56
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	16	0.56
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	16	0.56
(1,341)	1:40:B:ILE:HD11	1:53:B:MET:H	20	0.56
(1,341)	1:40:B:ILE:HD12	1:53:B:MET:H	20	0.56
(1,341)	1:40:B:ILE:HD13	1:53:B:MET:H	20	0.56
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	19	0.56
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	19	0.56
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	5	0.55
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	5	0.55
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	5	0.55
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	5	0.55
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	5	0.55
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	5	0.55
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	11	0.55
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	11	0.55
(1,71)	1:8:A:ILE:HD11	1:8:A:ILE:H	20	0.55
(1,71)	1:8:A:ILE:HD12	1:8:A:ILE:H	20	0.55
(1,71)	1:8:A:ILE:HD13	1:8:A:ILE:H	20	0.55
(1,337)	1:41:B:ILE:HG12	1:52:B:ARG:HE	16	0.54
(1,337)	1:41:B:ILE:HG13	1:52:B:ARG:HE	16	0.54
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	12	0.54
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	12	0.54
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	12	0.54
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	12	0.54
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	12	0.54
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	12	0.54
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	11	0.53
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	11	0.53
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	11	0.53
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	6	0.52
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	6	0.52
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	6	0.52
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	6	0.52
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	6	0.52
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	6	0.52
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	19	0.52
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	19	0.52
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	19	0.52
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	19	0.52
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	19	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	19	0.52
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	15	0.5
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	15	0.5
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	15	0.5
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	15	0.5
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	15	0.5
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	15	0.5
(1,293)	1:46:B:ARG:HG2	1:46:B:ARG:H	5	0.5
(1,293)	1:46:B:ARG:HG3	1:46:B:ARG:H	5	0.5
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	14	0.5
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	14	0.5
(1,106)	1:14:A:ARG:HG2	1:14:A:ARG:H	10	0.5
(1,106)	1:14:A:ARG:HG3	1:14:A:ARG:H	10	0.5
(1,106)	1:14:A:ARG:HG2	1:14:A:ARG:H	18	0.5
(1,106)	1:14:A:ARG:HG3	1:14:A:ARG:H	18	0.5
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	8	0.49
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	8	0.49
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	8	0.49
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	8	0.49
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	8	0.49
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	8	0.49
(1,293)	1:46:B:ARG:HG2	1:46:B:ARG:H	4	0.48
(1,293)	1:46:B:ARG:HG3	1:46:B:ARG:H	4	0.48
(1,154)	1:8:A:ILE:HD11	1:21:A:MET:H	9	0.48
(1,154)	1:8:A:ILE:HD12	1:21:A:MET:H	9	0.48
(1,154)	1:8:A:ILE:HD13	1:21:A:MET:H	9	0.48
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	17	0.47
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	13	0.47
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	13	0.47
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	13	0.47
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	13	0.47
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	13	0.47
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	13	0.47
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	17	0.47
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	17	0.47
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	17	0.47
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	17	0.47
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	17	0.47
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	17	0.47
(1,154)	1:8:A:ILE:HD11	1:21:A:MET:H	18	0.47
(1,154)	1:8:A:ILE:HD12	1:21:A:MET:H	18	0.47
(1,154)	1:8:A:ILE:HD13	1:21:A:MET:H	18	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:14:A:ARG:HG2	1:14:A:ARG:H	13	0.47
(1,106)	1:14:A:ARG:HG3	1:14:A:ARG:H	13	0.47
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	8	0.46
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	8	0.46
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	11	0.46
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	11	0.46
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	11	0.46
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	11	0.46
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	11	0.46
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	11	0.46
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	15	0.46
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	15	0.46
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	15	0.46
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	15	0.46
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	15	0.46
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	15	0.46
(1,154)	1:8:A:ILE:HD11	1:21:A:MET:H	19	0.46
(1,154)	1:8:A:ILE:HD12	1:21:A:MET:H	19	0.46
(1,154)	1:8:A:ILE:HD13	1:21:A:MET:H	19	0.46
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	16	0.45
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	16	0.45
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	16	0.45
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	16	0.45
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	16	0.45
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	16	0.45
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	6	0.45
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	6	0.45
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	15	0.45
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	15	0.45
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD2	7	0.45
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD3	7	0.45
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD2	7	0.45
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD3	7	0.45
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD2	7	0.45
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD3	7	0.45
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD2	7	0.45
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD3	7	0.45
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD2	7	0.45
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD3	7	0.45
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD2	7	0.45
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD3	7	0.45
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD2	20	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD3	20	0.45
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD2	20	0.45
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD3	20	0.45
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD2	20	0.45
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD3	20	0.45
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD2	20	0.45
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD3	20	0.45
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD2	20	0.45
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD3	20	0.45
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD2	20	0.45
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD3	20	0.45
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	13	0.45
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	13	0.45
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	13	0.45
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	13	0.45
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	13	0.45
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	13	0.45
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	20	0.44
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	20	0.44
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	20	0.44
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	20	0.44
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	20	0.44
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	20	0.44
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	14	0.44
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	14	0.44
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	14	0.44
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	14	0.44
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	14	0.44
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	14	0.44
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	1	0.44
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	1	0.44
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	1	0.44
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	1	0.44
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	1	0.44
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	1	0.44
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	6	0.44
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	6	0.44
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	6	0.44
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	6	0.44
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	6	0.44
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	6	0.44
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD2	18	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD3	18	0.44
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD2	18	0.44
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD3	18	0.44
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD2	18	0.44
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD3	18	0.44
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD2	18	0.44
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD3	18	0.44
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD2	18	0.44
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD3	18	0.44
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD2	18	0.44
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD3	18	0.44
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	11	0.43
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	20	0.43
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	18	0.43
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	18	0.43
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	18	0.43
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	18	0.43
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	18	0.43
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	18	0.43
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	1	0.43
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	1	0.43
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	1	0.43
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	1	0.43
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	1	0.43
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	1	0.43
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	5	0.43
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	5	0.43
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	5	0.43
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	5	0.43
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	5	0.43
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	5	0.43
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	8	0.43
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	8	0.43
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	8	0.43
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	8	0.43
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	8	0.43
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	8	0.43
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	14	0.43
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	14	0.43
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	14	0.43
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	14	0.43
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	14	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	14	0.43
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	20	0.43
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	20	0.43
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	20	0.43
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	20	0.43
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	20	0.43
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	20	0.43
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD2	9	0.43
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD3	9	0.43
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD2	9	0.43
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD3	9	0.43
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD2	9	0.43
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD3	9	0.43
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD2	9	0.43
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD3	9	0.43
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD2	9	0.43
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD3	9	0.43
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD2	9	0.43
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD3	9	0.43
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	2	0.42
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	2	0.42
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	2	0.42
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	2	0.42
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	2	0.42
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	2	0.42
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	3	0.42
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	3	0.42
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	3	0.42
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	3	0.42
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	3	0.42
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	3	0.42
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	2	0.42
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	2	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	2	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	2	0.42
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	2	0.42
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	2	0.42
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	4	0.42
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	4	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	4	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	4	0.42
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	4	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	4	0.42
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	7	0.42
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	7	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	7	0.42
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	7	0.42
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	7	0.42
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	7	0.42
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	19	0.42
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	19	0.42
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	19	0.41
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	11	0.41
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	11	0.41
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	11	0.41
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	11	0.41
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	11	0.41
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	11	0.41
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	4	0.41
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	3	0.41
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	3	0.41
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	3	0.41
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	3	0.41
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	3	0.41
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	3	0.41
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	16	0.41
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	16	0.41
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	16	0.41
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	16	0.41
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	16	0.41
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	16	0.41
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	10	0.41
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	13	0.41
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	9	0.4
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	9	0.4
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	9	0.4
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	9	0.4
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	9	0.4
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	9	0.4
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	12	0.4
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	12	0.4
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	12	0.4
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	12	0.4
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	12	0.4
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	10	0.4
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	10	0.4
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	10	0.4
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	10	0.4
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	10	0.4
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	10	0.4
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	18	0.4
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	18	0.4
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	18	0.4
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD2	19	0.4
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD3	19	0.4
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD2	19	0.4
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD3	19	0.4
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD2	19	0.4
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD3	19	0.4
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD2	19	0.4
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD3	19	0.4
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD2	19	0.4
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD3	19	0.4
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD2	19	0.4
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD3	19	0.4
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	9	0.39
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	12	0.39
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	4	0.39
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	4	0.39
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	4	0.39
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	4	0.39
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	4	0.39
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	4	0.39
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	10	0.39
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	10	0.39
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	10	0.39
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	10	0.39
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	10	0.39
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	10	0.39
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	14	0.39
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	14	0.39
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	14	0.39
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	14	0.39
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	14	0.39
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	18	0.39
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	18	0.39
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	5	0.39
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	9	0.39
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	9	0.39
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	9	0.39
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	9	0.39
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	9	0.39
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	9	0.39
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	20	0.39
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	20	0.39
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	20	0.39
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	20	0.38
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	17	0.38
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	17	0.38
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	17	0.38
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	20	0.37
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	20	0.37
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	20	0.37
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	7	0.37
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	7	0.37
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	7	0.37
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	7	0.37
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	7	0.37
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	7	0.37
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	19	0.37
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	19	0.37
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	19	0.37
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	19	0.37
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	19	0.37
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	19	0.37
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	16	0.37
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	16	0.37
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	17	0.37
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	17	0.37
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	17	0.37
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	17	0.37
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	17	0.37
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	17	0.37
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	19	0.37
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	19	0.37
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	19	0.37
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	19	0.37
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	19	0.37
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	18	0.37
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	18	0.37
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	18	0.37
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	18	0.37
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	18	0.37
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	18	0.37
(1,330)	1:53:B:MET:HG2	1:42:B:TYR:HD1	18	0.37
(1,330)	1:53:B:MET:HG2	1:42:B:TYR:HD2	18	0.37
(1,330)	1:53:B:MET:HG3	1:42:B:TYR:HD1	18	0.37
(1,330)	1:53:B:MET:HG3	1:42:B:TYR:HD2	18	0.37
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	17	0.37
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	17	0.37
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	16	0.37
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	16	0.37
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	18	0.37
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	18	0.37
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	18	0.37
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	18	0.37
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	18	0.37
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	18	0.37
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	9	0.37
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	9	0.37
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	14	0.37
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	7	0.37
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	7	0.37
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	12	0.37
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	12	0.37
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	12	0.37
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD2	5	0.37
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD3	5	0.37
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD2	5	0.37
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD3	5	0.37
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD2	5	0.37
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD3	5	0.37
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD2	5	0.37
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD3	5	0.37
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD2	5	0.37
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD3	5	0.37
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD2	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD3	5	0.37
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	12	0.37
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	7	0.36
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	9	0.36
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	9	0.36
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	9	0.36
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	18	0.36
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	18	0.36
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	18	0.36
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	9	0.36
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	9	0.36
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	9	0.36
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	9	0.36
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	9	0.36
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	9	0.36
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	13	0.36
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	13	0.36
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	13	0.36
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	13	0.36
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	13	0.36
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	13	0.36
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	10	0.36
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	10	0.36
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	9	0.36
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	9	0.36
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	17	0.36
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	17	0.36
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	8	0.36
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	8	0.36
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	3	0.36
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	3	0.36
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	18	0.35
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	5	0.35
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	17	0.35
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	17	0.35
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	17	0.35
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	17	0.35
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	17	0.35
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	17	0.35
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	6	0.35
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	6	0.35
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	15	0.35
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	15	0.35
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	15	0.35
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	16	0.35
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	16	0.35
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	7	0.35
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	7	0.35
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	7	0.35
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	7	0.35
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	7	0.35
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	7	0.35
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	16	0.35
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	16	0.35
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	16	0.35
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	16	0.35
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	16	0.35
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	16	0.35
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	15	0.35
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	15	0.35
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	15	0.35
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	15	0.35
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	15	0.35
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	15	0.35
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	16	0.35
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	16	0.35
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	16	0.35
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	16	0.35
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	16	0.35
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	16	0.35
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	15	0.35
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	15	0.35
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	1	0.35
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	1	0.35
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	17	0.35
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	17	0.35
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	20	0.35
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	20	0.35
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	13	0.35
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	13	0.35
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	20	0.35
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	11	0.35
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	20	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	9	0.34
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	18	0.34
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	19	0.34
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	19	0.34
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	19	0.34
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	7	0.34
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	7	0.34
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	7	0.34
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	8	0.34
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	8	0.34
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	8	0.34
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	8	0.34
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	8	0.34
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	8	0.34
(1,337)	1:41:B:ILE:HG12	1:52:B:ARG:HE	17	0.34
(1,337)	1:41:B:ILE:HG13	1:52:B:ARG:HE	17	0.34
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	2	0.34
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	2	0.34
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	5	0.34
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	5	0.34
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	10	0.34
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	10	0.34
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	13	0.34
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	13	0.34
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	19	0.34
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	19	0.34
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	14	0.34
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	14	0.34
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	4	0.34
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	4	0.34
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	6	0.34
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	6	0.34
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	18	0.34
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	18	0.34
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	14	0.34
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	14	0.34
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	2	0.34
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	2	0.34
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	2	0.34
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	2	0.34
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	2	0.34
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	6	0.34
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	6	0.34
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	6	0.34
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	6	0.34
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	6	0.34
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	6	0.34
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	12	0.34
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	12	0.34
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	12	0.34
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	12	0.34
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	12	0.34
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	12	0.34
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	13	0.34
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	13	0.34
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	13	0.34
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	13	0.34
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	13	0.34
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	13	0.34
(1,181)	1:6:A:VAL:HG11	1:3:A:LYS:H	14	0.34
(1,181)	1:6:A:VAL:HG12	1:3:A:LYS:H	14	0.34
(1,181)	1:6:A:VAL:HG13	1:3:A:LYS:H	14	0.34
(1,181)	1:6:A:VAL:HG21	1:3:A:LYS:H	14	0.34
(1,181)	1:6:A:VAL:HG22	1:3:A:LYS:H	14	0.34
(1,181)	1:6:A:VAL:HG23	1:3:A:LYS:H	14	0.34
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	3	0.34
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	3	0.34
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	6	0.34
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	6	0.34
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	15	0.34
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	15	0.34
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	18	0.34
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	18	0.34
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	10	0.34
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	10	0.34
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	15	0.33
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	15	0.33
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	15	0.33
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	15	0.33
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	15	0.33
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	15	0.33
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	1	0.33
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	1	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	1	0.33
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	1	0.33
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	1	0.33
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	1	0.33
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	4	0.33
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	4	0.33
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	4	0.33
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	4	0.33
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	4	0.33
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	4	0.33
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	9	0.33
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	9	0.33
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	9	0.33
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	9	0.33
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	9	0.33
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	9	0.33
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	14	0.33
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	14	0.33
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	14	0.33
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	14	0.33
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	14	0.33
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	14	0.33
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	19	0.33
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	19	0.33
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	19	0.33
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	19	0.33
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	19	0.33
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	19	0.33
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	1	0.33
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	1	0.33
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	3	0.33
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	3	0.33
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	4	0.33
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	4	0.33
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	7	0.33
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	7	0.33
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	9	0.33
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	9	0.33
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	3	0.33
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	3	0.33
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	5	0.33
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	12	0.33
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	12	0.33
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	4	0.33
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	4	0.33
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	4	0.33
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	4	0.33
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	4	0.33
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	4	0.33
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	11	0.33
