



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 PM UTC

PDB ID : 5XOL / pdb_00005xol
BMRB ID : 36094
Title : Thanatin R13R14AA in complex with LPS
Authors : Sinha, S.; Bhattacharjya, S.
Deposited on : 2017-05-29

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

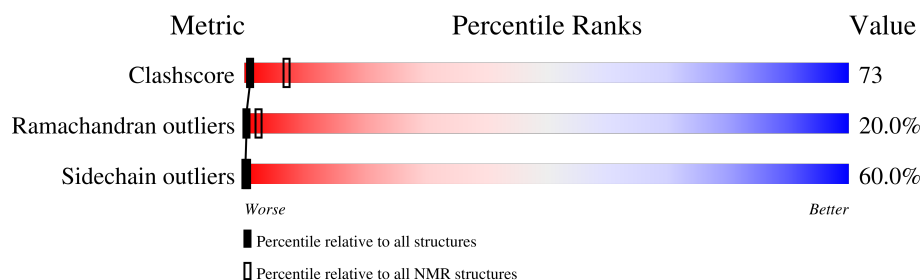
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 14%.

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	
1	B	21	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:4-A:21, B:40-B:52 (31)	0.33	17

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 640 atoms, of which 330 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
			320	97	165	29	26	3	
1	B	21	Total	C	H	N	O	S	0
			320	97	165	29	26	3	

There are 4 discrepancies between the modelled and reference sequences:

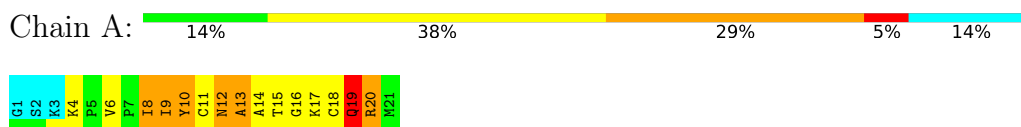
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ALA	ARG	engineered mutation	UNP P55788
A	14	ALA	ARG	engineered mutation	UNP P55788
B	45	ALA	ARG	engineered mutation	UNP P55788
B	46	ALA	ARG	engineered mutation	UNP P55788

4 Residue-property plots [i](#)

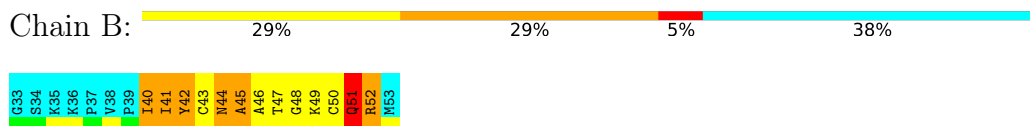
4.1 Average score per residue in the NMR ensemble

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

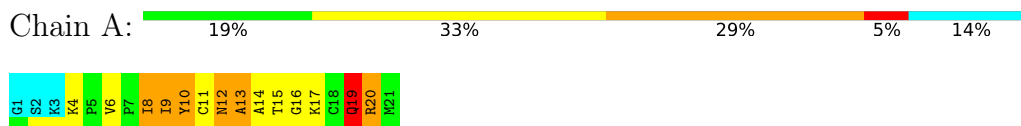


4.2 Scores per residue for each member of the ensemble

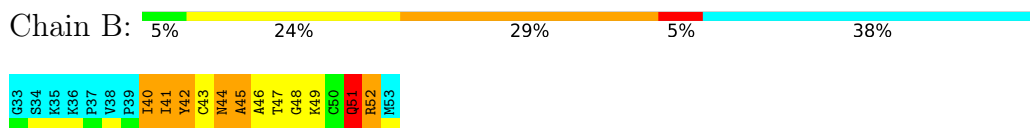
Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