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	11	0.33
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	11	0.33
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	11	0.33
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	11	0.33
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	11	0.33
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	15	0.33
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	15	0.33
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	15	0.33
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	15	0.33
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	15	0.33
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	15	0.33
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	17	0.33
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	17	0.33
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	17	0.33
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	17	0.33
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	17	0.33
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	17	0.33
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	19	0.33
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	19	0.33
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	19	0.33
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	19	0.33
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	19	0.33
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	19	0.33
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	2	0.33
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	2	0.33
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	2	0.33
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	2	0.33
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	2	0.33
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	2	0.33
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	4	0.33
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	4	0.33
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	4	0.33
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	4	0.33
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	4	0.33
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	6	0.33
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	6	0.33
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	6	0.33
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	6	0.33
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	6	0.33
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	6	0.33
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	7	0.33
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	7	0.33
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	7	0.33
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	7	0.33
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	7	0.33
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	7	0.33
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	9	0.33
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	9	0.33
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	10	0.33
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	10	0.33
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	2	0.33
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	2	0.33
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	5	0.33
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	1	0.32
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	13	0.32
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	2	0.32
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	2	0.32
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	2	0.32
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	2	0.32
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	2	0.32
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	2	0.32
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	3	0.32
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	3	0.32
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	3	0.32
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	3	0.32
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	3	0.32
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	3	0.32
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	12	0.32
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	12	0.32
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	12	0.32
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	12	0.32
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	12	0.32
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	12	0.32
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	16	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	16	0.32
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	11	0.32
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	11	0.32
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	12	0.32
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	12	0.32
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	14	0.32
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	14	0.32
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	18	0.32
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	18	0.32
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	20	0.32
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	20	0.32
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	13	0.32
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	1	0.32
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	1	0.32
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	1	0.32
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	1	0.32
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	1	0.32
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	1	0.32
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	3	0.32
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	3	0.32
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	3	0.32
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	3	0.32
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	3	0.32
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	3	0.32
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	10	0.32
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	10	0.32
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	10	0.32
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	10	0.32
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	10	0.32
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	10	0.32
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	13	0.32
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	13	0.32
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	13	0.32
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	13	0.32
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	13	0.32
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	13	0.32
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	4	0.32
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	4	0.32
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	2	0.32
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	2	0.32
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	4	0.32
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	4	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	7	0.32
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	7	0.32
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	13	0.32
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	13	0.32
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	16	0.32
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	16	0.32
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	12	0.32
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	12	0.32
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	15	0.32
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	15	0.32
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	5	0.31
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	5	0.31
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	5	0.31
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	5	0.31
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	5	0.31
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	5	0.31
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	10	0.31
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	10	0.31
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	10	0.31
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	10	0.31
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	10	0.31
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	10	0.31
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	11	0.31
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	11	0.31
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	11	0.31
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	11	0.31
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	11	0.31
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	11	0.31
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	13	0.31
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	13	0.31
(1,317)	1:52:B:ARG:HD2	1:52:B:ARG:H	8	0.31
(1,317)	1:52:B:ARG:HD3	1:52:B:ARG:H	8	0.31
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	11	0.31
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	6	0.31
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	17	0.31
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	17	0.31
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	17	0.31
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	17	0.31
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	17	0.31
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	17	0.31
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	8	0.31
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	3	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	3	0.31
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	4	0.31
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	4	0.31
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	5	0.31
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	5	0.31
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	9	0.31
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	9	0.31
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	20	0.31
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	20	0.31
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	14	0.31
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	14	0.31
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	14	0.31
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	14	0.31
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	6	0.3
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	6	0.3
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	6	0.3
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	6	0.3
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	6	0.3
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	6	0.3
(1,368)	1:38:B:VAL:HG11	1:35:B:LYS:H	16	0.3
(1,368)	1:38:B:VAL:HG12	1:35:B:LYS:H	16	0.3
(1,368)	1:38:B:VAL:HG13	1:35:B:LYS:H	16	0.3
(1,368)	1:38:B:VAL:HG21	1:35:B:LYS:H	16	0.3
(1,368)	1:38:B:VAL:HG22	1:35:B:LYS:H	16	0.3
(1,368)	1:38:B:VAL:HG23	1:35:B:LYS:H	16	0.3
(1,341)	1:40:B:ILE:HD11	1:53:B:MET:H	16	0.3
(1,341)	1:40:B:ILE:HD12	1:53:B:MET:H	16	0.3
(1,341)	1:40:B:ILE:HD13	1:53:B:MET:H	16	0.3
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	18	0.3
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	18	0.3
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	8	0.3
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	8	0.3
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	13	0.3
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	13	0.3
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	18	0.3
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	18	0.3
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	16	0.3
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	1	0.3
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	1	0.3
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	1	0.3
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	1	0.3
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	1	0.3
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	3	0.3
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	3	0.3
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	3	0.3
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	3	0.3
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	3	0.3
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	3	0.3
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	10	0.3
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	10	0.3
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	10	0.3
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	10	0.3
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	10	0.3
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	10	0.3
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	5	0.3
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	5	0.3
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	5	0.3
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	14	0.3
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	15	0.3
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	11	0.3
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	11	0.3
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	5	0.3
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	5	0.3
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	9	0.3
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	9	0.3
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	11	0.3
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	11	0.3
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	12	0.3
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	12	0.3
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	18	0.3
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	18	0.3
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	19	0.3
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	19	0.3
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	20	0.3
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	20	0.3
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	10	0.29
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	15	0.29
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	19	0.29
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	11	0.29
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	11	0.29
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	1	0.29
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	1	0.29
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	12	0.29
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	8	0.29
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	8	0.29
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	12	0.29
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	12	0.29
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	1	0.29
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	17	0.29
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	17	0.29
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	17	0.29
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	1	0.29
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	1	0.29
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	9	0.29
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	9	0.29
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	16	0.29
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	16	0.29
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	16	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	1	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	1	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	2	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	2	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	3	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	3	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	6	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	6	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	7	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	7	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	8	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	8	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	10	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	10	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	13	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	13	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	15	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	15	0.29
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	17	0.29
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	17	0.29
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	11	0.28
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	12	0.28
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	6	0.28
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	6	0.28
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	6	0.28
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	13	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	13	0.28
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	13	0.28
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	6	0.28
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	10	0.28
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	10	0.28
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	11	0.28
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	11	0.28
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	20	0.28
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	20	0.28
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	20	0.28
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	20	0.28
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	8	0.28
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	8	0.28
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	20	0.28
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	20	0.28
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	12	0.28
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	12	0.28
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	12	0.28
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	12	0.28
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	12	0.28
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	12	0.28
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	14	0.28
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	14	0.28
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	12	0.28
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	12	0.28
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	12	0.28
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	12	0.28
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	12	0.28
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	12	0.28
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	9	0.28
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	14	0.28
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	14	0.28
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	4	0.28
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	4	0.28
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	9	0.28
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	9	0.28
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	16	0.28
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	16	0.28
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	19	0.28
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	19	0.28
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	13	0.28
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	19	0.28
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	19	0.28
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	6	0.28
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	6	0.28
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	15	0.28
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	15	0.28
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	17	0.28
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	17	0.28
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	15	0.28
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	4	0.28
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	4	0.28
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	16	0.28
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	16	0.28
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	4	0.27
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	5	0.27
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	14	0.27
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	3	0.27
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	4	0.27
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	4	0.27
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	4	0.27
(1,372)	1:38:B:VAL:HG11	1:52:B:ARG:HE	18	0.27
(1,372)	1:38:B:VAL:HG12	1:52:B:ARG:HE	18	0.27
(1,372)	1:38:B:VAL:HG13	1:52:B:ARG:HE	18	0.27
(1,372)	1:38:B:VAL:HG21	1:52:B:ARG:HE	18	0.27
(1,372)	1:38:B:VAL:HG22	1:52:B:ARG:HE	18	0.27
(1,372)	1:38:B:VAL:HG23	1:52:B:ARG:HE	18	0.27
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	14	0.27
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	7	0.27
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	16	0.27
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	16	0.27
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	16	0.27
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	16	0.27
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	19	0.27
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	19	0.27
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	19	0.27
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	19	0.27
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	2	0.27
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	2	0.27
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	12	0.27
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	12	0.27
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	4	0.27
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	5	0.27
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	5	0.27
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	11	0.27
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	11	0.27
(1,300)	1:49:B:LYS:HB2	1:49:B:LYS:H	2	0.27
(1,300)	1:49:B:LYS:HB3	1:49:B:LYS:H	2	0.27
(1,300)	1:49:B:LYS:HB2	1:49:B:LYS:H	19	0.27
(1,300)	1:49:B:LYS:HB3	1:49:B:LYS:H	19	0.27
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	10	0.27
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	11	0.27
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	2	0.27
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	2	0.27
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	12	0.27
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	12	0.27
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	13	0.27
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	13	0.27
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	15	0.27
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	15	0.27
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	17	0.27
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	17	0.27
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	20	0.27
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	12	0.27
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	12	0.27
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	12	0.27
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	12	0.27
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	3	0.27
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	18	0.27
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	1	0.27
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	1	0.27
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	3	0.27
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	3	0.27
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	10	0.27
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	10	0.27
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	13	0.27
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	13	0.27
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	14	0.27
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	14	0.27
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	17	0.27
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	17	0.27
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	1	0.27
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	1	0.27
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	15	0.27
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	14	0.27
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	14	0.27
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	5	0.27
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	5	0.27
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	12	0.27
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	12	0.27
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	14	0.27
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	14	0.27
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	19	0.27
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	19	0.27
(1,19)	1:7:A:PRO:HB2	1:8:A:ILE:H	14	0.27
(1,19)	1:7:A:PRO:HB3	1:8:A:ILE:H	14	0.27
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	16	0.26
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	17	0.26
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	8	0.26
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	8	0.26
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	8	0.26
(1,368)	1:38:B:VAL:HG11	1:35:B:LYS:H	6	0.26
(1,368)	1:38:B:VAL:HG12	1:35:B:LYS:H	6	0.26
(1,368)	1:38:B:VAL:HG13	1:35:B:LYS:H	6	0.26
(1,368)	1:38:B:VAL:HG21	1:35:B:LYS:H	6	0.26
(1,368)	1:38:B:VAL:HG22	1:35:B:LYS:H	6	0.26
(1,368)	1:38:B:VAL:HG23	1:35:B:LYS:H	6	0.26
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	8	0.26
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	16	0.26
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	6	0.26
(1,337)	1:41:B:ILE:HG12	1:52:B:ARG:HE	15	0.26
(1,337)	1:41:B:ILE:HG13	1:52:B:ARG:HE	15	0.26
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	10	0.26
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	3	0.26
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	3	0.26
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	14	0.26
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	14	0.26
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	20	0.26
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	20	0.26
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	3	0.26
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	3	0.26
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	8	0.26
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	8	0.26
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	12	0.26
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	12	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	13	0.26
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	13	0.26
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	15	0.26
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	15	0.26
(1,300)	1:49:B:LYS:HB2	1:49:B:LYS:H	1	0.26
(1,300)	1:49:B:LYS:HB3	1:49:B:LYS:H	1	0.26
(1,300)	1:49:B:LYS:HB2	1:49:B:LYS:H	10	0.26
(1,300)	1:49:B:LYS:HB3	1:49:B:LYS:H	10	0.26
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	1	0.26
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	2	0.26
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	3	0.26
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	5	0.26
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	6	0.26
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	12	0.26
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	14	0.26
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	7	0.26
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	7	0.26
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	16	0.26
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	16	0.26
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	1	0.26
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	1	0.26
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	6	0.26
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	6	0.26
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	15	0.26
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	15	0.26
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	12	0.26
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	4	0.26
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	19	0.26
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	20	0.26
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	20	0.26
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	4	0.26
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	8	0.26
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	17	0.26
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	14	0.26
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	14	0.26
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	14	0.26
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	14	0.26
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	15	0.26
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	10	0.26
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	10	0.26
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	2	0.26
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	5	0.26
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	5	0.26
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	11	0.26
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	11	0.26
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	20	0.26
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	20	0.26
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	8	0.26
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	8	0.26
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	18	0.26
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	18	0.26
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	3	0.26
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	10	0.26
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	12	0.26
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	12	0.26
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	16	0.26
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	16	0.26
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	3	0.26
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	3	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	2	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	2	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	5	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	5	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	6	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	6	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	8	0.26
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	8	0.26
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	10	0.25
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	4	0.25
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	5	0.25
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	8	0.25
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	13	0.25
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	15	0.25
(1,337)	1:41:B:ILE:HG12	1:52:B:ARG:HE	6	0.25
(1,337)	1:41:B:ILE:HG13	1:52:B:ARG:HE	6	0.25
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	13	0.25
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	13	0.25
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	6	0.25
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	6	0.25
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	16	0.25
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	16	0.25
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	17	0.25
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	18	0.25
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	18	0.25
(1,300)	1:49:B:LYS:HB2	1:49:B:LYS:H	7	0.25
(1,300)	1:49:B:LYS:HB3	1:49:B:LYS:H	7	0.25
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	9	0.25
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	4	0.25
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	4	0.25
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	19	0.25
(1,178)	1:15:A:THR:HG21	1:14:A:ARG:HE	4	0.25
(1,178)	1:15:A:THR:HG22	1:14:A:ARG:HE	4	0.25
(1,178)	1:15:A:THR:HG23	1:14:A:ARG:HE	4	0.25
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD2	11	0.25
(1,172)	1:8:A:ILE:HD11	1:7:A:PRO:HD3	11	0.25
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD2	11	0.25
(1,172)	1:8:A:ILE:HD12	1:7:A:PRO:HD3	11	0.25
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD2	11	0.25
(1,172)	1:8:A:ILE:HD13	1:7:A:PRO:HD3	11	0.25
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	5	0.25
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	16	0.25
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	16	0.25
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	2	0.25
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	6	0.25
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	13	0.25
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	15	0.25
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	15	0.25
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	15	0.25
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	15	0.25
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	7	0.25
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	7	0.25
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	7	0.25
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	7	0.25
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	15	0.25
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	15	0.25
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	19	0.25
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	19	0.25
(1,113)	1:17:A:LYS:HB2	1:17:A:LYS:H	6	0.25
(1,113)	1:17:A:LYS:HB3	1:17:A:LYS:H	6	0.25
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	2	0.25
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	6	0.25
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	15	0.25
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	15	0.25
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	20	0.25
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	2	0.25
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	7	0.25
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	19	0.25
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	8	0.25
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	8	0.25
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	8	0.25
(1,16)	1:2:A:SER:HB2	1:3:A:LYS:H	8	0.25
(1,16)	1:2:A:SER:HB3	1:3:A:LYS:H	8	0.25
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	4	0.25
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	8	0.25
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	2	0.24
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	3	0.24
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	11	0.24
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	11	0.24
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	11	0.24
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	15	0.24
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	15	0.24
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	15	0.24
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	13	0.24
(1,330)	1:53:B:MET:HG2	1:42:B:TYR:HD1	8	0.24
(1,330)	1:53:B:MET:HG2	1:42:B:TYR:HD2	8	0.24
(1,330)	1:53:B:MET:HG3	1:42:B:TYR:HD1	8	0.24
(1,330)	1:53:B:MET:HG3	1:42:B:TYR:HD2	8	0.24
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	2	0.24
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	1	0.24
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	1	0.24
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	5	0.24
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	5	0.24
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	8	0.24
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	8	0.24
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	9	0.24
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	9	0.24
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	6	0.24
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	6	0.24
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	15	0.24
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	15	0.24
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	19	0.24
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	19	0.24
(1,318)	1:53:B:MET:HB2	1:53:B:MET:H	8	0.24
(1,318)	1:53:B:MET:HB3	1:53:B:MET:H	8	0.24
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	9	0.24
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	8	0.24
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	18	0.24
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	16	0.24
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	16	0.24
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	14	0.24
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	14	0.24
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	9	0.24
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	9	0.24
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	18	0.24
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	2	0.24
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	2	0.24
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	5	0.24
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	5	0.24
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	15	0.24
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	15	0.24
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	14	0.24
(1,187)	1:6:A:VAL:HG11	1:9:A:ILE:H	20	0.24
(1,187)	1:6:A:VAL:HG12	1:9:A:ILE:H	20	0.24
(1,187)	1:6:A:VAL:HG13	1:9:A:ILE:H	20	0.24
(1,187)	1:6:A:VAL:HG21	1:9:A:ILE:H	20	0.24
(1,187)	1:6:A:VAL:HG22	1:9:A:ILE:H	20	0.24
(1,187)	1:6:A:VAL:HG23	1:9:A:ILE:H	20	0.24
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	14	0.24
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	14	0.24
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	14	0.24
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	14	0.24
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	14	0.24
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	14	0.24
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	20	0.24