- Molecule 1: Thanatin



- Molecule 1: Thanatin

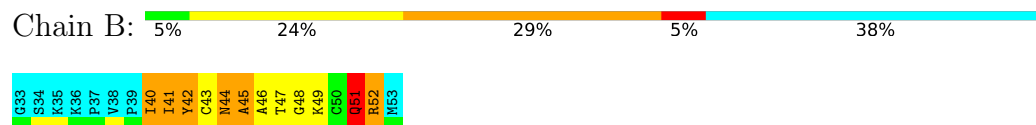


4.2.2 Score per residue for model 2

- Molecule 1: Thanatin

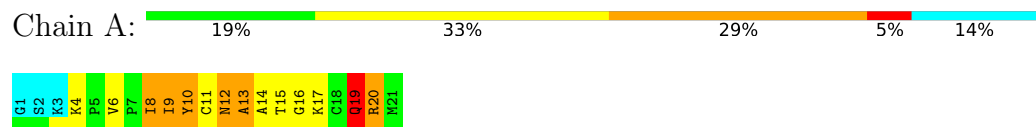


- Molecule 1: Thanatin

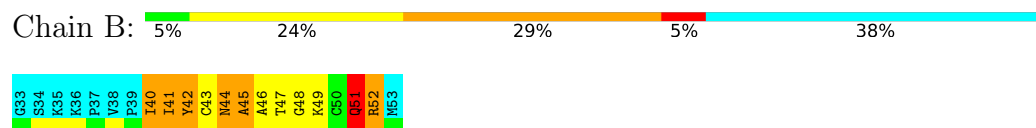


4.2.3 Score per residue for model 3

- Molecule 1: Thanatin

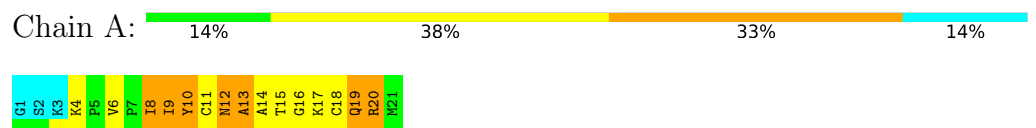


- Molecule 1: Thanatin

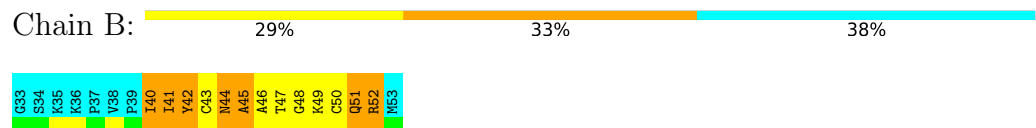


4.2.4 Score per residue for model 4

- Molecule 1: Thanatin

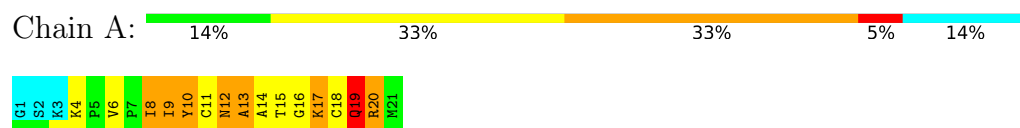


- Molecule 1: Thanatin

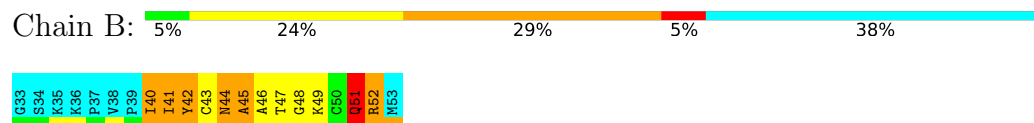


4.2.5 Score per residue for model 5

- Molecule 1: Thanatin

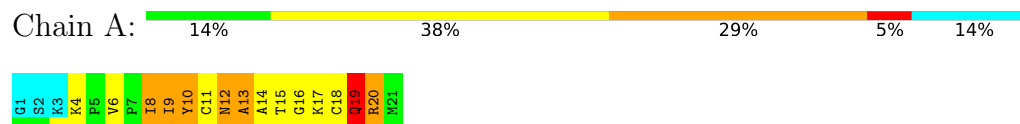


- Molecule 1: Thanatin

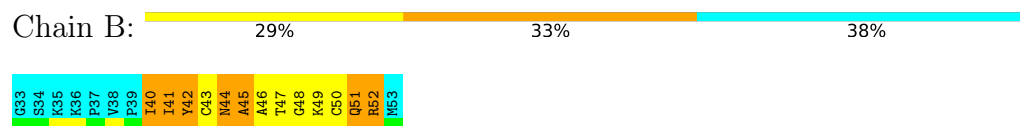


4.2.6 Score per residue for model 6

- Molecule 1: Thanatin

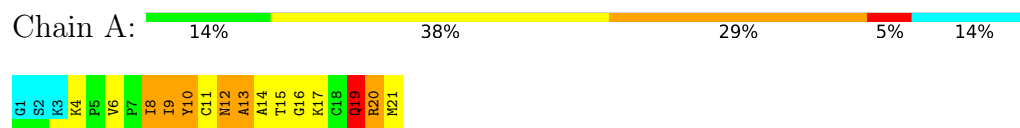


- Molecule 1: Thanatin

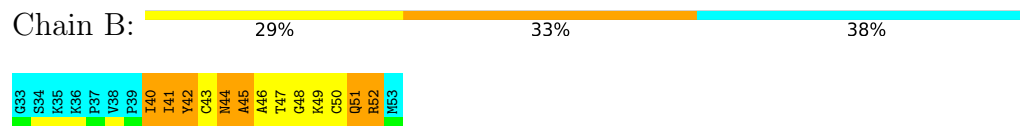


4.2.7 Score per residue for model 7

- Molecule 1: Thanatin

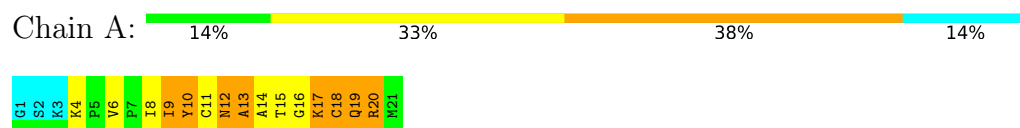


- Molecule 1: Thanatin

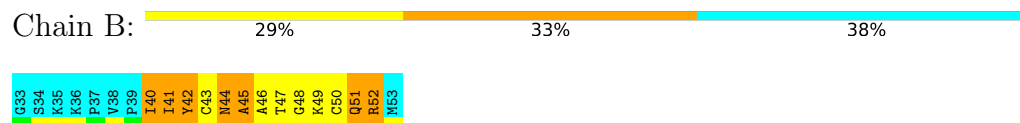


4.2.8 Score per residue for model 8

- Molecule 1: Thanatin