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	20	0.24
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	20	0.24
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	20	0.24
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	20	0.24
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	20	0.24
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	11	0.24
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	1	0.24
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	15	0.24
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	1	0.24
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	8	0.24
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	17	0.24
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	17	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	7	0.24
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	7	0.24
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	4	0.24
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	8	0.24
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	3	0.24
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	18	0.24
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	18	0.24
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	3	0.24
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	13	0.24
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	4	0.23
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	15	0.23
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	1	0.23
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	1	0.23
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	1	0.23
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	16	0.23
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	16	0.23
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	16	0.23
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	12	0.23
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	20	0.23
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	1	0.23
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	2	0.23
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	14	0.23
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	18	0.23
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	20	0.23
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	17	0.23
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	7	0.23
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	7	0.23
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	15	0.23
(1,239)	1:35:B:LYS:HB2	1:35:B:LYS:H	10	0.23
(1,239)	1:35:B:LYS:HB3	1:35:B:LYS:H	10	0.23
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	10	0.23
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	10	0.23
(1,226)	1:46:B:ARG:HB2	1:47:B:THR:H	17	0.23
(1,226)	1:46:B:ARG:HB3	1:47:B:THR:H	17	0.23
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	17	0.23
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	12	0.23
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	6	0.23
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	6	0.23
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	7	0.23
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	7	0.23
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	8	0.23
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	17	0.23
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	17	0.23
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	1	0.23
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	1	0.23
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	1	0.23
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	2	0.23
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	2	0.23
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	2	0.23
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	6	0.23
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	6	0.23
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	6	0.23
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	13	0.23
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	13	0.23
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	13	0.23
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	11	0.23
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	11	0.23
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	12	0.23
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	12	0.23
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	14	0.23
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	14	0.23
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	16	0.23
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	16	0.23
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	10	0.23
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	11	0.23
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	2	0.23
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	16	0.23
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	17	0.23
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	20	0.23
(1,150)	1:9:A:ILE:HG12	1:20:A:ARG:HE	8	0.23
(1,150)	1:9:A:ILE:HG13	1:20:A:ARG:HE	8	0.23
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	16	0.23
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	16	0.23
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	16	0.23
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	16	0.23
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	20	0.23
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	20	0.23
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	20	0.23
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	20	0.23
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	13	0.23
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	13	0.23
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	7	0.23
(1,52)	1:3:A:LYS:HB2	1:3:A:LYS:H	13	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:3:A:LYS:HB3	1:3:A:LYS:H	13	0.23
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	3	0.23
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	3	0.23
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	12	0.23
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	12	0.23
(1,39)	1:14:A:ARG:HB2	1:15:A:THR:H	7	0.23
(1,39)	1:14:A:ARG:HB3	1:15:A:THR:H	7	0.23
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	7	0.23
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	5	0.23
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	8	0.23
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	8	0.23
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	12	0.23
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	12	0.23
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	12	0.23
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	12	0.23
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	12	0.23
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	12	0.23
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	1	0.23
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	1	0.23
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	3	0.23
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	3	0.23
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	11	0.23
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	11	0.23
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	10	0.23
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	2	0.22
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	7	0.22
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG11	11	0.22
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG12	11	0.22
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG13	11	0.22
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG21	11	0.22
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG22	11	0.22
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG23	11	0.22
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	20	0.22
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	20	0.22
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	20	0.22
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	5	0.22
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	5	0.22
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	5	0.22
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	17	0.22
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	17	0.22
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	17	0.22
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	18	0.22
(1,336)	1:40:B:ILE:HG12	1:52:B:ARG:HE	17	0.22
(1,336)	1:40:B:ILE:HG13	1:52:B:ARG:HE	17	0.22
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	11	0.22
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	11	0.22
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	11	0.22
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	11	0.22
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	1	0.22
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	16	0.22
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	14	0.22
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	14	0.22
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	17	0.22
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	17	0.22
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	9	0.22
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	11	0.22
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	3	0.22
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	5	0.22
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	7	0.22
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	7	0.22
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	15	0.22
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	15	0.22
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	16	0.22
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	16	0.22
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	19	0.22
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	19	0.22
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	18	0.22
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	18	0.22
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	18	0.22
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	18	0.22
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	18	0.22
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	18	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	3	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	3	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	10	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	10	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	12	0.22
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	12	0.22
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	12	0.22
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	12	0.22
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	12	0.22
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD2	16	0.22
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD3	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD2	16	0.22
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD3	16	0.22
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD2	16	0.22
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD3	16	0.22
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD2	16	0.22
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD3	16	0.22
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD2	16	0.22
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD3	16	0.22
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD2	16	0.22
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD3	16	0.22
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	2	0.22
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	2	0.22
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	3	0.22
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	3	0.22
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	4	0.22
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	4	0.22
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	6	0.22
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	6	0.22
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	9	0.22
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	9	0.22
(1,203)	1:34:B:SER:HB2	1:35:B:LYS:H	17	0.22
(1,203)	1:34:B:SER:HB3	1:35:B:LYS:H	17	0.22
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	13	0.22
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	11	0.22
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	11	0.22
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	11	0.22
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	11	0.22
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	9	0.22
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	13	0.22
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	13	0.22
(1,130)	1:20:A:ARG:HD2	1:20:A:ARG:H	5	0.22
(1,130)	1:20:A:ARG:HD3	1:20:A:ARG:H	5	0.22
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	18	0.22
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	18	0.22
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	3	0.22
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	10	0.22
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	11	0.22
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	14	0.22
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	12	0.22
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	12	0.22
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	14	0.22
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	14	0.22
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	14	0.22
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	14	0.22
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	14	0.22
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	10	0.22
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	10	0.22
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	14	0.22
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	14	0.22
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	17	0.22
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	17	0.22
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	15	0.22
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	16	0.22
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	19	0.22
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	11	0.21
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	11	0.21
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	11	0.21
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	1	0.21
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	1	0.21
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	1	0.21
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	1	0.21
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	1	0.21
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	1	0.21
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	5	0.21
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	5	0.21
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	5	0.21
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	5	0.21
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	5	0.21
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	5	0.21
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	18	0.21
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	18	0.21
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	18	0.21
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	18	0.21
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	18	0.21
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	18	0.21
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	1	0.21
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	1	0.21
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	5	0.21
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB2	11	0.21
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB3	11	0.21
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	12	0.21
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	17	0.21
(1,341)	1:40:B:ILE:HD11	1:53:B:MET:H	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:40:B:ILE:HD12	1:53:B:MET:H	19	0.21
(1,341)	1:40:B:ILE:HD13	1:53:B:MET:H	19	0.21
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	9	0.21
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	9	0.21
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	17	0.21
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	17	0.21
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	9	0.21
(1,239)	1:35:B:LYS:HB2	1:35:B:LYS:H	4	0.21
(1,239)	1:35:B:LYS:HB3	1:35:B:LYS:H	4	0.21
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	14	0.21
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	18	0.21
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	17	0.21
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	17	0.21
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	9	0.21
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	9	0.21
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	19	0.21
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	19	0.21
(1,219)	1:42:B:TYR:HD1	1:43:B:CYS:H	16	0.21
(1,219)	1:42:B:TYR:HD2	1:43:B:CYS:H	16	0.21
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	2	0.21
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	8	0.21
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	20	0.21
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	4	0.21
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	4	0.21
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	17	0.21
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	17	0.21
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	1	0.21
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	1	0.21
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	1	0.21
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	1	0.21
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	1	0.21
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	1	0.21
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	19	0.21
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	19	0.21
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	19	0.21
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	19	0.21
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	19	0.21
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	19	0.21
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	9	0.21
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	9	0.21
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	3	0.21
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	3	0.21
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	7	0.21
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	7	0.21
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	7	0.21
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	7	0.21
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	6	0.21
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	14	0.21
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	2	0.21
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	2	0.21
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	16	0.21
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	16	0.21
(1,126)	1:20:A:ARG:HA	1:20:A:ARG:HE	20	0.21
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	7	0.21
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	7	0.21
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	7	0.21
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	7	0.21
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	6	0.21
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	17	0.21
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	18	0.21
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	1	0.21
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	1	0.21
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	2	0.21
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	2	0.21
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	9	0.21
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	9	0.21
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	13	0.21
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	13	0.21
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	3	0.21
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	3	0.21
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	3	0.21
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	1	0.2
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	8	0.2
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	8	0.2
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	8	0.2
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	1	0.2
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	1	0.2
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	2	0.2
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	2	0.2
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	14	0.2
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	14	0.2
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	14	0.2
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD2	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:40:B:ILE:HD11	1:39:B:PRO:HD3	13	0.2
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD2	13	0.2
(1,359)	1:40:B:ILE:HD12	1:39:B:PRO:HD3	13	0.2
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD2	13	0.2
(1,359)	1:40:B:ILE:HD13	1:39:B:PRO:HD3	13	0.2
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	9	0.2
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	9	0.2
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	9	0.2
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	9	0.2
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	7	0.2
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	14	0.2
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	3	0.2
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	3	0.2
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	16	0.2
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	16	0.2
(1,295)	1:46:B:ARG:HD2	1:46:B:ARG:H	19	0.2
(1,295)	1:46:B:ARG:HD3	1:46:B:ARG:H	19	0.2
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	19	0.2
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	19	0.2
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	7	0.2
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	7	0.2
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	12	0.2
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	13	0.2
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	13	0.2
(1,219)	1:42:B:TYR:HD1	1:43:B:CYS:H	19	0.2
(1,219)	1:42:B:TYR:HD2	1:43:B:CYS:H	19	0.2
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	1	0.2
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	10	0.2
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	14	0.2
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	1	0.2
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	1	0.2
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	13	0.2
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	13	0.2
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	5	0.2
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	5	0.2
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	5	0.2
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	5	0.2
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	5	0.2
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	5	0.2
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	14	0.2
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	14	0.2
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	20	0.2
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	7	0.2
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	7	0.2
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	13	0.2
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	13	0.2
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	20	0.2
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	20	0.2
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	3	0.2
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	3	0.2
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	5	0.2
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	9	0.2
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	9	0.2
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	9	0.2
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	9	0.2
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	10	0.2
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	10	0.2
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	10	0.2
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	10	0.2
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	11	0.2
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	11	0.2
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	17	0.2
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	17	0.2
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	7	0.2
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	19	0.2
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	6	0.2
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	6	0.2
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	15	0.2
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	15	0.2
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	3	0.2
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	3	0.2
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	18	0.2
(1,52)	1:3:A:LYS:HB2	1:3:A:LYS:H	6	0.2
(1,52)	1:3:A:LYS:HB3	1:3:A:LYS:H	6	0.2
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	20	0.2
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	20	0.2
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	20	0.2
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	20	0.2
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	20	0.2
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	20	0.2
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	9	0.2
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	13	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	1	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	1	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	1	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	1	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	1	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	2	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	2	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	2	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	2	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	2	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	2	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	6	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	6	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	6	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	6	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	6	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	6	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	17	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	17	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	17	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	17	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	17	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	17	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	20	0.2
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	20	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	20	0.2
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	20	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	20	0.2
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	20	0.2
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	7	0.2
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	7	0.2
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	7	0.2
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	9	0.2
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	9	0.2
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	9	0.2
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	10	0.2
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	10	0.2
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	10	0.2
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	18	0.2
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	18	0.2
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	18	0.2
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	19	0.19
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	17	0.19
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	17	0.19
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	17	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	2	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	2	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	2	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	15	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	15	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	15	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	19	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	19	0.19
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	19	0.19
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	7	0.19
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	7	0.19
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	7	0.19
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	7	0.19
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	7	0.19
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	7	0.19
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	16	0.19
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	16	0.19
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	16	0.19
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	16	0.19
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	16	0.19
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	16	0.19
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	12	0.19
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	3	0.19
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	11	0.19
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	10	0.19
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	3	0.19
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	3	0.19
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	3	0.19
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	3	0.19
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	5	0.19
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	5	0.19
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	5	0.19
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	5	0.19
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	5	0.19
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	5	0.19
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	11	0.19
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	11	0.19
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	4	0.19
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	4	0.19
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	4	0.19
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	9	0.19
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	9	0.19
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	7	0.19
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	7	0.19
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	19	0.19
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	19	0.19
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	7	0.19
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	20	0.19
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	19	0.19
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	19	0.19
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	16	0.19
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	2	0.19
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	2	0.19
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	6	0.19
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	6	0.19
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	9	0.19
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	9	0.19
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	15	0.19
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	15	0.19
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	16	0.19
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	16	0.19
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	2	0.19
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	2	0.19
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	10	0.19
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	10	0.19
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	14	0.19
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	14	0.19
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	2	0.19
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	2	0.19
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	2	0.19
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	2	0.19
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	2	0.19
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	2	0.19
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	4	0.19
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	4	0.19
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	4	0.19
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	4	0.19
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	4	0.19
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	8	0.19
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	8	0.19
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	8	0.19
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	8	0.19
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	8	0.19
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	8	0.19
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	11	0.19
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	11	0.19
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	15	0.19
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	15	0.19
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	15	0.19
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	1	0.19
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	1	0.19
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	2	0.19
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	2	0.19
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	3	0.19
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	3	0.19
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	2	0.19
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	1	0.19
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	1	0.19
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	6	0.19
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	6	0.19
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	3	0.19
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	17	0.19
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	17	0.19
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	17	0.19
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	17	0.19
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	10	0.19
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	12	0.19
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	12	0.19
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	16	0.19
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	16	0.19
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	18	0.19
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	18	0.19
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	7	0.19
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	7	0.19
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	15	0.19
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	15	0.19
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	3	0.19
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	3	0.19
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	12	0.19
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	20	0.19
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	5	0.19
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	5	0.19
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	6	0.19
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	6	0.19
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	8	0.19
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	8	0.19
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	11	0.19
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	11	0.19
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	17	0.19
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	17	0.19
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	19	0.19
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	19	0.19
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	2	0.19
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	4	0.19
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	4	0.19
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	4	0.19
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	6	0.19
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	6	0.19
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	13	0.19
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	13	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	3	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	3	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	3	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	3	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	3	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	3	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	11	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	11	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	11	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	11	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	11	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	11	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	13	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	13	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	13	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	13	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	13	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	13	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	15	0.19
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	15	0.19
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	15	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	15	0.19