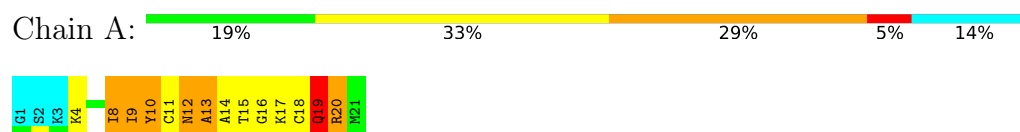


- Molecule 1: Thanatin

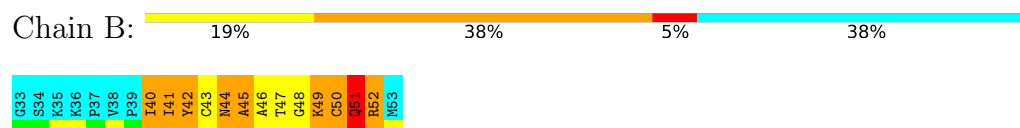


4.2.9 Score per residue for model 9

- Molecule 1: Thanatin

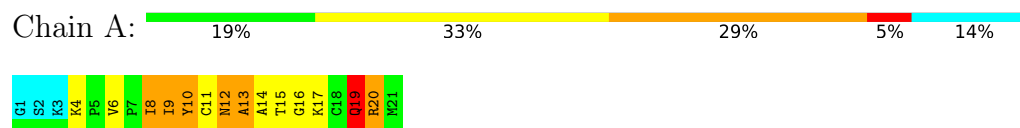


- Molecule 1: Thanatin

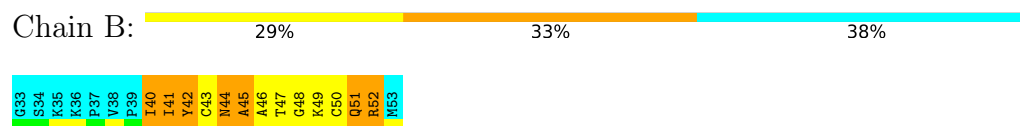


4.2.10 Score per residue for model 10

- Molecule 1: Thanatin

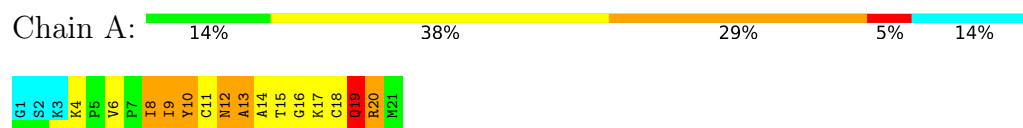


- Molecule 1: Thanatin

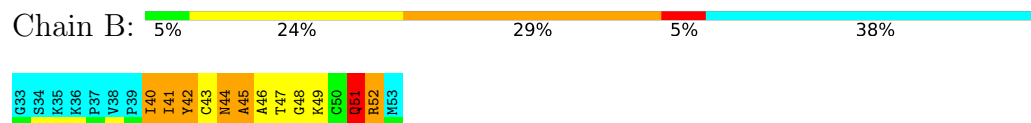


4.2.11 Score per residue for model 11

- Molecule 1: Thanatin



- Molecule 1: Thanatin

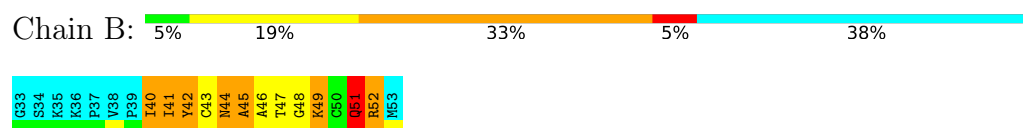


4.2.12 Score per residue for model 12

- Molecule 1: Thanatin



- Molecule 1: Thanatin

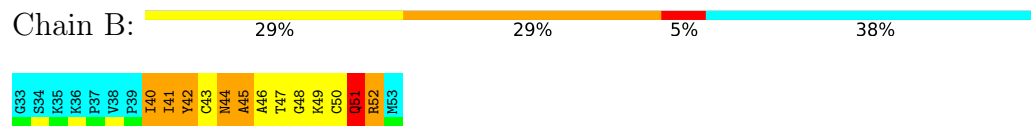


4.2.13 Score per residue for model 13

- Molecule 1: Thanatin



- Molecule 1: Thanatin

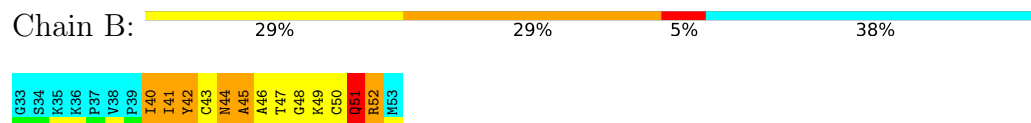


4.2.14 Score per residue for model 14

- Molecule 1: Thanatin

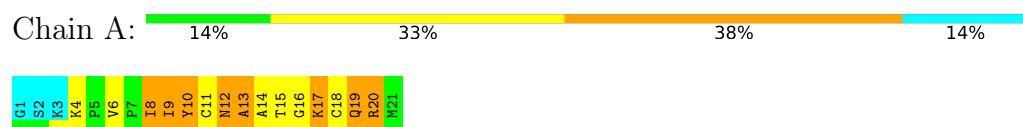


- Molecule 1: Thanatin

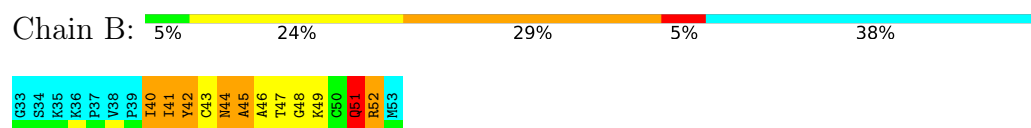


4.2.15 Score per residue for model 15

- Molecule 1: Thanatin



- Molecule 1: Thanatin

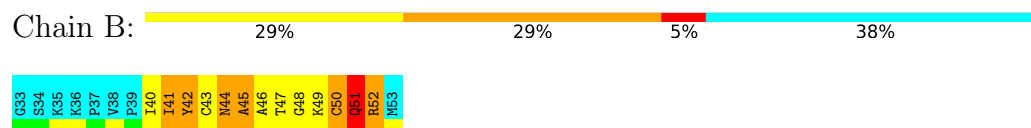


4.2.16 Score per residue for model 16

- Molecule 1: Thanatin

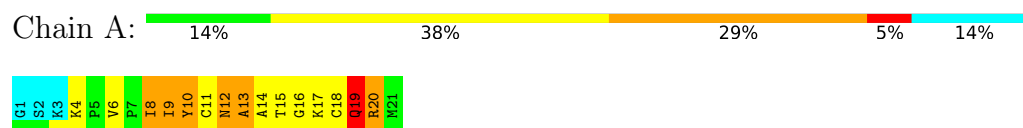


- Molecule 1: Thanatin

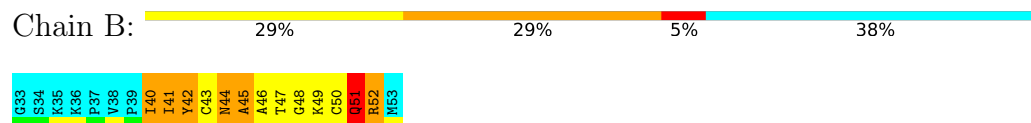


4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Thanatin



- Molecule 1: Thanatin

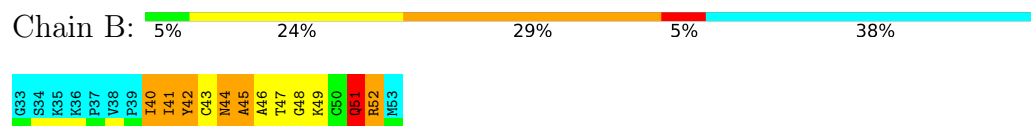


4.2.18 Score per residue for model 18

- Molecule 1: Thanatin

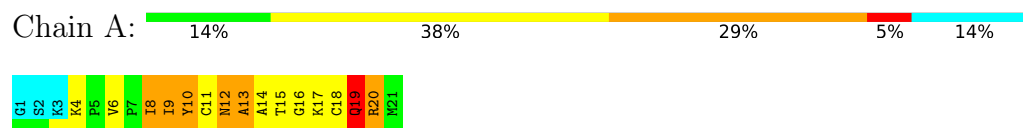


- Molecule 1: Thanatin

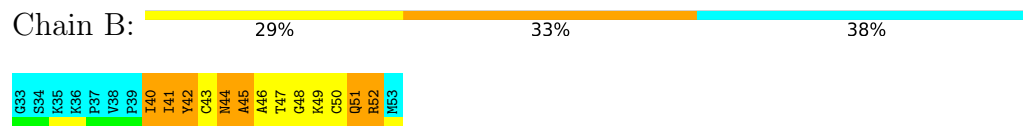


4.2.19 Score per residue for model 19

- Molecule 1: Thanatin

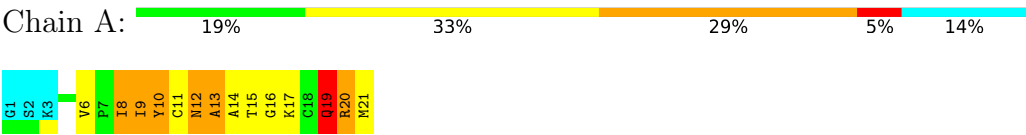


- Molecule 1: Thanatin

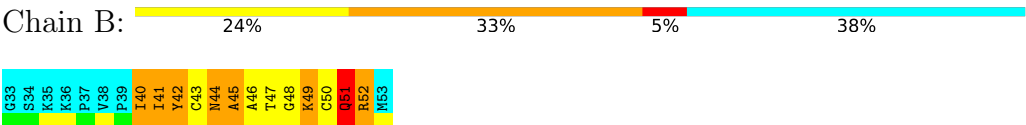


4.2.20 Score per residue for model 20

● 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	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	74
Number of shifts mapped to atoms	74
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	14%

6 Model quality

6.1 Standard geometry

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

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	136	144	144	19±1
1	B	98	99	99	16±1
All	All	4680	4860	4860	698

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 73.