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	15	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	4	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	4	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	7	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	7	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	12	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	12	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	15	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	15	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	19	0.19
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	19	0.19
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	10	0.18
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	10	0.18
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	10	0.18
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	20	0.18
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	20	0.18
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	20	0.18
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	20	0.18
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	20	0.18
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	20	0.18
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	5	0.18
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	5	0.18
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	9	0.18
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	9	0.18
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	17	0.18
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	17	0.18
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	3	0.18
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	3	0.18
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	3	0.18
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	4	0.18
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	4	0.18
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	4	0.18
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	5	0.18
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	5	0.18
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	5	0.18
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	15	0.18
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	17	0.18
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	9	0.18
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	16	0.18
(1,341)	1:40:B:ILE:HD11	1:53:B:MET:H	18	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,341)	1:40:B:ILE:HD12	1:53:B:MET:H	18	0.18
(1,341)	1:40:B:ILE:HD13	1:53:B:MET:H	18	0.18
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	18	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	2	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	2	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	2	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	2	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	4	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	4	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	4	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	4	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	8	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	8	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	8	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	8	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	10	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	10	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	10	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	10	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	12	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	12	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	12	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	12	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	14	0.18
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	14	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	14	0.18
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	14	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	1	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	1	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	3	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	3	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	9	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	9	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	13	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	13	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	18	0.18
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	18	0.18
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	3	0.18
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	9	0.18
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	1	0.18
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	1	0.18
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	12	0.18
(1,319)	1:53:B:MET:HG2	1:53:B:MET:H	18	0.18
(1,319)	1:53:B:MET:HG3	1:53:B:MET:H	18	0.18
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	2	0.18
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	2	0.18
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	10	0.18
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	10	0.18
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	19	0.18
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	19	0.18
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	14	0.18
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	14	0.18
(1,228)	1:47:B:THR:HG21	1:48:B:GLY:H	19	0.18
(1,228)	1:47:B:THR:HG22	1:48:B:GLY:H	19	0.18
(1,228)	1:47:B:THR:HG23	1:48:B:GLY:H	19	0.18
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	1	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	1	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	1	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	3	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	3	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	8	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	8	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	10	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	10	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	12	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	12	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	18	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	18	0.18
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	20	0.18
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	20	0.18
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	4	0.18
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	19	0.18
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	3	0.18
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	3	0.18
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	5	0.18
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	5	0.18
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	8	0.18
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	8	0.18
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	18	0.18
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	18	0.18
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	20	0.18
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	20	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	3	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	3	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	3	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	3	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	3	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	9	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	9	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	9	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	9	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	9	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	9	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	10	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	10	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	10	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	10	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	10	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	10	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	13	0.18
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	13	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	13	0.18
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	13	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	13	0.18
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	13	0.18
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	16	0.18
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	16	0.18
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	13	0.18
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	13	0.18
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	19	0.18
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	19	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	4	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	4	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	5	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	5	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	6	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	6	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	8	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	8	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	9	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	9	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	10	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	10	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	11	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	12	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	12	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	15	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	15	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	18	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	18	0.18
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	19	0.18
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	19	0.18
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	3	0.18
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	7	0.18
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	7	0.18
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	12	0.18
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	12	0.18
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	14	0.18
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	14	0.18
(1,178)	1:15:A:THR:HG21	1:14:A:ARG:HE	11	0.18
(1,178)	1:15:A:THR:HG22	1:14:A:ARG:HE	11	0.18
(1,178)	1:15:A:THR:HG23	1:14:A:ARG:HE	11	0.18
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	15	0.18
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	16	0.18
(1,174)	1:10:A:TYR:HA	1:9:A:ILE:H	11	0.18
(1,174)	1:10:A:TYR:HA	1:9:A:ILE:H	14	0.18
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	10	0.18
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	3	0.18
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	7	0.18
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	12	0.18
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	14	0.18
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	16	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	2	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	2	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	2	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	2	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	3	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	3	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	3	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	3	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	6	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	6	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	6	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	6	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	8	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	8	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	8	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	13	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	13	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	13	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	13	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	18	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	18	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	18	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	18	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	19	0.18
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	19	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	19	0.18
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	19	0.18
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	6	0.18
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	6	0.18
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	10	0.18
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	10	0.18
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	16	0.18
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	16	0.18
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	5	0.18
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	16	0.18
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	4	0.18
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	4	0.18
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	9	0.18
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	9	0.18
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	6	0.18
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	6	0.18
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	15	0.18
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	15	0.18
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	9	0.18
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	1	0.18
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	12	0.18
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	1	0.18
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	1	0.18
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	3	0.18
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	3	0.18
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	4	0.18
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	4	0.18
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	9	0.18
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	14	0.18
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	14	0.18
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	16	0.18
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	16	0.18
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	7	0.18
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	7	0.18
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	12	0.18
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	12	0.18
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	1	0.18
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	3	0.18
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	3	0.18
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	5	0.18
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	5	0.18
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	9	0.18
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	9	0.18
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	17	0.18
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	17	0.18
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	18	0.18
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	18	0.18
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	4	0.18
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	4	0.18
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	4	0.18
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	4	0.18
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	4	0.18
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	4	0.18
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	5	0.18
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	5	0.18
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	5	0.18
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	5	0.18
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	5	0.18
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	5	0.18
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	10	0.18
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	10	0.18
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	10	0.18
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	10	0.18
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	10	0.18
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	10	0.18
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	4	0.18
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	4	0.18
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	4	0.18
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	1	0.18
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	3	0.17
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	3	0.17
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	3	0.17
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	16	0.17
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	16	0.17
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	16	0.17
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	6	0.17
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	6	0.17
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	6	0.17
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	10	0.17
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	10	0.17
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	10	0.17
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	13	0.17
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	13	0.17
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	6	0.17
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	6	0.17
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	6	0.17
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	7	0.17
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	8	0.17
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	15	0.17
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	6	0.17
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	9	0.17
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	19	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	1	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	1	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	1	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	1	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	6	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	6	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	6	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	6	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	15	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	15	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	15	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	15	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	17	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	17	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	17	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	17	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	18	0.17
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	18	0.17
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	18	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	2	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	2	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	6	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	6	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	10	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	10	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	17	0.17
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	17	0.17
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	8	0.17
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	7	0.17
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	7	0.17
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	9	0.17
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	9	0.17
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	18	0.17
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	18	0.17
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	4	0.17
(1,245)	1:36:B:LYS:HD2	1:36:B:LYS:H	13	0.17
(1,245)	1:36:B:LYS:HD3	1:36:B:LYS:H	13	0.17
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	9	0.17
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	9	0.17
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	13	0.17
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	15	0.17
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	4	0.17
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	4	0.17
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	5	0.17
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	5	0.17
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	11	0.17
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	11	0.17
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	1	0.17
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	1	0.17
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	12	0.17
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	12	0.17
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	16	0.17
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	16	0.17
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	6	0.17
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	13	0.17
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	15	0.17
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	12	0.17
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	12	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	7	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	7	0.17
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	7	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	7	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	7	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	11	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	11	0.17
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	11	0.17
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	11	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	11	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	11	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	12	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	12	0.17
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	12	0.17
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	12	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	12	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	12	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	14	0.17
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	14	0.17
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	14	0.17
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	14	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	14	0.17
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	14	0.17
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	17	0.17
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	17	0.17
(1,209)	1:41:B:ILE:HD11	1:42:B:TYR:H	17	0.17
(1,209)	1:41:B:ILE:HD12	1:42:B:TYR:H	17	0.17
(1,209)	1:41:B:ILE:HD13	1:42:B:TYR:H	17	0.17
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	11	0.17
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	11	0.17
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	11	0.17
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	14	0.17
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	14	0.17
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	17	0.17
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	17	0.17
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	5	0.17
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	5	0.17
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	19	0.17
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	19	0.17
(1,178)	1:15:A:THR:HG21	1:14:A:ARG:HE	13	0.17
(1,178)	1:15:A:THR:HG22	1:14:A:ARG:HE	13	0.17
(1,178)	1:15:A:THR:HG23	1:14:A:ARG:HE	13	0.17
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:10:A:TYR:HA	1:9:A:ILE:H	9	0.17
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	17	0.17
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	17	0.17
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	17	0.17
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	3	0.17
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	3	0.17
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	6	0.17
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	10	0.17
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	15	0.17
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	1	0.17
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	1	0.17
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	1	0.17
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	1	0.17
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	4	0.17
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	4	0.17
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	4	0.17
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	4	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	1	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	1	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	2	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	2	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	3	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	3	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	4	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	4	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	7	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	7	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	8	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	8	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	13	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	13	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	14	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	14	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	18	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	18	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	19	0.17
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	19	0.17
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	11	0.17
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	2	0.17
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	2	0.17
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	10	0.17
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	11	0.17
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	11	0.17
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	20	0.17
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	20	0.17
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	3	0.17
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	3	0.17
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	16	0.17
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	16	0.17
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	6	0.17
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	6	0.17
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	7	0.17
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	7	0.17
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	5	0.17
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	16	0.17
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	19	0.17
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	2	0.17
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	2	0.17
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	10	0.17
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	10	0.17
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	13	0.17
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	13	0.17
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	8	0.17
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	8	0.17
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	15	0.17
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	15	0.17
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	12	0.17
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	10	0.17
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	10	0.17
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	11	0.17
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	11	0.17
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	14	0.17
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	14	0.17
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	7	0.17
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	7	0.17
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	7	0.17
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	7	0.17
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	7	0.17
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	7	0.17
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	16	0.17
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	16	0.17
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	16	0.17
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	16	0.17
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	16	0.17
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	18	0.17
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	18	0.17
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	18	0.17
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	18	0.17
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	18	0.17
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	18	0.17
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	14	0.17
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	14	0.17
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	16	0.17
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	16	0.17
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	11	0.17
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	14	0.17
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	16	0.17
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	16	0.17
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	16	0.17
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	9	0.17
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	18	0.17
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	8	0.16
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	12	0.16
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	12	0.16
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	12	0.16
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	9	0.16
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	9	0.16
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	9	0.16
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	18	0.16
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	18	0.16
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	18	0.16
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	17	0.16
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	17	0.16
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	17	0.16
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	17	0.16
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	17	0.16
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	17	0.16
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	8	0.16
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	8	0.16
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	9	0.16
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	9	0.16
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	16	0.16
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	16	0.16
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	20	0.16
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	13	0.16
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	20	0.16
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	3	0.16
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	19	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	4	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	4	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	12	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	12	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	14	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	14	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	15	0.16
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	15	0.16
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	11	0.16
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	12	0.16
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	10	0.16
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	10	0.16
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	1	0.16
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	1	0.16
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	8	0.16
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	8	0.16
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	11	0.16
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	11	0.16
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	13	0.16
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	13	0.16
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	15	0.16
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	15	0.16
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	20	0.16
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	20	0.16
(1,260)	1:40:B:ILE:HG21	1:40:B:ILE:H	16	0.16
(1,260)	1:40:B:ILE:HG22	1:40:B:ILE:H	16	0.16
(1,260)	1:40:B:ILE:HG23	1:40:B:ILE:H	16	0.16
(1,239)	1:35:B:LYS:HB2	1:35:B:LYS:H	8	0.16
(1,239)	1:35:B:LYS:HB3	1:35:B:LYS:H	8	0.16
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	17	0.16
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	17	0.16
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	10	0.16
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	10	0.16
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	11	0.16
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	11	0.16
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	2	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	4	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	4	0.16
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	12	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	12	0.16
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	15	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	15	0.16
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	16	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	16	0.16
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	17	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	17	0.16
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	18	0.16
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	18	0.16
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	7	0.16
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	7	0.16
(1,222)	1:44:B:ASN:HD21	1:45:B:ARG:H	19	0.16
(1,222)	1:44:B:ASN:HD22	1:45:B:ARG:H	19	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	2	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	2	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	3	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	3	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	4	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	4	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	6	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	6	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	10	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	10	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	11	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	11	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	13	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	13	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	15	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	15	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	17	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	17	0.16
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	18	0.16
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	18	0.16
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	7	0.16
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	16	0.16
(1,218)	1:42:B:TYR:H	1:43:B:CYS:H	17	0.16
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	6	0.16
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	6	0.16
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	6	0.16
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	6	0.16
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	6	0.16
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	15	0.16
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	15	0.16
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	15	0.16
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	15	0.16
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	15	0.16
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	15	0.16
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	19	0.16
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	19	0.16
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD1	16	0.16
(1,212)	1:41:B:ILE:HA	1:42:B:TYR:HD2	16	0.16
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	4	0.16
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	4	0.16
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	4	0.16
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	10	0.16
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	10	0.16
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	10	0.16
(1,206)	1:39:B:PRO:HB2	1:40:B:ILE:H	16	0.16
(1,206)	1:39:B:PRO:HB3	1:40:B:ILE:H	16	0.16
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	7	0.16
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	20	0.16
(1,181)	1:6:A:VAL:HG11	1:3:A:LYS:H	8	0.16
(1,181)	1:6:A:VAL:HG12	1:3:A:LYS:H	8	0.16
(1,181)	1:6:A:VAL:HG13	1:3:A:LYS:H	8	0.16
(1,181)	1:6:A:VAL:HG21	1:3:A:LYS:H	8	0.16
(1,181)	1:6:A:VAL:HG22	1:3:A:LYS:H	8	0.16
(1,181)	1:6:A:VAL:HG23	1:3:A:LYS:H	8	0.16
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	9	0.16
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	9	0.16
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	17	0.16
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	17	0.16
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	5	0.16
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	19	0.16
(1,174)	1:10:A:TYR:HA	1:9:A:ILE:H	19	0.16