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:HD12	1:A:19:GLN:O	0.69	1.87	9	20
1:B:41:ILE:HD12	1:B:51:GLN:O	0.66	1.90	12	20
1:B:44:ASN:O	1:B:45:ALA:O	0.65	2.15	9	20
1:A:12:ASN:O	1:A:13:ALA:O	0.64	2.16	5	20
1:B:52:ARG:N	1:B:52:ARG:HE	0.64	1.89	16	3
1:A:9:ILE:HD11	1:A:11:CYS:HB3	0.61	1.72	10	20
1:B:41:ILE:HD11	1:B:43:CYS:HB3	0.61	1.71	14	20
1:B:44:ASN:ND2	1:B:45:ALA:N	0.60	2.50	4	20
1:A:12:ASN:ND2	1:A:13:ALA:N	0.59	2.50	4	20
1:A:12:ASN:CG	1:A:13:ALA:N	0.59	2.61	9	19
1:B:44:ASN:CG	1:B:45:ALA:N	0.58	2.61	18	20
1:A:12:ASN:OD1	1:A:15:THR:HG21	0.57	1.99	18	1
1:A:12:ASN:HD22	1:A:13:ALA:N	0.57	1.98	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:CYS:O	1:A:19:GLN:HB3	0.53	2.04	11	7
1:B:47:THR:OG1	1:B:48:GLY:N	0.53	2.42	12	20
1:A:15:THR:OG1	1:A:16:GLY:N	0.53	2.42	5	20
1:B:50:CYS:O	1:B:51:GLN:HB3	0.52	2.05	17	8
1:A:10:TYR:CD1	1:A:10:TYR:N	0.51	2.77	12	12
1:A:10:TYR:N	1:A:10:TYR:CD2	0.51	2.77	14	8
1:B:45:ALA:O	1:B:47:THR:HG22	0.51	2.05	9	20
1:B:42:TYR:N	1:B:42:TYR:CD1	0.50	2.77	17	13
1:B:42:TYR:CD2	1:B:42:TYR:N	0.50	2.78	4	6
1:A:21:MET:HE2	1:B:49:LYS:HE2	0.50	1.83	12	1
1:B:42:TYR:HE1	1:B:51:GLN:HG2	0.50	1.66	17	5
1:A:10:TYR:HE2	1:A:19:GLN:HG2	0.50	1.67	14	3
1:A:10:TYR:CD1	1:A:21:MET:HE3	0.50	2.42	14	1
1:A:9:ILE:HD11	1:A:11:CYS:CB	0.49	2.37	8	18
1:A:10:TYR:CD2	1:A:21:MET:HE3	0.49	2.42	20	1
1:A:13:ALA:O	1:A:15:THR:HG22	0.48	2.08	5	19
1:A:20:ARG:N	1:A:20:ARG:NE	0.48	2.61	12	19
1:B:41:ILE:HD11	1:B:43:CYS:CB	0.48	2.38	4	15
1:A:18:CYS:H	1:A:19:GLN:NE2	0.48	2.07	11	3
1:B:52:ARG:N	1:B:52:ARG:NE	0.48	2.61	15	19
1:A:10:TYR:HE1	1:A:19:GLN:HG2	0.48	1.68	11	4
1:A:6:VAL:CG1	1:A:20:ARG:CG	0.48	2.92	8	15
1:A:6:VAL:HG12	1:A:20:ARG:CG	0.47	2.39	7	9
1:B:42:TYR:CD1	1:B:42:TYR:O	0.47	2.67	16	1
1:B:50:CYS:H	1:B:51:GLN:NE2	0.47	2.07	17	1
1:A:12:ASN:C	1:A:13:ALA:O	0.46	2.59	16	20
1:B:44:ASN:C	1:B:45:ALA:O	0.46	2.59	14	20
1:B:40:ILE:HG12	1:B:40:ILE:O	0.46	2.11	3	7
1:B:51:GLN:NE2	1:B:52:ARG:O	0.45	2.49	12	12
1:A:8:ILE:O	1:A:8:ILE:HG12	0.45	2.10	20	18
1:A:20:ARG:H	1:A:20:ARG:NE	0.45	2.10	9	1
1:A:12:ASN:ND2	1:A:12:ASN:C	0.45	2.75	17	12
1:B:44:ASN:ND2	1:B:44:ASN:C	0.45	2.75	11	13
1:B:42:TYR:CD1	1:B:42:TYR:N	0.45	2.80	11	1
1:A:19:GLN:NE2	1:A:20:ARG:O	0.45	2.50	9	13
1:B:40:ILE:O	1:B:40:ILE:HG12	0.44	2.12	1	11
1:A:20:ARG:NE	1:A:20:ARG:H	0.44	2.11	20	1
1:B:45:ALA:O	1:B:47:THR:N	0.44	2.51	20	19
1:B:52:ARG:NE	1:B:52:ARG:H	0.44	2.11	12	5
1:A:13:ALA:O	1:A:15:THR:N	0.43	2.52	16	18
1:B:50:CYS:C	1:B:51:GLN:CD	0.43	2.87	7	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ARG:N	1:A:20:ARG:HE	0.43	2.12	12	2
1:A:20:ARG:NE	1:A:20:ARG:N	0.43	2.66	9	1
1:A:8:ILE:O	1:A:8:ILE:CG1	0.43	2.67	1	2
1:A:18:CYS:C	1:A:19:GLN:CG	0.42	2.93	9	8
1:B:40:ILE:O	1:B:40:ILE:CG1	0.42	2.67	18	1
1:A:18:CYS:C	1:A:19:GLN:CD	0.42	2.87	4	4
1:A:12:ASN:O	1:A:13:ALA:C	0.42	2.62	18	18
1:B:42:TYR:HE2	1:B:51:GLN:HG2	0.42	1.74	8	3
1:A:19:GLN:CG	1:A:20:ARG:N	0.42	2.83	19	2
1:B:44:ASN:O	1:B:45:ALA:C	0.42	2.63	18	15
1:A:21:MET:HE2	1:B:49:LYS:HD3	0.42	1.91	20	1
1:A:12:ASN:C	1:A:12:ASN:ND2	0.42	2.78	18	1
1:A:15:THR:HG23	1:A:17:LYS:H	0.41	1.75	15	2
1:A:6:VAL:O	1:A:6:VAL:HG13	0.41	2.16	12	5
1:B:50:CYS:C	1:B:51:GLN:CG	0.41	2.94	20	3
1:B:47:THR:HG23	1:B:49:LYS:O	0.40	2.16	9	1
1:A:15:THR:HG23	1:A:17:LYS:O	0.40	2.16	8	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	17/21 (81%)	10±0 (62±3%)	4±0 (21±3%)	3±0 (18±0%)	0	3
1	B	13/21 (62%)	7±0 (57±4%)	3±0 (20±4%)	3±0 (23±0%)	0	2
All	All	600/840 (71%)	358 (60%)	122 (20%)	120 (20%)	0	2

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	13	ALA	20
1	A	14	ALA	20
1	A	19	GLN	20
1	B	45	ALA	20

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Mol	Chain	Res	Type	Models (Total)
1	B	46	ALA	20
1	B	51	GLN	20

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	15/17 (88%)	7±1 (46±4%)	8±1 (54±4%)	0	1
1	B	10/17 (59%)	3±1 (32±7%)	7±1 (68±7%)	0	0
All	All	500/680 (74%)	200 (40%)	300 (60%)	0	0

All 18 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	9	ILE	20
1	A	10	TYR	20
1	A	12	ASN	20
1	A	17	LYS	20
1	A	20	ARG	20
1	B	40	ILE	20
1	B	41	ILE	20
1	B	42	TYR	20
1	B	44	ASN	20
1	B	49	LYS	20
1	B	52	ARG	20
1	A	4	LYS	19
1	A	19	GLN	17
1	B	51	GLN	14
1	A	21	MET	6
1	B	50	CYS	3
1	A	18	CYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 14% for the well-defined parts and 13% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *R2A-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	74
Number of shifts mapped to atoms	74
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 14%, i.e. 60 atoms were assigned a chemical shift out of a possible 416. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	60/153 (39%)	60/62 (97%)	0/62 (0%)	0/29 (0%)
Sidechain	0/245 (0%)	0/160 (0%)	0/72 (0%)	0/13 (0%)
Aromatic	0/18 (0%)	0/8 (0%)	0/10 (0%)	0/0 (—%)
Overall	60/416 (14%)	60/230 (26%)	0/144 (0%)	0/42 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 13%, i.e. 74 atoms were assigned a chemical shift out of a possible 552. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	74/206 (36%)	74/84 (88%)	0/84 (0%)	0/38 (0%)
Sidechain	0/328 (0%)	0/214 (0%)	0/98 (0%)	0/16 (0%)
Aromatic	0/18 (0%)	0/8 (0%)	0/10 (0%)	0/0 (—%)
Overall	74/552 (13%)	74/306 (24%)	0/192 (0%)	0/54 (0%)