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	7	0.16
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB2	16	0.16
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB3	16	0.16
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	7	0.16
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	12	0.16
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	18	0.16
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	2	0.16
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	2	0.16
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	18	0.16
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	19	0.16
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	9	0.16
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	9	0.16
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	4	0.16
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	6	0.16
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	6	0.16
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	14	0.16
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	14	0.16
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	19	0.16
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	19	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	1	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	1	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	5	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	5	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	9	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	9	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	12	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	12	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	14	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	14	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	16	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	16	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	17	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	17	0.16
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	19	0.16
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	19	0.16
(1,52)	1:3:A:LYS:HB2	1:3:A:LYS:H	2	0.16
(1,52)	1:3:A:LYS:HB3	1:3:A:LYS:H	2	0.16
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	2	0.16
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	2	0.16
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	5	0.16
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	5	0.16
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	13	0.16
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	13	0.16
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	18	0.16
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	18	0.16
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	12	0.16
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	1	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	1	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	3	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	3	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	4	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	4	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	5	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	5	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	11	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	11	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	12	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	12	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	13	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	13	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	16	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	16	0.16
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	18	0.16
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	18	0.16
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	20	0.16
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	20	0.16
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	9	0.16
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	9	0.16
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	9	0.16
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	9	0.16
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	9	0.16
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	9	0.16
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD1	20	0.16
(1,25)	1:9:A:ILE:HA	1:10:A:TYR:HD2	20	0.16
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	9	0.16
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	18	0.16
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	19	0.16
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	1	0.16
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	1	0.16
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	1	0.16
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	7	0.16
(2,2)	1:35:B:LYS:HA	1:40:B:ILE:HA	6	0.15
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	2	0.15
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	2	0.15
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	2	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	1	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	1	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	12	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	12	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	12	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	14	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	14	0.15
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	14	0.15
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	15	0.15
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	15	0.15
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	15	0.15
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	15	0.15
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	15	0.15
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	15	0.15
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	18	0.15
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	18	0.15
(1,368)	1:38:B:VAL:HG11	1:35:B:LYS:H	7	0.15
(1,368)	1:38:B:VAL:HG12	1:35:B:LYS:H	7	0.15
(1,368)	1:38:B:VAL:HG13	1:35:B:LYS:H	7	0.15
(1,368)	1:38:B:VAL:HG21	1:35:B:LYS:H	7	0.15
(1,368)	1:38:B:VAL:HG22	1:35:B:LYS:H	7	0.15
(1,368)	1:38:B:VAL:HG23	1:35:B:LYS:H	7	0.15
(1,368)	1:38:B:VAL:HG11	1:35:B:LYS:H	15	0.15
(1,368)	1:38:B:VAL:HG12	1:35:B:LYS:H	15	0.15
(1,368)	1:38:B:VAL:HG13	1:35:B:LYS:H	15	0.15
(1,368)	1:38:B:VAL:HG21	1:35:B:LYS:H	15	0.15
(1,368)	1:38:B:VAL:HG22	1:35:B:LYS:H	15	0.15
(1,368)	1:38:B:VAL:HG23	1:35:B:LYS:H	15	0.15
(1,368)	1:38:B:VAL:HG11	1:35:B:LYS:H	20	0.15
(1,368)	1:38:B:VAL:HG12	1:35:B:LYS:H	20	0.15
(1,368)	1:38:B:VAL:HG13	1:35:B:LYS:H	20	0.15
(1,368)	1:38:B:VAL:HG21	1:35:B:LYS:H	20	0.15
(1,368)	1:38:B:VAL:HG22	1:35:B:LYS:H	20	0.15
(1,368)	1:38:B:VAL:HG23	1:35:B:LYS:H	20	0.15
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	7	0.15
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	7	0.15
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	16	0.15
(1,352)	1:43:B:CYS:HA	1:50:B:CYS:HB2	11	0.15
(1,352)	1:43:B:CYS:HA	1:50:B:CYS:HB3	11	0.15
(1,336)	1:40:B:ILE:HG12	1:52:B:ARG:HE	20	0.15
(1,336)	1:40:B:ILE:HG13	1:52:B:ARG:HE	20	0.15
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	7	0.15
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	7	0.15
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	7	0.15
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	13	0.15
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	13	0.15
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	13	0.15
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	13	0.15
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	8	0.15
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	8	0.15
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	16	0.15
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	16	0.15
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	20	0.15
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	20	0.15
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	17	0.15
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	19	0.15
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	19	0.15
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	2	0.15
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	2	0.15
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	1	0.15
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	1	0.15
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	19	0.15
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	19	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	3	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	4	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	5	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	6	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	8	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	9	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	11	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	12	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	13	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	14	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	15	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	16	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	17	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	18	0.15
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	20	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	1	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	2	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	7	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	8	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	9	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	10	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	13	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	15	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	16	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	17	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	19	0.15
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	20	0.15
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	16	0.15
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	16	0.15
(1,265)	1:41:B:ILE:HG21	1:41:B:ILE:H	6	0.15
(1,265)	1:41:B:ILE:HG22	1:41:B:ILE:H	6	0.15
(1,265)	1:41:B:ILE:HG23	1:41:B:ILE:H	6	0.15
(1,265)	1:41:B:ILE:HG21	1:41:B:ILE:H	15	0.15
(1,265)	1:41:B:ILE:HG22	1:41:B:ILE:H	15	0.15
(1,265)	1:41:B:ILE:HG23	1:41:B:ILE:H	15	0.15
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	17	0.15
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	1	0.15
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	1	0.15
(1,233)	1:49:B:LYS:HG2	1:50:B:CYS:H	2	0.15
(1,233)	1:49:B:LYS:HG3	1:50:B:CYS:H	2	0.15
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	1	0.15
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	1	0.15
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	5	0.15
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	5	0.15
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	6	0.15
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	6	0.15
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	8	0.15
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	8	0.15
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	13	0.15
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	13	0.15
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	5	0.15
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	5	0.15
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	7	0.15
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	7	0.15
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	8	0.15
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	8	0.15
(1,217)	1:42:B:TYR:HB2	1:43:B:CYS:H	9	0.15
(1,217)	1:42:B:TYR:HB3	1:43:B:CYS:H	9	0.15
(1,215)	1:41:B:ILE:HA	1:42:B:TYR:HE1	18	0.15
(1,215)	1:41:B:ILE:HA	1:42:B:TYR:HE2	18	0.15
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	20	0.15
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	20	0.15
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	20	0.15
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	20	0.15
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	20	0.15
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	8	0.15
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	8	0.15
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	16	0.15
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	19	0.15
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	20	0.15
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	8	0.15
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	8	0.15
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	8	0.15
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	19	0.15
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	19	0.15
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	19	0.15
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	8	0.15
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	1	0.15
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	1	0.15
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	13	0.15
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	13	0.15
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	15	0.15
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	15	0.15
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	11	0.15
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	11	0.15
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	11	0.15
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	11	0.15
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	11	0.15
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	11	0.15
(1,178)	1:15:A:THR:HG21	1:14:A:ARG:HE	10	0.15
(1,178)	1:15:A:THR:HG22	1:14:A:ARG:HE	10	0.15
(1,178)	1:15:A:THR:HG23	1:14:A:ARG:HE	10	0.15
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	14	0.15
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	20	0.15
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	2	0.15
(1,174)	1:10:A:TYR:HA	1:9:A:ILE:H	18	0.15
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	18	0.15
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	20	0.15
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	12	0.15
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	12	0.15
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	10	0.15
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	5	0.15
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	11	0.15
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE1	5	0.15
(1,147)	1:19:A:GLN:HG2	1:10:A:TYR:HE2	5	0.15
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE1	5	0.15
(1,147)	1:19:A:GLN:HG3	1:10:A:TYR:HE2	5	0.15
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	15	0.15
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	15	0.15
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	20	0.15
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	20	0.15
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	13	0.15
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	1	0.15
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	1	0.15
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	3	0.15
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	3	0.15
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	10	0.15
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	10	0.15
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	17	0.15
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	17	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	2	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	4	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	5	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	7	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	9	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	10	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	11	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	13	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	14	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	16	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	17	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	19	0.15
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	20	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	1	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	3	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	5	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	6	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	7	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	9	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	12	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	14	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	15	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	16	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	17	0.15
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	20	0.15
(1,78)	1:9:A:ILE:HG21	1:9:A:ILE:H	8	0.15
(1,78)	1:9:A:ILE:HG22	1:9:A:ILE:H	8	0.15
(1,78)	1:9:A:ILE:HG23	1:9:A:ILE:H	8	0.15
(1,59)	1:4:A:LYS:HG2	1:4:A:LYS:H	19	0.15
(1,59)	1:4:A:LYS:HG3	1:4:A:LYS:H	19	0.15
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	1	0.15
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	1	0.15
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	6	0.15
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	6	0.15
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	8	0.15
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	8	0.15
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	4	0.15
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	4	0.15
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	9	0.15
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	9	0.15
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	10	0.15
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	10	0.15
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	16	0.15
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	16	0.15
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	20	0.15
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	20	0.15
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	6	0.15
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	6	0.15
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	9	0.15
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	9	0.15
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	10	0.15
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	10	0.15
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	14	0.15
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	14	0.15
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	17	0.15
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	17	0.15
(1,31)	1:10:A:TYR:H	1:11:A:CYS:H	8	0.15
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	7	0.15
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	7	0.15
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	8	0.15
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	8	0.15
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	8	0.15
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	8	0.15
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	8	0.15
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	8	0.15
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	2	0.15
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	2	0.15
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	2	0.15
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	6	0.15
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	6	0.15
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	6	0.15
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	2	0.15
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	14	0.14
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG11	12	0.14
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG12	12	0.14
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG13	12	0.14
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG21	12	0.14
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG22	12	0.14
(1,380)	1:46:B:ARG:H	1:6:A:VAL:HG23	12	0.14
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	4	0.14
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	4	0.14
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	4	0.14
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	4	0.14
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	4	0.14
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	4	0.14
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	6	0.14
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	6	0.14
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	6	0.14
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	6	0.14
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	6	0.14
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	6	0.14
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	8	0.14
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	8	0.14
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	12	0.14
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	12	0.14
(1,367)	1:48:B:GLY:HA2	1:47:B:THR:H	15	0.14
(1,367)	1:48:B:GLY:HA3	1:47:B:THR:H	15	0.14
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	1	0.14
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	2	0.14
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	9	0.14
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	14	0.14
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB2	10	0.14
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB3	10	0.14
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	1	0.14
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	3	0.14
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	11	0.14
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:40:B:ILE:HG12	1:52:B:ARG:HE	7	0.14
(1,336)	1:40:B:ILE:HG13	1:52:B:ARG:HE	7	0.14
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE1	20	0.14
(1,334)	1:51:B:GLN:HG2	1:42:B:TYR:HE2	20	0.14
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE1	20	0.14
(1,334)	1:51:B:GLN:HG3	1:42:B:TYR:HE2	20	0.14
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	4	0.14
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	3	0.14
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	3	0.14
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	5	0.14
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	5	0.14
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	8	0.14
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	8	0.14
(1,301)	1:49:B:LYS:HD2	1:49:B:LYS:H	2	0.14
(1,301)	1:49:B:LYS:HD3	1:49:B:LYS:H	2	0.14
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	3	0.14
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	4	0.14
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	5	0.14
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	6	0.14
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	11	0.14
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	14	0.14
(1,296)	1:47:B:THR:HA	1:47:B:THR:H	18	0.14
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	12	0.14
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	12	0.14
(1,290)	1:46:B:ARG:HB2	1:46:B:ARG:HE	7	0.14
(1,290)	1:46:B:ARG:HB3	1:46:B:ARG:HE	7	0.14
(1,287)	1:46:B:ARG:HA	1:46:B:ARG:HE	3	0.14
(1,287)	1:46:B:ARG:HA	1:46:B:ARG:HE	6	0.14
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	3	0.14
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	3	0.14
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	11	0.14
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	11	0.14
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	13	0.14
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	13	0.14
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	14	0.14
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	14	0.14
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	3	0.14
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	3	0.14
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	11	0.14
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	11	0.14
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	20	0.14
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	2	0.14
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	3	0.14
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	20	0.14
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	20	0.14
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	13	0.14
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	13	0.14
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	7	0.14
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	17	0.14
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	9	0.14
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	9	0.14
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	9	0.14
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	14	0.14
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	14	0.14
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	14	0.14
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	6	0.14
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	6	0.14
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	11	0.14
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	11	0.14
(1,181)	1:6:A:VAL:HG11	1:3:A:LYS:H	9	0.14
(1,181)	1:6:A:VAL:HG12	1:3:A:LYS:H	9	0.14
(1,181)	1:6:A:VAL:HG13	1:3:A:LYS:H	9	0.14
(1,181)	1:6:A:VAL:HG21	1:3:A:LYS:H	9	0.14
(1,181)	1:6:A:VAL:HG22	1:3:A:LYS:H	9	0.14
(1,181)	1:6:A:VAL:HG23	1:3:A:LYS:H	9	0.14
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	15	0.14
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	15	0.14
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	1	0.14
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	6	0.14
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	9	0.14
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	12	0.14
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	12	0.14
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	12	0.14
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	12	0.14
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB2	20	0.14
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB3	20	0.14
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	9	0.14
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	1	0.14
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	15	0.14
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	5	0.14
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	5	0.14
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	2	0.14
(1,135)	1:21:A:MET:HG2	1:8:A:ILE:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:21:A:MET:HG3	1:8:A:ILE:H	20	0.14
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	1	0.14
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	1	0.14
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	2	0.14
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	4	0.14
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	8	0.14
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	10	0.14
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	11	0.14
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	13	0.14
(1,109)	1:15:A:THR:HA	1:15:A:THR:H	18	0.14
(1,103)	1:14:A:ARG:HB2	1:14:A:ARG:HE	9	0.14
(1,103)	1:14:A:ARG:HB3	1:14:A:ARG:HE	9	0.14
(1,100)	1:14:A:ARG:HA	1:14:A:ARG:HE	11	0.14
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	14	0.14
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	14	0.14
(1,64)	1:6:A:VAL:HB	1:6:A:VAL:H	19	0.14
(1,52)	1:3:A:LYS:HB2	1:3:A:LYS:H	7	0.14
(1,52)	1:3:A:LYS:HB3	1:3:A:LYS:H	7	0.14
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	8	0.14
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	8	0.14
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	10	0.14
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	10	0.14
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	11	0.14
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	11	0.14
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	19	0.14
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	19	0.14
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	4	0.14
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	4	0.14
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	8	0.14
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	8	0.14
(1,46)	1:17:A:LYS:HG2	1:18:A:CYS:H	15	0.14
(1,46)	1:17:A:LYS:HG3	1:18:A:CYS:H	15	0.14
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	1	0.14
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	1	0.14
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	8	0.14
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	8	0.14
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	11	0.14
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	11	0.14
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	14	0.14
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	14	0.14
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	17	0.14
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,45)	1:17:A:LYS:HD2	1:18:A:CYS:H	19	0.14
(1,45)	1:17:A:LYS:HD3	1:18:A:CYS:H	19	0.14
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	6	0.14
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	11	0.14
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	19	0.14
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	19	0.14
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	15	0.14
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	15	0.14
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	19	0.14
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	19	0.14
(1,28)	1:9:A:ILE:HA	1:10:A:TYR:HE1	5	0.14
(1,28)	1:9:A:ILE:HA	1:10:A:TYR:HE2	5	0.14
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD1	19	0.14
(1,27)	1:9:A:ILE:HG21	1:10:A:TYR:HD2	19	0.14
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD1	19	0.14
(1,27)	1:9:A:ILE:HG22	1:10:A:TYR:HD2	19	0.14
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD1	19	0.14
(1,27)	1:9:A:ILE:HG23	1:10:A:TYR:HD2	19	0.14
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	9	0.14
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	9	0.14
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	11	0.14
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	11	0.14
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	12	0.14
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	20	0.14
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	15	0.14
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	15	0.14
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	15	0.14
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	17	0.14
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	17	0.14
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	17	0.14
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	17	0.14
(2,1)	1:3:A:LYS:HA	1:8:A:ILE:HA	8	0.13
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD11	3	0.13
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD12	3	0.13
(1,377)	1:14:A:ARG:H	1:40:B:ILE:HD13	3	0.13
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	16	0.13
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	16	0.13
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	16	0.13
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	16	0.13
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	16	0.13
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	16	0.13
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	13	0.13
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	13	0.13
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	13	0.13
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	13	0.13
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	13	0.13
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	4	0.13
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	4	0.13
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	10	0.13
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	10	0.13
(1,368)	1:38:B:VAL:HG11	1:35:B:LYS:H	13	0.13
(1,368)	1:38:B:VAL:HG12	1:35:B:LYS:H	13	0.13
(1,368)	1:38:B:VAL:HG13	1:35:B:LYS:H	13	0.13
(1,368)	1:38:B:VAL:HG21	1:35:B:LYS:H	13	0.13
(1,368)	1:38:B:VAL:HG22	1:35:B:LYS:H	13	0.13
(1,368)	1:38:B:VAL:HG23	1:35:B:LYS:H	13	0.13
(1,360)	1:41:B:ILE:HG21	1:40:B:ILE:H	16	0.13
(1,360)	1:41:B:ILE:HG22	1:40:B:ILE:H	16	0.13
(1,360)	1:41:B:ILE:HG23	1:40:B:ILE:H	16	0.13
(1,360)	1:41:B:ILE:HG21	1:40:B:ILE:H	18	0.13
(1,360)	1:41:B:ILE:HG22	1:40:B:ILE:H	18	0.13
(1,360)	1:41:B:ILE:HG23	1:40:B:ILE:H	18	0.13
(1,355)	1:44:B:ASN:H	1:49:B:LYS:H	14	0.13
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	4	0.13
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	9	0.13
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	12	0.13
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	4	0.13
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	7	0.13
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	7	0.13
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	7	0.13
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE1	19	0.13
(1,332)	1:51:B:GLN:HA	1:42:B:TYR:HE2	19	0.13
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	18	0.13
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	20	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	2	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	3	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	8	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	10	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	11	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	12	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	14	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	16	0.13
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	20	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	1	0.13
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	2	0.13
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	7	0.13
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	10	0.13
(1,299)	1:49:B:LYS:HA	1:49:B:LYS:H	19	0.13
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	3	0.13
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	3	0.13
(1,287)	1:46:B:ARG:HA	1:46:B:ARG:HE	11	0.13
(1,270)	1:42:B:TYR:HA	1:42:B:TYR:HD1	16	0.13
(1,270)	1:42:B:TYR:HA	1:42:B:TYR:HD2	16	0.13
(1,270)	1:42:B:TYR:HA	1:42:B:TYR:HD1	19	0.13
(1,270)	1:42:B:TYR:HA	1:42:B:TYR:HD2	19	0.13
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	16	0.13
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	16	0.13
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	6	0.13
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	6	0.13
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	9	0.13
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	9	0.13
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	10	0.13
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	10	0.13
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	14	0.13
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	14	0.13
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	6	0.13
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	6	0.13
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	7	0.13
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	7	0.13
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	6	0.13
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	20	0.13
(1,221)	1:44:B:ASN:HB2	1:45:B:ARG:H	14	0.13
(1,221)	1:44:B:ASN:HB3	1:45:B:ARG:H	14	0.13
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD1	16	0.13
(1,214)	1:41:B:ILE:HG21	1:42:B:TYR:HD2	16	0.13
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD1	16	0.13
(1,214)	1:41:B:ILE:HG22	1:42:B:TYR:HD2	16	0.13
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD1	16	0.13
(1,214)	1:41:B:ILE:HG23	1:42:B:TYR:HD2	16	0.13
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	4	0.13
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	8	0.13
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD2	15	0.13
(1,205)	1:38:B:VAL:HG11	1:39:B:PRO:HD3	15	0.13
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD2	15	0.13
(1,205)	1:38:B:VAL:HG12	1:39:B:PRO:HD3	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD2	15	0.13
(1,205)	1:38:B:VAL:HG13	1:39:B:PRO:HD3	15	0.13
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD2	15	0.13
(1,205)	1:38:B:VAL:HG21	1:39:B:PRO:HD3	15	0.13
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD2	15	0.13
(1,205)	1:38:B:VAL:HG22	1:39:B:PRO:HD3	15	0.13
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD2	15	0.13
(1,205)	1:38:B:VAL:HG23	1:39:B:PRO:HD3	15	0.13
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	1	0.13
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	1	0.13
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	1	0.13
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	1	0.13
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	2	0.13
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	2	0.13
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	2	0.13
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	2	0.13
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	19	0.13
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	19	0.13
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	19	0.13
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	19	0.13
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	12	0.13
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	20	0.13
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	2	0.13
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	2	0.13
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	7	0.13
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	7	0.13
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	16	0.13
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	16	0.13
(1,181)	1:6:A:VAL:HG11	1:3:A:LYS:H	18	0.13
(1,181)	1:6:A:VAL:HG12	1:3:A:LYS:H	18	0.13
(1,181)	1:6:A:VAL:HG13	1:3:A:LYS:H	18	0.13
(1,181)	1:6:A:VAL:HG21	1:3:A:LYS:H	18	0.13
(1,181)	1:6:A:VAL:HG22	1:3:A:LYS:H	18	0.13
(1,181)	1:6:A:VAL:HG23	1:3:A:LYS:H	18	0.13
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	20	0.13
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	20	0.13
(1,178)	1:15:A:THR:HG21	1:14:A:ARG:HE	2	0.13
(1,178)	1:15:A:THR:HG22	1:14:A:ARG:HE	2	0.13
(1,178)	1:15:A:THR:HG23	1:14:A:ARG:HE	2	0.13
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	19	0.13
(1,174)	1:10:A:TYR:HA	1:9:A:ILE:H	5	0.13
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	6	0.13
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	6	0.13
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	14	0.13
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	14	0.13
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	14	0.13
(1,166)	1:11:A:CYS:HA	1:17:A:LYS:H	12	0.13
(1,155)	1:8:A:ILE:HG12	1:21:A:MET:H	5	0.13
(1,155)	1:8:A:ILE:HG13	1:21:A:MET:H	5	0.13
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	12	0.13
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	6	0.13
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE1	12	0.13
(1,145)	1:19:A:GLN:HA	1:10:A:TYR:HE2	12	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	3	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	4	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	5	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	12	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	13	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	15	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	16	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	17	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	19	0.13
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	20	0.13
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	6	0.13
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	6	0.13
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	8	0.13
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	8	0.13
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	18	0.13
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	18	0.13
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	6	0.13
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	8	0.13
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	15	0.13
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	18	0.13
(1,94)	1:13:A:ARG:HA	1:13:A:ARG:HE	7	0.13
(1,94)	1:13:A:ARG:HA	1:13:A:ARG:HE	10	0.13
(1,83)	1:10:A:TYR:HA	1:10:A:TYR:HD1	12	0.13
(1,83)	1:10:A:TYR:HA	1:10:A:TYR:HD2	12	0.13
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	16	0.13
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	16	0.13
(1,59)	1:4:A:LYS:HG2	1:4:A:LYS:H	8	0.13
(1,59)	1:4:A:LYS:HG3	1:4:A:LYS:H	8	0.13
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	3	0.13
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	7	0.13
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	7	0.13
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	16	0.13
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	16	0.13
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	17	0.13
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	17	0.13
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	7	0.13
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	7	0.13
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	4	0.13
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	14	0.13
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	14	0.13
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	14	0.13
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	15	0.13
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	15	0.13
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	4	0.13
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	4	0.13
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	2	0.13
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	16	0.13
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	1	0.13
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	1	0.13
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	1	0.13
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	1	0.13
(1,16)	1:2:A:SER:HB2	1:3:A:LYS:H	11	0.13
(1,16)	1:2:A:SER:HB3	1:3:A:LYS:H	11	0.13
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	16	0.13
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	17	0.13
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	14	0.12
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	14	0.12
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	14	0.12
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	1	0.12
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	1	0.12
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	1	0.12
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	1	0.12
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	1	0.12
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	1	0.12
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	2	0.12
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	2	0.12
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	2	0.12
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	2	0.12
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	2	0.12
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	2	0.12
(1,375)	1:6:A:VAL:HG11	1:43:B:CYS:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:6:A:VAL:HG12	1:43:B:CYS:H	8	0.12
(1,375)	1:6:A:VAL:HG13	1:43:B:CYS:H	8	0.12
(1,375)	1:6:A:VAL:HG21	1:43:B:CYS:H	8	0.12
(1,375)	1:6:A:VAL:HG22	1:43:B:CYS:H	8	0.12
(1,375)	1:6:A:VAL:HG23	1:43:B:CYS:H	8	0.12
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	2	0.12
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	2	0.12
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	11	0.12
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	11	0.12
(1,364)	1:47:B:THR:H	1:46:B:ARG:H	11	0.12
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	5	0.12
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	8	0.12
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	14	0.12
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	20	0.12
(1,360)	1:41:B:ILE:HG21	1:40:B:ILE:H	5	0.12
(1,360)	1:41:B:ILE:HG22	1:40:B:ILE:H	5	0.12
(1,360)	1:41:B:ILE:HG23	1:40:B:ILE:H	5	0.12
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	19	0.12
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB2	7	0.12
(1,351)	1:50:B:CYS:HA	1:43:B:CYS:HB3	7	0.12
(1,347)	1:43:B:CYS:HA	1:51:B:GLN:H	11	0.12
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	2	0.12
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	5	0.12
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	20	0.12
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	7	0.12
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	7	0.12
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	7	0.12
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	7	0.12
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	5	0.12
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	13	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	1	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	4	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	5	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	6	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	7	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	9	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	13	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	15	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	17	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	18	0.12
(1,306)	1:51:B:GLN:HA	1:51:B:GLN:H	19	0.12
(1,294)	1:46:B:ARG:HB2	1:46:B:ARG:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:46:B:ARG:HB3	1:46:B:ARG:H	6	0.12
(1,281)	1:45:B:ARG:HA	1:45:B:ARG:HE	17	0.12
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	8	0.12
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	8	0.12
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	17	0.12
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	17	0.12
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	19	0.12
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	19	0.12
(1,251)	1:38:B:VAL:HB	1:38:B:VAL:H	16	0.12
(1,245)	1:36:B:LYS:HD2	1:36:B:LYS:H	6	0.12
(1,245)	1:36:B:LYS:HD3	1:36:B:LYS:H	6	0.12
(1,241)	1:35:B:LYS:HE2	1:35:B:LYS:H	18	0.12
(1,241)	1:35:B:LYS:HE3	1:35:B:LYS:H	18	0.12
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	1	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	1	0.12
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	2	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	2	0.12
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	5	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	5	0.12
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	12	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	12	0.12
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	15	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	15	0.12
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	18	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	18	0.12
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	20	0.12
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	20	0.12
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	3	0.12
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	3	0.12
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	15	0.12
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	15	0.12
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	7	0.12
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	8	0.12
(1,223)	1:45:B:ARG:HA	1:46:B:ARG:HE	10	0.12
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE1	13	0.12
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE2	13	0.12
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE1	13	0.12
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE2	13	0.12
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE1	13	0.12
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE2	13	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	1	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	3	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	5	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	9	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	10	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	11	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	12	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	13	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	14	0.12
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	18	0.12
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	3	0.12
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	3	0.12
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	3	0.12
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	3	0.12
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	9	0.12
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	9	0.12
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	9	0.12
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	9	0.12
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	8	0.12
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	13	0.12
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	15	0.12
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	4	0.12
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	4	0.12
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	4	0.12
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	19	0.12
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	19	0.12
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	2	0.12
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	2	0.12
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	2	0.12
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	2	0.12
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	2	0.12
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	2	0.12
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	17	0.12
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	17	0.12
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	17	0.12
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	17	0.12
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	17	0.12
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	17	0.12
(1,180)	1:16:A:GLY:HA2	1:15:A:THR:H	16	0.12
(1,180)	1:16:A:GLY:HA3	1:15:A:THR:H	16	0.12
(1,178)	1:15:A:THR:HG21	1:14:A:ARG:HE	18	0.12
(1,178)	1:15:A:THR:HG22	1:14:A:ARG:HE	18	0.12
(1,178)	1:15:A:THR:HG23	1:14:A:ARG:HE	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	10	0.12
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	14	0.12
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	16	0.12
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	17	0.12
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	1	0.12
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	1	0.12
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	1	0.12
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	11	0.12
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	11	0.12
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	11	0.12
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	20	0.12
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	20	0.12
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	20	0.12
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	11	0.12
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	9	0.12
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	13	0.12
(1,141)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	6	0.12
(1,141)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	6	0.12
(1,141)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	6	0.12
(1,141)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	6	0.12
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	17	0.12
(1,138)	1:18:A:CYS:HA	1:10:A:TYR:H	20	0.12
(1,137)	1:20:A:ARG:HD2	1:9:A:ILE:H	20	0.12
(1,137)	1:20:A:ARG:HD3	1:9:A:ILE:H	20	0.12
(1,126)	1:20:A:ARG:HA	1:20:A:ARG:HE	12	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	1	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	2	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	6	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	7	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	8	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	9	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	10	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	11	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	14	0.12
(1,119)	1:19:A:GLN:HA	1:19:A:GLN:H	18	0.12
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	3	0.12
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	3	0.12
(1,114)	1:17:A:LYS:HD2	1:17:A:LYS:H	12	0.12
(1,114)	1:17:A:LYS:HD3	1:17:A:LYS:H	12	0.12
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	1	0.12
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	3	0.12
(1,112)	1:17:A:LYS:HA	1:17:A:LYS:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,100)	1:14:A:ARG:HA	1:14:A:ARG:HE	4	0.12
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	9	0.12
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	9	0.12
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	11	0.12
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	11	0.12
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	1	0.12
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	1	0.12
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	2	0.12
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	2	0.12
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	4	0.12
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	4	0.12
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	5	0.12
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	5	0.12
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	6	0.12
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	6	0.12
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	10	0.12
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	10	0.12
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	8	0.12
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	15	0.12
(1,34)	1:12:A:ASN:HB2	1:13:A:ARG:H	2	0.12
(1,34)	1:12:A:ASN:HB3	1:13:A:ARG:H	2	0.12
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	16	0.12
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	16	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	12	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	12	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	16	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	16	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	18	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	18	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	20	0.12
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	20	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	1	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	3	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	4	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	6	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	7	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	10	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	13	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	15	0.12
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	17	0.12
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD2	8	0.12
(1,18)	1:6:A:VAL:HG11	1:7:A:PRO:HD3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD2	8	0.12
(1,18)	1:6:A:VAL:HG12	1:7:A:PRO:HD3	8	0.12
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD2	8	0.12
(1,18)	1:6:A:VAL:HG13	1:7:A:PRO:HD3	8	0.12
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD2	8	0.12
(1,18)	1:6:A:VAL:HG21	1:7:A:PRO:HD3	8	0.12
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD2	8	0.12
(1,18)	1:6:A:VAL:HG22	1:7:A:PRO:HD3	8	0.12
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD2	8	0.12
(1,18)	1:6:A:VAL:HG23	1:7:A:PRO:HD3	8	0.12
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	7	0.12
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	7	0.12
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	7	0.12
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	7	0.12
(1,16)	1:2:A:SER:HB2	1:3:A:LYS:H	10	0.12
(1,16)	1:2:A:SER:HB3	1:3:A:LYS:H	10	0.12
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	5	0.12
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	9	0.12
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	14	0.12
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	15	0.12
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	19	0.12
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	20	0.12
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	17	0.12
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD11	5	0.11
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD12	5	0.11
(1,378)	1:46:B:ARG:H	1:8:A:ILE:HD13	5	0.11
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	11	0.11
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	11	0.11
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	11	0.11
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	11	0.11
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	11	0.11
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	11	0.11
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	13	0.11
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	13	0.11
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	13	0.11
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	13	0.11
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	13	0.11
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	13	0.11
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	4	0.11
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	4	0.11
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	4	0.11
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	4	0.11
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	4	0.11
(1,374)	1:38:B:VAL:HG11	1:41:B:ILE:H	14	0.11
(1,374)	1:38:B:VAL:HG12	1:41:B:ILE:H	14	0.11
(1,374)	1:38:B:VAL:HG13	1:41:B:ILE:H	14	0.11
(1,374)	1:38:B:VAL:HG21	1:41:B:ILE:H	14	0.11
(1,374)	1:38:B:VAL:HG22	1:41:B:ILE:H	14	0.11
(1,374)	1:38:B:VAL:HG23	1:41:B:ILE:H	14	0.11
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	3	0.11
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	3	0.11
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	1	0.11
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	1	0.11
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	1	0.11
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	1	0.11
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	1	0.11
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	1	0.11
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	5	0.11
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	5	0.11
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	5	0.11
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	5	0.11
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	5	0.11
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	5	0.11
(1,371)	1:38:B:VAL:HG11	1:53:B:MET:H	17	0.11
(1,371)	1:38:B:VAL:HG12	1:53:B:MET:H	17	0.11
(1,371)	1:38:B:VAL:HG13	1:53:B:MET:H	17	0.11
(1,371)	1:38:B:VAL:HG21	1:53:B:MET:H	17	0.11
(1,371)	1:38:B:VAL:HG22	1:53:B:MET:H	17	0.11
(1,371)	1:38:B:VAL:HG23	1:53:B:MET:H	17	0.11
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	4	0.11
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	6	0.11
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	11	0.11
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	15	0.11
(1,361)	1:42:B:TYR:HA	1:41:B:ILE:H	16	0.11
(1,360)	1:41:B:ILE:HG21	1:40:B:ILE:H	1	0.11
(1,360)	1:41:B:ILE:HG22	1:40:B:ILE:H	1	0.11
(1,360)	1:41:B:ILE:HG23	1:40:B:ILE:H	1	0.11
(1,360)	1:41:B:ILE:HG21	1:40:B:ILE:H	20	0.11
(1,360)	1:41:B:ILE:HG22	1:40:B:ILE:H	20	0.11
(1,360)	1:41:B:ILE:HG23	1:40:B:ILE:H	20	0.11
(1,354)	1:50:B:CYS:HA	1:44:B:ASN:H	14	0.11
(1,353)	1:43:B:CYS:HA	1:49:B:LYS:H	10	0.11
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD1	17	0.11
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD2	17	0.11
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD1	17	0.11
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD2	17	0.11
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	1	0.11
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	1	0.11
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	1	0.11
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	1	0.11
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	18	0.11
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	18	0.11
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	18	0.11
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	18	0.11
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	20	0.11
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	20	0.11
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	20	0.11
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	20	0.11
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	15	0.11
(1,322)	1:53:B:MET:HG2	1:40:B:ILE:H	11	0.11
(1,322)	1:53:B:MET:HG3	1:40:B:ILE:H	11	0.11
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	1	0.11
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	1	0.11
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	11	0.11
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	11	0.11
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	13	0.11
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	13	0.11
(1,235)	1:51:B:GLN:HG2	1:52:B:ARG:H	4	0.11
(1,235)	1:51:B:GLN:HG3	1:52:B:ARG:H	4	0.11
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	2	0.11
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	2	0.11
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	8	0.11
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	8	0.11
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	9	0.11
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	9	0.11
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	12	0.11
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	12	0.11
(1,234)	1:51:B:GLN:HE21	1:52:B:ARG:H	17	0.11
(1,234)	1:51:B:GLN:HE22	1:52:B:ARG:H	17	0.11
(1,232)	1:49:B:LYS:HD2	1:50:B:CYS:H	7	0.11
(1,232)	1:49:B:LYS:HD3	1:50:B:CYS:H	7	0.11
(1,228)	1:47:B:THR:HG21	1:48:B:GLY:H	14	0.11
(1,228)	1:47:B:THR:HG22	1:48:B:GLY:H	14	0.11
(1,228)	1:47:B:THR:HG23	1:48:B:GLY:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE1	11	0.11
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE2	11	0.11
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE1	11	0.11
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE2	11	0.11
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE1	11	0.11
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE2	11	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	4	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	4	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	6	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	6	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	7	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	7	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	15	0.11
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	15	0.11
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	6	0.11
(1,208)	1:41:B:ILE:H	1:42:B:TYR:H	15	0.11
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	8	0.11
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	8	0.11
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	8	0.11
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	8	0.11
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	17	0.11
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	17	0.11
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	17	0.11
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	17	0.11
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	1	0.11
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	2	0.11
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	9	0.11
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	16	0.11
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	17	0.11
(1,186)	1:20:A:ARG:HD2	1:6:A:VAL:H	3	0.11
(1,186)	1:20:A:ARG:HD3	1:6:A:VAL:H	3	0.11
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	6	0.11
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	6	0.11
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	6	0.11
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	6	0.11
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	6	0.11
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	6	0.11
(1,177)	1:15:A:THR:H	1:14:A:ARG:H	4	0.11
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	5	0.11
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	9	0.11
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	13	0.11
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	2	0.11
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	2	0.11
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB2	15	0.11
(1,165)	1:11:A:CYS:HA	1:18:A:CYS:HB3	15	0.11
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	6	0.11
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	6	0.11
(1,162)	1:10:A:TYR:HB2	1:19:A:GLN:HE21	18	0.11
(1,162)	1:10:A:TYR:HB2	1:19:A:GLN:HE22	18	0.11
(1,162)	1:10:A:TYR:HB3	1:19:A:GLN:HE21	18	0.11
(1,162)	1:10:A:TYR:HB3	1:19:A:GLN:HE22	18	0.11
(1,156)	1:10:A:TYR:HA	1:19:A:GLN:H	8	0.11
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	1	0.11
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	4	0.11
(1,152)	1:8:A:ILE:HA	1:21:A:MET:H	20	0.11
(1,126)	1:20:A:ARG:HA	1:20:A:ARG:HE	14	0.11
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	1	0.11
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	1	0.11
(1,107)	1:14:A:ARG:HB2	1:14:A:ARG:H	11	0.11
(1,107)	1:14:A:ARG:HB3	1:14:A:ARG:H	11	0.11
(1,100)	1:14:A:ARG:HA	1:14:A:ARG:HE	9	0.11
(1,94)	1:13:A:ARG:HA	1:13:A:ARG:HE	3	0.11
(1,83)	1:10:A:TYR:HA	1:10:A:TYR:HD1	14	0.11
(1,83)	1:10:A:TYR:HA	1:10:A:TYR:HD2	14	0.11
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	4	0.11
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	4	0.11
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	12	0.11
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	12	0.11
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	15	0.11
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	15	0.11
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	17	0.11
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	17	0.11
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	18	0.11
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	18	0.11
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	19	0.11
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	19	0.11
(1,58)	1:4:A:LYS:HD2	1:4:A:LYS:H	2	0.11
(1,58)	1:4:A:LYS:HD3	1:4:A:LYS:H	2	0.11
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	9	0.11
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	9	0.11
(1,48)	1:19:A:GLN:HG2	1:20:A:ARG:H	13	0.11
(1,48)	1:19:A:GLN:HG3	1:20:A:ARG:H	13	0.11
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	1	0.11
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	13	0.11
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	13	0.11
(1,36)	1:13:A:ARG:HA	1:14:A:ARG:HE	17	0.11
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	15	0.11
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	15	0.11
(1,35)	1:12:A:ASN:HD21	1:13:A:ARG:H	18	0.11
(1,35)	1:12:A:ASN:HD22	1:13:A:ARG:H	18	0.11
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	11	0.11
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	11	0.11
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE1	14	0.11
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE2	14	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE1	14	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE2	14	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE1	14	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE2	14	0.11
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE1	16	0.11
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE2	16	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE1	16	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE2	16	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE1	16	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE2	16	0.11
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE1	17	0.11
(1,29)	1:9:A:ILE:HG21	1:10:A:TYR:HE2	17	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE1	17	0.11
(1,29)	1:9:A:ILE:HG22	1:10:A:TYR:HE2	17	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE1	17	0.11
(1,29)	1:9:A:ILE:HG23	1:10:A:TYR:HE2	17	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	8	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	8	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	13	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	13	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	15	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	15	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	17	0.11
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	17	0.11
(1,21)	1:9:A:ILE:H	1:10:A:TYR:H	8	0.11
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	13	0.11
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	13	0.11
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	13	0.11
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	17	0.11
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	17	0.11
(1,16)	1:2:A:SER:HB2	1:3:A:LYS:H	5	0.11
(1,16)	1:2:A:SER:HB3	1:3:A:LYS:H	5	0.11
(1,16)	1:2:A:SER:HB2	1:3:A:LYS:H	13	0.11
(1,16)	1:2:A:SER:HB3	1:3:A:LYS:H	13	0.11
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	1	0.11
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	6	0.11
(1,8)	1:13:A:ARG:HA	1:14:A:ARG:H	12	0.11
(1,2)	1:3:A:LYS:HA	1:4:A:LYS:H	6	0.11
(1,376)	1:38:B:VAL:HG11	1:11:A:CYS:H	10	0.1
(1,376)	1:38:B:VAL:HG12	1:11:A:CYS:H	10	0.1
(1,376)	1:38:B:VAL:HG13	1:11:A:CYS:H	10	0.1
(1,376)	1:38:B:VAL:HG21	1:11:A:CYS:H	10	0.1
(1,376)	1:38:B:VAL:HG22	1:11:A:CYS:H	10	0.1
(1,376)	1:38:B:VAL:HG23	1:11:A:CYS:H	10	0.1
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	14	0.1
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	14	0.1
(1,373)	1:52:B:ARG:HD2	1:38:B:VAL:H	17	0.1
(1,373)	1:52:B:ARG:HD3	1:38:B:VAL:H	17	0.1
(1,365)	1:47:B:THR:HG21	1:46:B:ARG:HE	10	0.1
(1,365)	1:47:B:THR:HG22	1:46:B:ARG:HE	10	0.1
(1,365)	1:47:B:THR:HG23	1:46:B:ARG:HE	10	0.1
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	2	0.1
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	3	0.1
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	12	0.1
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	13	0.1
(1,362)	1:45:B:ARG:H	1:44:B:ASN:H	17	0.1
(1,361)	1:42:B:TYR:HA	1:41:B:ILE:H	20	0.1
(1,340)	1:40:B:ILE:H	1:53:B:MET:H	13	0.1
(1,339)	1:40:B:ILE:HA	1:53:B:MET:H	3	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD1	6	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD2	6	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD1	6	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD2	6	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD1	9	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD2	9	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD1	9	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD2	9	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD1	13	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD2	13	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD1	13	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD2	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD1	15	0.1
(1,329)	1:51:B:GLN:HG2	1:42:B:TYR:HD2	15	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD1	15	0.1
(1,329)	1:51:B:GLN:HG3	1:42:B:TYR:HD2	15	0.1
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	13	0.1
(1,328)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	13	0.1
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	13	0.1
(1,328)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	13	0.1
(1,325)	1:50:B:CYS:HA	1:42:B:TYR:H	6	0.1
(1,324)	1:52:B:ARG:HD2	1:41:B:ILE:H	7	0.1
(1,324)	1:52:B:ARG:HD3	1:41:B:ILE:H	7	0.1
(1,304)	1:50:B:CYS:HB2	1:50:B:CYS:H	7	0.1
(1,304)	1:50:B:CYS:HB3	1:50:B:CYS:H	7	0.1
(1,269)	1:42:B:TYR:HE1	1:42:B:TYR:H	9	0.1
(1,269)	1:42:B:TYR:HE2	1:42:B:TYR:H	9	0.1
(1,219)	1:42:B:TYR:HD1	1:43:B:CYS:H	8	0.1
(1,219)	1:42:B:TYR:HD2	1:43:B:CYS:H	8	0.1
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE1	3	0.1
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE2	3	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE1	3	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE2	3	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE1	3	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE2	3	0.1
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE1	8	0.1
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE2	8	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE1	8	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE2	8	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE1	8	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE2	8	0.1
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE1	18	0.1
(1,216)	1:41:B:ILE:HG21	1:42:B:TYR:HE2	18	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE1	18	0.1
(1,216)	1:41:B:ILE:HG22	1:42:B:TYR:HE2	18	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE1	18	0.1
(1,216)	1:41:B:ILE:HG23	1:42:B:TYR:HE2	18	0.1
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD1	18	0.1
(1,213)	1:41:B:ILE:HB	1:42:B:TYR:HD2	18	0.1
(1,207)	1:40:B:ILE:HG21	1:41:B:ILE:H	5	0.1
(1,207)	1:40:B:ILE:HG22	1:41:B:ILE:H	5	0.1
(1,207)	1:40:B:ILE:HG23	1:41:B:ILE:H	5	0.1
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	5	0.1
(1,204)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	5	0.1
(1,204)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	5	0.1
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	7	0.1
(1,195)	1:45:B:ARG:HA	1:46:B:ARG:H	11	0.1
(1,189)	1:35:B:LYS:HA	1:36:B:LYS:H	1	0.1
(1,185)	1:6:A:VAL:HG11	1:20:A:ARG:HE	5	0.1
(1,185)	1:6:A:VAL:HG12	1:20:A:ARG:HE	5	0.1
(1,185)	1:6:A:VAL:HG13	1:20:A:ARG:HE	5	0.1
(1,185)	1:6:A:VAL:HG21	1:20:A:ARG:HE	5	0.1
(1,185)	1:6:A:VAL:HG22	1:20:A:ARG:HE	5	0.1
(1,185)	1:6:A:VAL:HG23	1:20:A:ARG:HE	5	0.1
(1,184)	1:6:A:VAL:HG11	1:21:A:MET:H	15	0.1
(1,184)	1:6:A:VAL:HG12	1:21:A:MET:H	15	0.1
(1,184)	1:6:A:VAL:HG13	1:21:A:MET:H	15	0.1
(1,184)	1:6:A:VAL:HG21	1:21:A:MET:H	15	0.1
(1,184)	1:6:A:VAL:HG22	1:21:A:MET:H	15	0.1
(1,184)	1:6:A:VAL:HG23	1:21:A:MET:H	15	0.1
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	4	0.1
(1,175)	1:13:A:ARG:H	1:12:A:ASN:H	6	0.1
(1,173)	1:9:A:ILE:HG21	1:8:A:ILE:H	15	0.1
(1,173)	1:9:A:ILE:HG22	1:8:A:ILE:H	15	0.1
(1,173)	1:9:A:ILE:HG23	1:8:A:ILE:H	15	0.1
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB2	18	0.1
(1,164)	1:18:A:CYS:HA	1:11:A:CYS:HB3	18	0.1
(1,160)	1:11:A:CYS:HA	1:19:A:GLN:H	14	0.1
(1,153)	1:8:A:ILE:H	1:21:A:MET:H	4	0.1
(1,142)	1:19:A:GLN:HG2	1:10:A:TYR:HD1	8	0.1
(1,142)	1:19:A:GLN:HG2	1:10:A:TYR:HD2	8	0.1
(1,142)	1:19:A:GLN:HG3	1:10:A:TYR:HD1	8	0.1
(1,142)	1:19:A:GLN:HG3	1:10:A:TYR:HD2	8	0.1
(1,117)	1:18:A:CYS:HB2	1:18:A:CYS:H	8	0.1
(1,117)	1:18:A:CYS:HB3	1:18:A:CYS:H	8	0.1
(1,100)	1:14:A:ARG:HA	1:14:A:ARG:HE	8	0.1
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	7	0.1
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	7	0.1
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	10	0.1
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	10	0.1
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	13	0.1
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	13	0.1
(1,82)	1:10:A:TYR:HE1	1:10:A:TYR:H	20	0.1
(1,82)	1:10:A:TYR:HE2	1:10:A:TYR:H	20	0.1
(1,54)	1:3:A:LYS:HE2	1:3:A:LYS:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:3:A:LYS:HE3	1:3:A:LYS:H	10	0.1
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	5	0.1
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	5	0.1
(1,47)	1:19:A:GLN:HE21	1:20:A:ARG:H	18	0.1
(1,47)	1:19:A:GLN:HE22	1:20:A:ARG:H	18	0.1
(1,32)	1:10:A:TYR:HD1	1:11:A:CYS:H	7	0.1
(1,32)	1:10:A:TYR:HD2	1:11:A:CYS:H	7	0.1
(1,30)	1:10:A:TYR:HB2	1:11:A:CYS:H	16	0.1
(1,30)	1:10:A:TYR:HB3	1:11:A:CYS:H	16	0.1
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	1	0.1
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	1	0.1
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD1	7	0.1
(1,26)	1:9:A:ILE:HB	1:10:A:TYR:HD2	7	0.1
(1,20)	1:8:A:ILE:HG21	1:9:A:ILE:H	19	0.1
(1,20)	1:8:A:ILE:HG22	1:9:A:ILE:H	19	0.1
(1,20)	1:8:A:ILE:HG23	1:9:A:ILE:H	19	0.1
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	6	0.1
(1,17)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	6	0.1
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	6	0.1
(1,17)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	6	0.1
(1,4)	1:9:A:ILE:HA	1:10:A:TYR:H	5	0.1