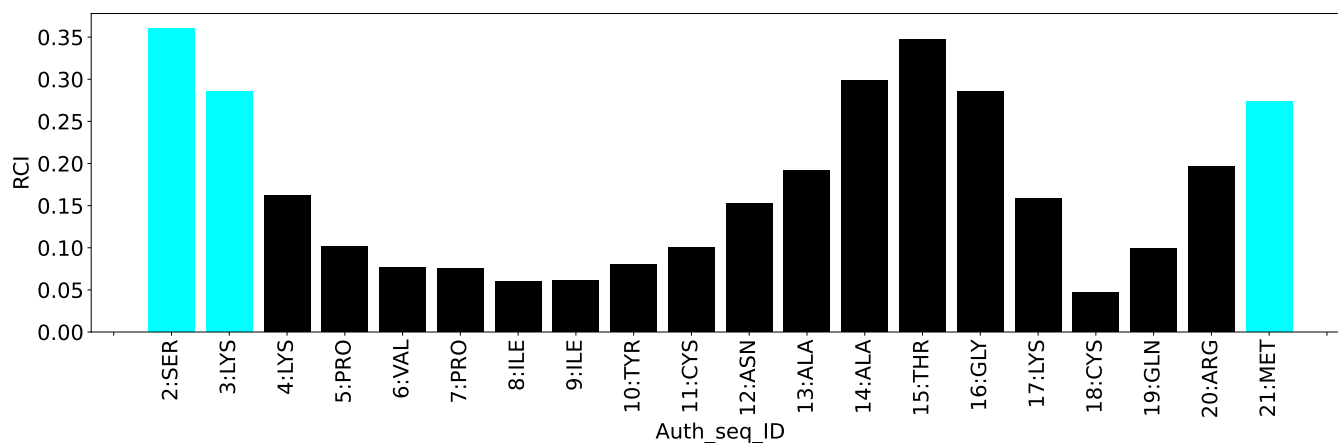
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

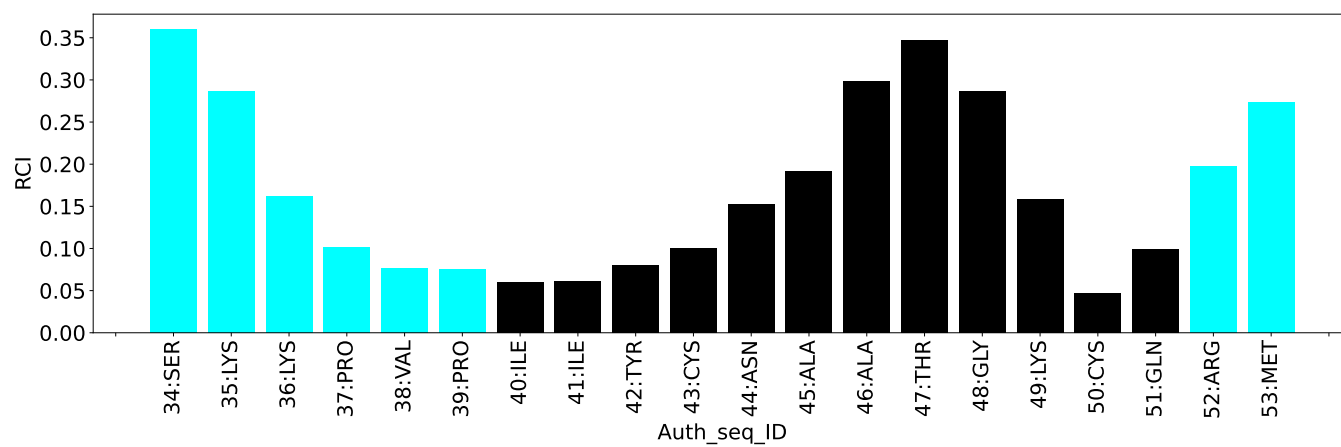
7.1.5 Random Coil Index (RCI) plots [i](#)

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	390
Intra-residue ($ i-j =0$)	148
Sequential ($ i-j =1$)	146
Medium range ($ i-j >1$ and $ i-j <5$)	16
Long range ($ i-j \geq 5$)	80
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	64
Number of unmapped restraints	0
Number of restraints per residue	10.8
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)	52.0	0.2
0.2-0.5 (Medium)	32.0	0.49
>0.5 (Large)	1.3	0.71

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)	17.2	9.69
10.0-20.0 (Medium)	5.7	19.95
>20.0 (Large)	10.3	43.98