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

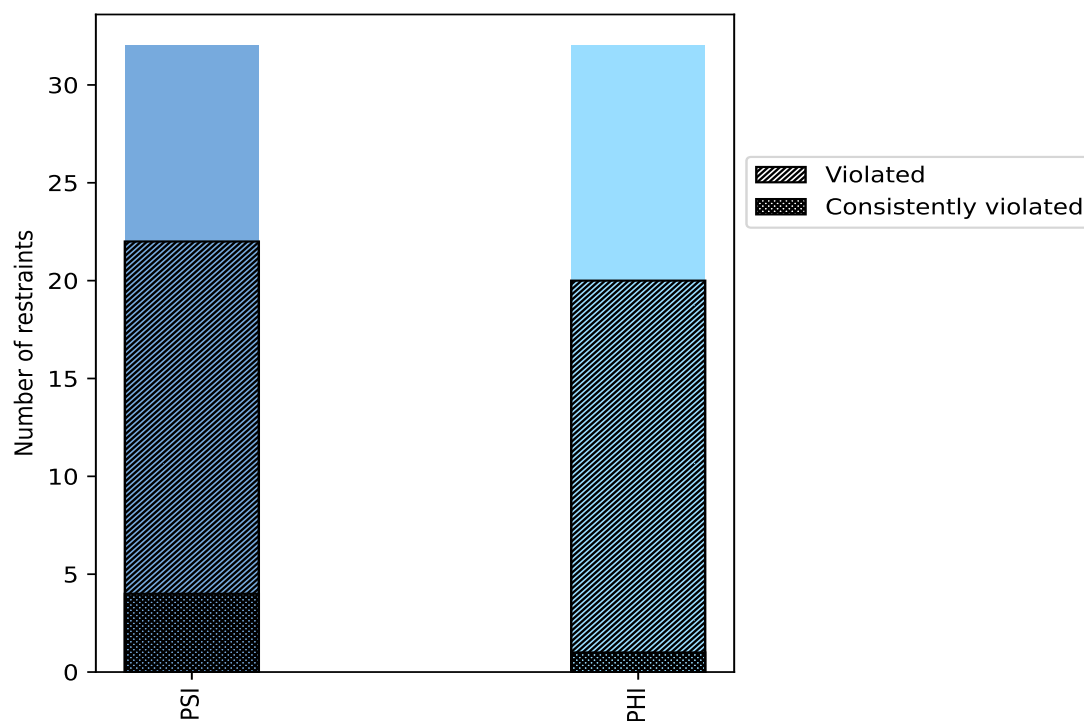
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	32	50.0	22	68.8	34.4	4	12.5	6.2
PHI	32	50.0	20	62.5	31.2	1	3.1	1.6
Total	64	100.0	42	65.6	65.6	5	7.8	7.8

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

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



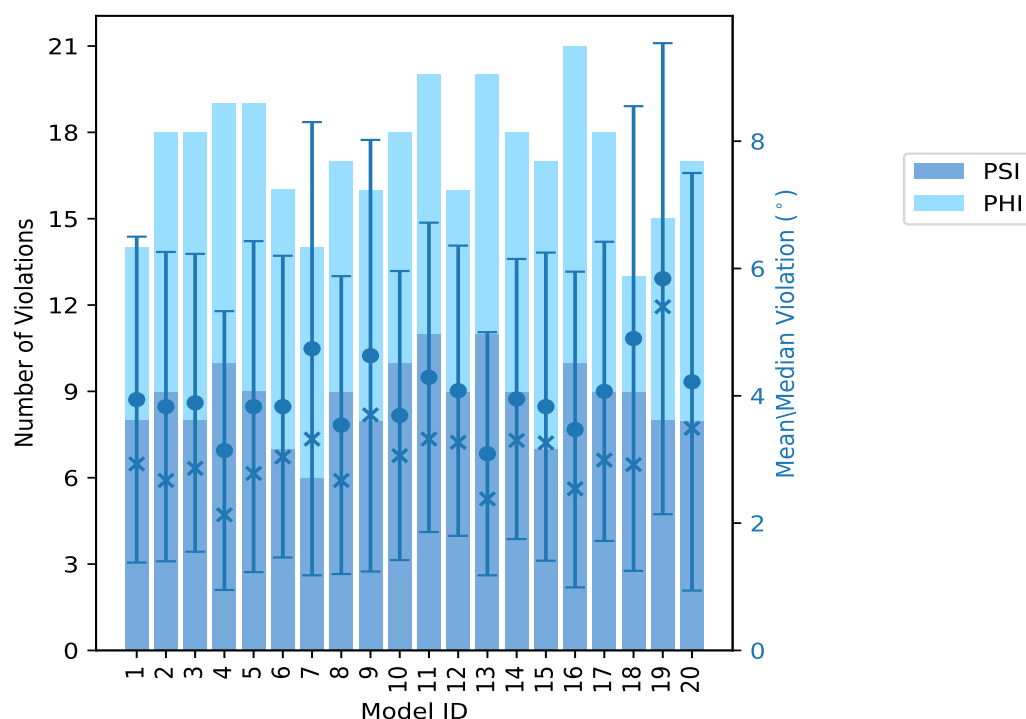
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	8	6	14	3.94	8.87	2.56	2.93
2	9	9	18	3.83	9.05	2.43	2.67
3	8	10	18	3.89	8.99	2.34	2.86
4	10	9	19	3.14	9.0	2.19	2.13
5	9	10	19	3.83	10.94	2.6	2.78
6	7	9	16	3.83	9.32	2.37	3.04
7	6	8	14	4.74	14.72	3.56	3.32
8	9	8	17	3.54	8.99	2.34	2.67
9	8	8	16	4.63	14.33	3.39	3.7
10	10	8	18	3.69	8.97	2.27	3.06
11	11	9	20	4.29	9.09	2.43	3.32
12	9	7	16	4.08	9.09	2.28	3.27
13	11	9	20	3.09	8.59	1.91	2.38
14	9	9	18	3.95	8.61	2.2	3.3
15	7	10	17	3.83	9.12	2.42	3.26
16	10	11	21	3.47	8.88	2.48	2.54
17	9	9	18	4.07	8.71	2.35	2.99
18	9	4	13	4.9	14.51	3.65	2.92
19	8	7	15	5.84	14.59	3.7	5.4
20	8	9	17	4.22	14.72	3.28	3.49

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



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

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

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

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

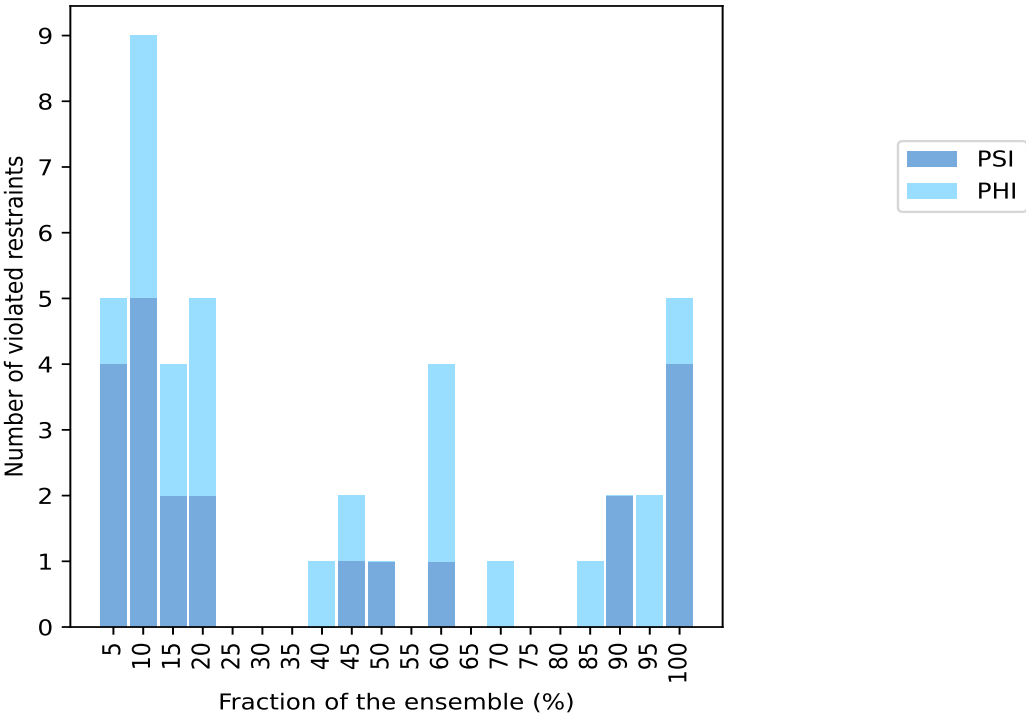
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	3	4	12	60.0
0	0	0	13	65.0
0	1	1	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	1	1	17	85.0
2	0	2	18	90.0
0	2	2	19	95.0
4	1	5	20	100.0