9 Distance violation analysis ⓘ

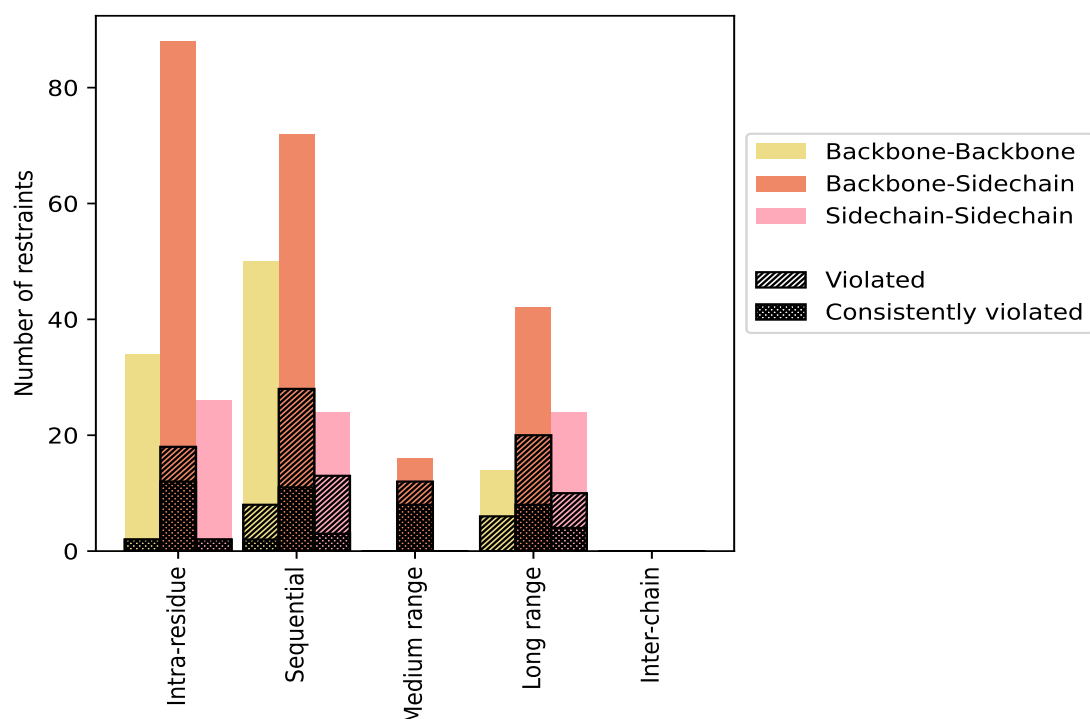
9.1 Summary of distance violations ⓘ

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)	148	37.9	22	14.9	5.6	16	10.8	4.1
Backbone-Backbone	34	8.7	2	5.9	0.5	2	5.9	0.5
Backbone-Sidechain	88	22.6	18	20.5	4.6	12	13.6	3.1
Sidechain-Sidechain	26	6.7	2	7.7	0.5	2	7.7	0.5
Sequential (i-j =1)	146	37.4	49	33.6	12.6	16	11.0	4.1
Backbone-Backbone	50	12.8	8	16.0	2.1	2	4.0	0.5
Backbone-Sidechain	72	18.5	28	38.9	7.2	11	15.3	2.8
Sidechain-Sidechain	24	6.2	13	54.2	3.3	3	12.5	0.8
Medium range (i-j >1 & i-j <5)	16	4.1	12	75.0	3.1	8	50.0	2.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	16	4.1	12	75.0	3.1	8	50.0	2.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	80	20.5	36	45.0	9.2	12	15.0	3.1
Backbone-Backbone	14	3.6	6	42.9	1.5	0	0.0	0.0
Backbone-Sidechain	42	10.8	20	47.6	5.1	8	19.0	2.1
Sidechain-Sidechain	24	6.2	10	41.7	2.6	4	16.7	1.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	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	390	100.0	119	30.5	30.5	52	13.3	13.3
Backbone-Backbone	98	25.1	16	16.3	4.1	4	4.1	1.0
Backbone-Sidechain	218	55.9	78	35.8	20.0	39	17.9	10.0
Sidechain-Sidechain	74	19.0	25	33.8	6.4	9	12.2	2.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	20	28	11	21	0	80	0.2	0.54	0.09	0.19
2	20	27	11	26	0	84	0.2	0.53	0.09	0.19
3	20	27	11	21	0	79	0.21	0.54	0.09	0.19
4	20	32	12	30	0	94	0.19	0.41	0.06	0.19
5	19	28	12	28	0	87	0.2	0.55	0.09	0.19
6	20	30	12	29	0	91	0.19	0.54	0.07	0.19
7	20	27	12	27	0	86	0.19	0.54	0.08	0.18
8	19	34	12	28	0	93	0.19	0.35	0.06	0.19
9	18	31	12	29	0	90	0.2	0.55	0.09	0.19
10	19	31	12	29	0	91	0.19	0.54	0.08	0.19