¹ Number of models with violations

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

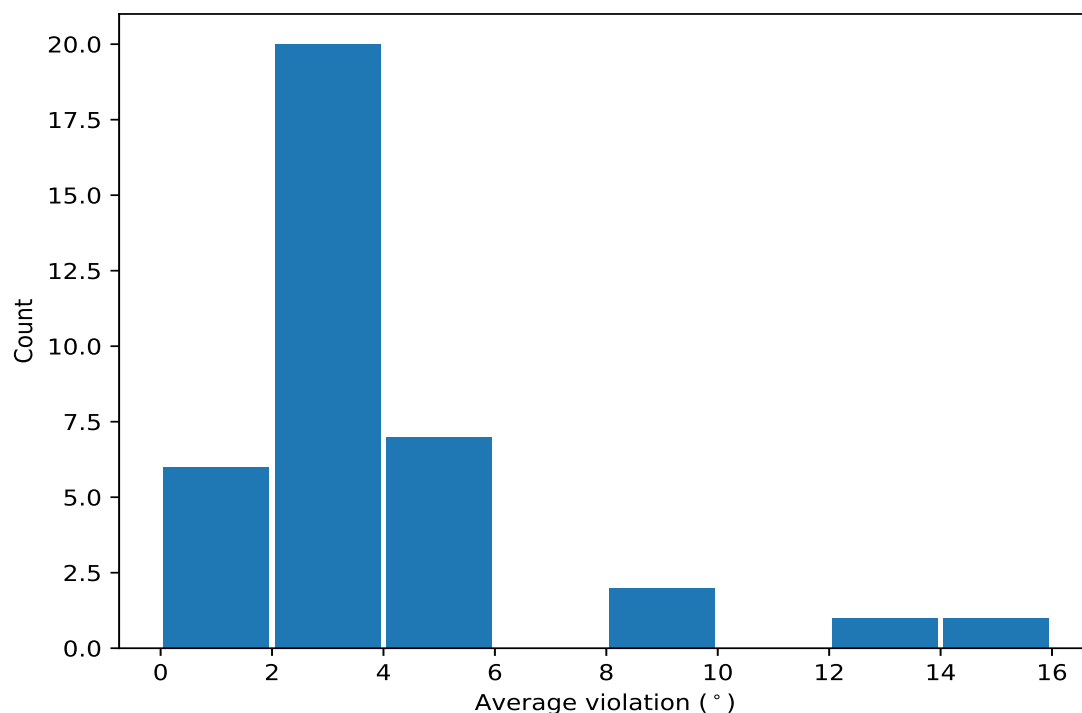


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints ⓘ

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	20	8.94	0.63	8.91
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	20	8.68	0.37	8.71
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	20	4.16	1.39	4.3
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	20	4.14	1.92	2.93
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	20	3.9	2.45	2.85
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	19	3.49	1.45	3.72
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	19	2.93	1.23	2.93
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	18	2.63	0.85	2.56
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	18	2.32	0.68	2.27
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	17	4.04	1.49	3.94
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	14	2.48	0.49	2.55
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	12	2.97	0.94	2.88
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	12	2.47	1.18	2.58
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	12	2.05	0.55	2.06
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	12	1.95	0.26	2.03
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	10	3.45	1.53	3.1
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	9	5.71	0.59	5.51
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	9	2.42	0.73	2.51
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	8	4.61	2.4	4.04
(1,9)	1:7:A:PRO:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	4	12.63	3.2	14.42

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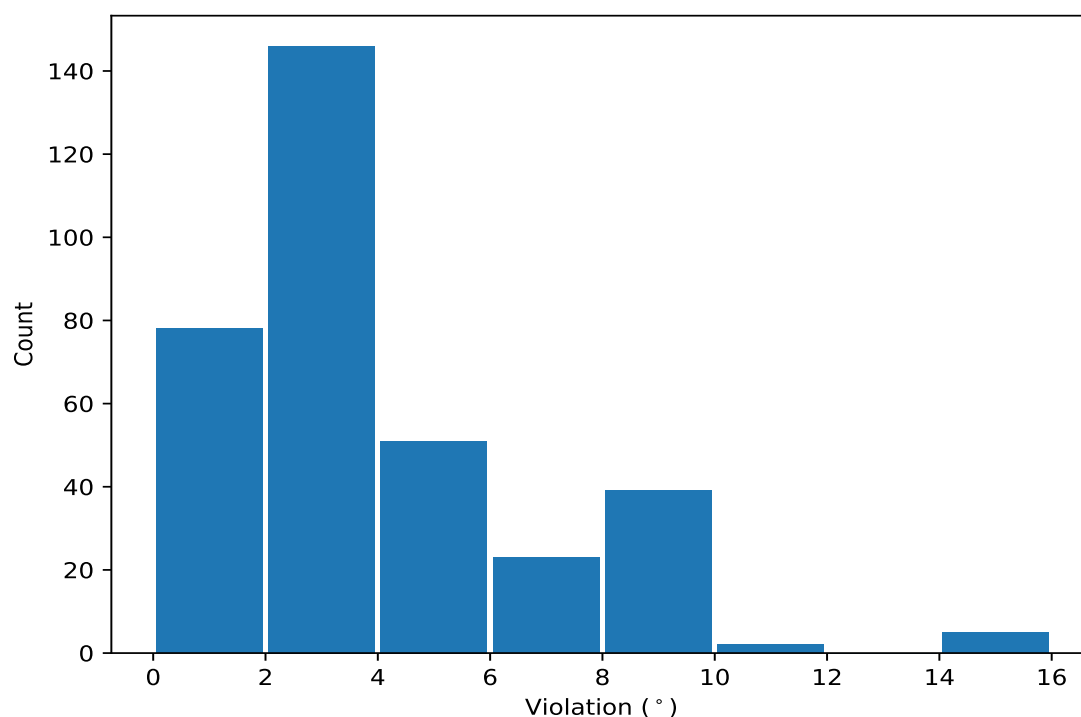
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	4	2.88	1.32	3.1
(1,26)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:CYS:N	4	2.79	1.31	2.19
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	4	2.38	1.1	2.23
(1,22)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:THR:N	4	1.43	0.41	1.28
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:LYS:N	3	4.09	1.41	3.14
(1,54)	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	1:47:B:THR:N	3	3.06	2.46	1.49
(1,39)	1:37:B:PRO:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	3	2.93	0.39	2.99
(1,55)	1:46:B:ARG:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	3	1.32	0.15	1.38
(1,41)	1:39:B:PRO:C	1:40:B:ILE:N	1:40:B:ILE:CA	1:40:B:ILE:C	2	14.72	0.0	14.72
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:PRO:N	2	4.38	0.75	4.38
(1,42)	1:40:B:ILE:N	1:40:B:ILE:CA	1:40:B:ILE:C	1:41:B:ILE:N	2	3.84	0.0	3.84
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	2	2.33	1.12	2.33
(1,7)	1:5:A:PRO:C	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	2	2.18	0.48	2.18
(1,58)	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	1:50:B:CYS:N	2	2.1	0.15	2.1
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	2	1.76	0.03	1.76
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	2	1.56	0.01	1.56
(1,23)	1:14:A:ARG:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	2	1.42	0.34	1.42

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,41)	1:39:B:PRO:C	1:40:B:ILE:N	1:40:B:ILE:CA	1:40:B:ILE:C	7	14.72
(1,41)	1:39:B:PRO:C	1:40:B:ILE:N	1:40:B:ILE:CA	1:40:B:ILE:C	20	14.72
(1,9)	1:7:A:PRO:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	19	14.59
(1,9)	1:7:A:PRO:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	18	14.51
(1,9)	1:7:A:PRO:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	9	14.33
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	5	10.94
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	19	10.88
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	19	9.52
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	18	9.38
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	9	9.34
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	6	9.32
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	15	9.12
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	11	9.09
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	12	9.09
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	2	9.05
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	11	9.03
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	4	9.0
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	3	8.99
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	8	8.99
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	10	8.97
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	3	8.93
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	16	8.88
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	1	8.87
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	2	8.85
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	5	8.84
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	15	8.79
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	6	8.75
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	20	8.72
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	17	8.71
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	7	8.7
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	9	8.69
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	12	8.69
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	10	8.65
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	1	8.65
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	8	8.64
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	17	8.61
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	14	8.61
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	18	8.6
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	17	8.59
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	13	8.59
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	7	8.58
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	16	8.53
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	14	8.52
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	4	8.2
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	19	8.18
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	19	8.09
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	11	7.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	20	7.55
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	13	7.4
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	16	7.34
(1,9)	1:7:A:PRO:C	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	5	7.09
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	11	6.97
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	3	6.93
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	15	6.85
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	1	6.82
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	12	6.77
(1,10)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:ILE:N	5	6.76
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	1	6.75
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	6	6.72
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	16	6.69
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	2	6.68
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	14	6.65
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	10	6.62
(1,54)	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	1:47:B:THR:N	19	6.53
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	8	6.42
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	16	6.38
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	7	6.36
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	18	6.32
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:LYS:N	11	6.09
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	17	5.97
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	19	5.74
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	2	5.72
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	17	5.61
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	11	5.57
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	10	5.56
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	3	5.54
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	14	5.51
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	9	5.47
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	4	5.46
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	11	5.41
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	19	5.4
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	11	5.35
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	2	5.32
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	3	5.3
(1,34)	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	1:35:B:LYS:N	12	5.3
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	9	5.23
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:PRO:N	12	5.13
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	15	5.08
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	20	5.05
(1,26)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:CYS:N	15	5.03
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	14	5.02
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	2	5.01
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	14	4.96
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	19	4.82
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	13	4.81
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	13	4.79
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	9	4.78
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	12	4.61

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	16	4.6
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	2	4.53
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	6	4.51
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	3	4.51
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	8	4.5
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	14	4.5
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	3	4.47
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	17	4.44
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	4	4.42
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	8	4.34
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	6	4.3
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	15	4.3
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	7	4.28
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	9	4.27
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	5	4.19
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	20	4.13
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	4	4.1
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	15	4.1
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	18	4.05
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	9	4.04
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	14	4.02
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	5	4.02
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	2	3.99
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	20	3.98
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	8	3.97
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	11	3.95
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	15	3.94
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	20	3.93
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	6	3.93
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	10	3.91
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	4	3.85
(1,42)	1:40:B:ILE:N	1:40:B:ILE:CA	1:40:B:ILE:C	1:41:B:ILE:N	7	3.84
(1,42)	1:40:B:ILE:N	1:40:B:ILE:CA	1:40:B:ILE:C	1:41:B:ILE:N	20	3.84
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	8	3.82
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	5	3.8
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	10	3.77
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1	3.75
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	10	3.72
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	17	3.66
(1,8)	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	1:7:A:PRO:N	11	3.63
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	12	3.57
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	17	3.54
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	13	3.53
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	20	3.49
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	19	3.47
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	16	3.45
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	3	3.43
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	18	3.42
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	12	3.41
(1,39)	1:37:B:PRO:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	6	3.37
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	9	3.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1	3.35
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	7	3.34
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	14	3.32
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	7	3.31
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	13	3.29
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	14	3.27
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	15	3.26
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	5	3.25
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	14	3.17
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	10	3.17
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	6	3.16
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:LYS:N	13	3.14
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	12	3.13
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	10	3.08
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	3	3.06
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1	3.06
(1,2)	1:2:A:SER:N	1:2:A:SER:CA	1:2:A:SER:C	1:3:A:LYS:N	10	3.05
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	11	3.01
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	17	2.99
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	11	2.99
(1,39)	1:37:B:PRO:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	16	2.99
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	17	2.98
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	16	2.97
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	14	2.94
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	6	2.93
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	17	2.93
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	10	2.93
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	18	2.92
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	18	2.92
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	5	2.9
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	6	2.89
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	20	2.89
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	2	2.85
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	10	2.85
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	16	2.83
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	18	2.83
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	17	2.82
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	4	2.81
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	7	2.8
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	12	2.8
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	19	2.8
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1	2.8
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	5	2.78
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	14	2.78
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	15	2.76
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	6	2.76
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	19	2.74
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	8	2.72
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	18	2.71
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	17	2.71
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	13	2.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	13	2.68
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	5	2.68
(1,7)	1:5:A:PRO:C	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	8	2.67
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	3	2.65
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	3	2.63
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	9	2.62
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	12	2.62
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	20	2.59
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	9	2.54
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	16	2.54
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	16	2.51
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	3	2.51
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	2	2.49
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	13	2.49
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	7	2.49
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	12	2.47
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	9	2.47
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	4	2.47
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	8	2.46
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	11	2.46
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	11	2.46
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	5	2.44
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	2	2.44
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	11	2.43
(1,39)	1:37:B:PRO:C	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	15	2.43
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	4	2.4
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	2	2.39
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	11	2.38
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1	2.38
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	3	2.34
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	3	2.34
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	7	2.33
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	2	2.33
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	3	2.26
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	13	2.26
(1,58)	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	1:50:B:CYS:N	2	2.25
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	11	2.24
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	13	2.23
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	12	2.21
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	10	2.2
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	20	2.19
(1,26)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:CYS:N	1	2.19
(1,26)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:CYS:N	6	2.19
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	17	2.18
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	20	2.16
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	9	2.15
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	13	2.15
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	20	2.14
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	4	2.13
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	10	2.13
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	15	2.11

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	11	2.1
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	13	2.1
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	5	2.09
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	5	2.09
(1,22)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:THR:N	18	2.08
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	8	2.07
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	18	2.07
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	10	2.06
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	9	2.04
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	14	2.04
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	8	2.03
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	13	2.03
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	12	2.02
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	5	2.01
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	7	2.01
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	5	1.98
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	17	1.98
(1,58)	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	1:50:B:CYS:N	1	1.96
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	5	1.95
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	13	1.93
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	7	1.93
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	4	1.93
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	1	1.91
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	5	1.9
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	18	1.89
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	4	1.87
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	4	1.87
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	12	1.86
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	17	1.84
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	13	1.83
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	4	1.83
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	17	1.82
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	19	1.82
(1,15)	1:10:A:TYR:C	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	4	1.82
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	16	1.8
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	17	1.79
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	15	1.78
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	6	1.78
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	19	1.78
(1,23)	1:14:A:ARG:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	4	1.75
(1,26)	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1:18:A:CYS:N	8	1.74
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	6	1.73
(1,20)	1:13:A:ARG:N	1:13:A:ARG:CA	1:13:A:ARG:C	1:14:A:ARG:N	2	1.73
(1,7)	1:5:A:PRO:C	1:6:A:VAL:N	1:6:A:VAL:CA	1:6:A:VAL:C	14	1.7
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	4	1.68
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	20	1.68
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	12	1.67
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	3	1.66
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	15	1.65
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	7	1.64
(1,33)	1:33:B:GLY:C	1:34:B:SER:N	1:34:B:SER:CA	1:34:B:SER:C	16	1.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	13	1.63
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	15	1.63
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	16	1.57
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	20	1.57
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	16	1.56
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	9	1.56
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	16	1.56
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	6	1.51
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ARG:N	8	1.5
(1,54)	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	1:47:B:THR:N	10	1.49
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	8	1.48
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	16	1.47
(1,55)	1:46:B:ARG:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	14	1.46
(1,22)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:THR:N	8	1.46
(1,35)	1:34:B:SER:C	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	8	1.43
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	14	1.41
(1,55)	1:46:B:ARG:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	11	1.38
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1	1.38
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	6	1.37
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	1	1.36
(1,49)	1:43:B:CYS:C	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	3	1.34
(1,47)	1:42:B:TYR:C	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	16	1.32
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	19	1.27
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	14	1.26
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	2	1.25
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ARG:N	16	1.23
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	11	1.21
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	15	1.2
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	9	1.16
(1,54)	1:46:B:ARG:N	1:46:B:ARG:CA	1:46:B:ARG:C	1:47:B:THR:N	4	1.15
(1,40)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:PRO:N	13	1.13
(1,55)	1:46:B:ARG:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	3	1.11
(1,45)	1:41:B:ILE:C	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	15	1.11
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	20	1.11
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	10	1.11
(1,22)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:THR:N	13	1.1
(1,13)	1:9:A:ILE:C	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	5	1.1
(1,23)	1:14:A:ARG:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	2	1.08
(1,22)	1:14:A:ARG:N	1:14:A:ARG:CA	1:14:A:ARG:C	1:15:A:THR:N	10	1.07
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	2	1.02
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	16	1.01
(1,17)	1:11:A:CYS:C	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	4	1.01