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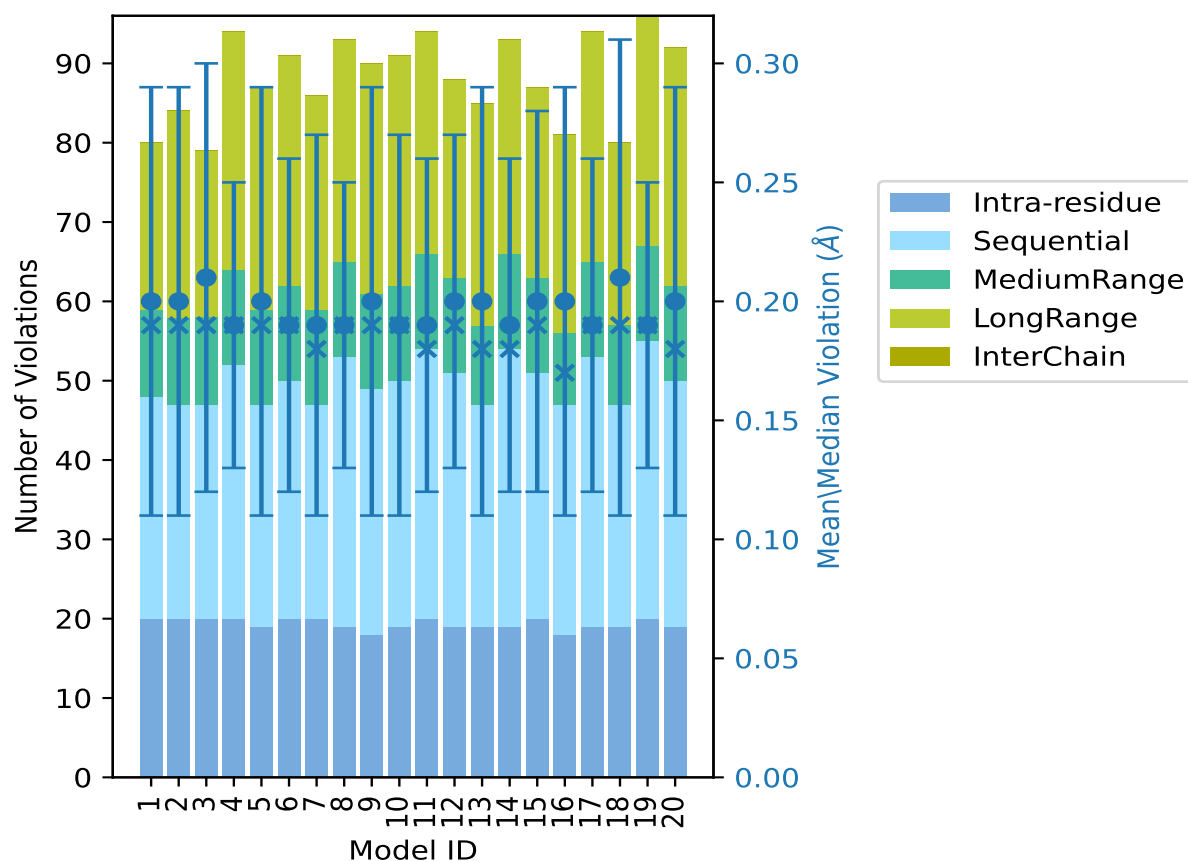
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	20	34	12	28	0	94	0.19	0.52	0.07	0.18
12	19	32	12	25	0	88	0.2	0.55	0.07	0.19
13	19	28	10	28	0	85	0.2	0.54	0.09	0.18
14	19	35	12	27	0	93	0.19	0.54	0.07	0.18
15	20	31	12	24	0	87	0.2	0.51	0.08	0.19
16	18	29	9	25	0	81	0.2	0.55	0.09	0.17
17	19	34	12	29	0	94	0.19	0.53	0.07	0.19
18	19	28	10	23	0	80	0.21	0.71	0.1	0.19
19	20	35	12	29	0	96	0.19	0.42	0.06	0.19
20	19	31	12	30	0	92	0.2	0.55	0.09	0.18

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

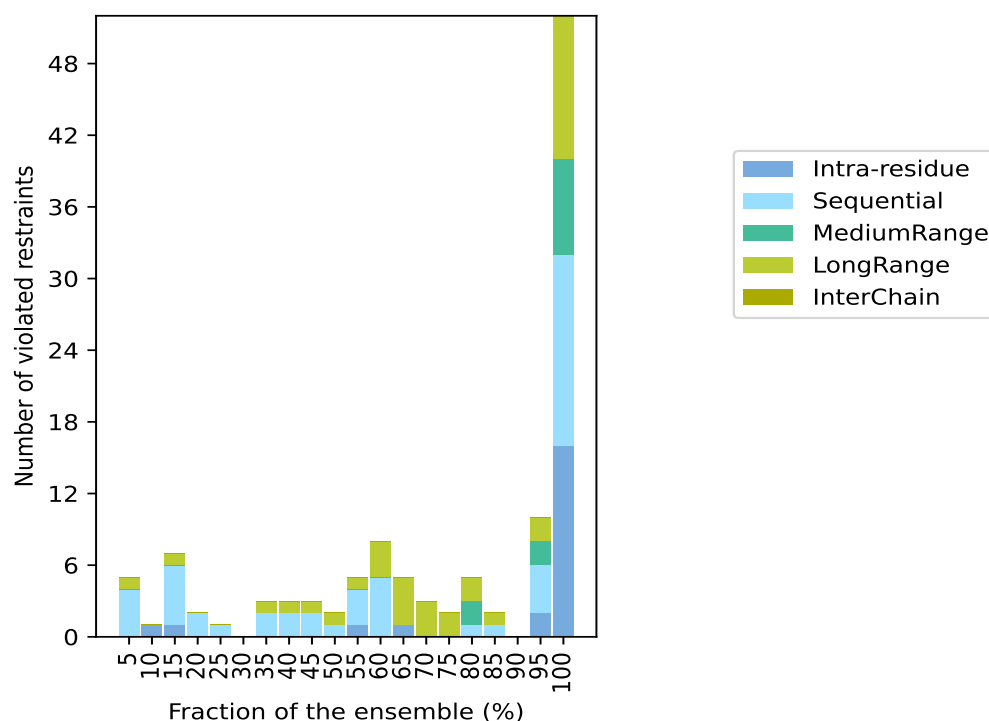
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 271(IR:126, SQ:97, MR:4, LR:44, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	4	0	1	0	5	1	5.0
1	0	0	0	0	1	2	10.0
1	5	0	1	0	7	3	15.0
0	2	0	0	0	2	4	20.0
0	1	0	0	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	2	0	1	0	3	7	35.0
0	2	0	1	0	3	8	40.0
0	2	0	1	0	3	9	45.0
0	1	0	1	0	2	10	50.0
1	3	0	1	0	5	11	55.0
0	5	0	3	0	8	12	60.0
1	0	0	4	0	5	13	65.0
0	0	0	3	0	3	14	70.0
0	0	0	2	0	2	15	75.0
0	1	2	2	0	5	16	80.0
0	1	0	1	0	2	17	85.0
0	0	0	0	0	0	18	90.0
2	4	2	2	0	10	19	95.0
16	16	8	12	0	52	20	100.0

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

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

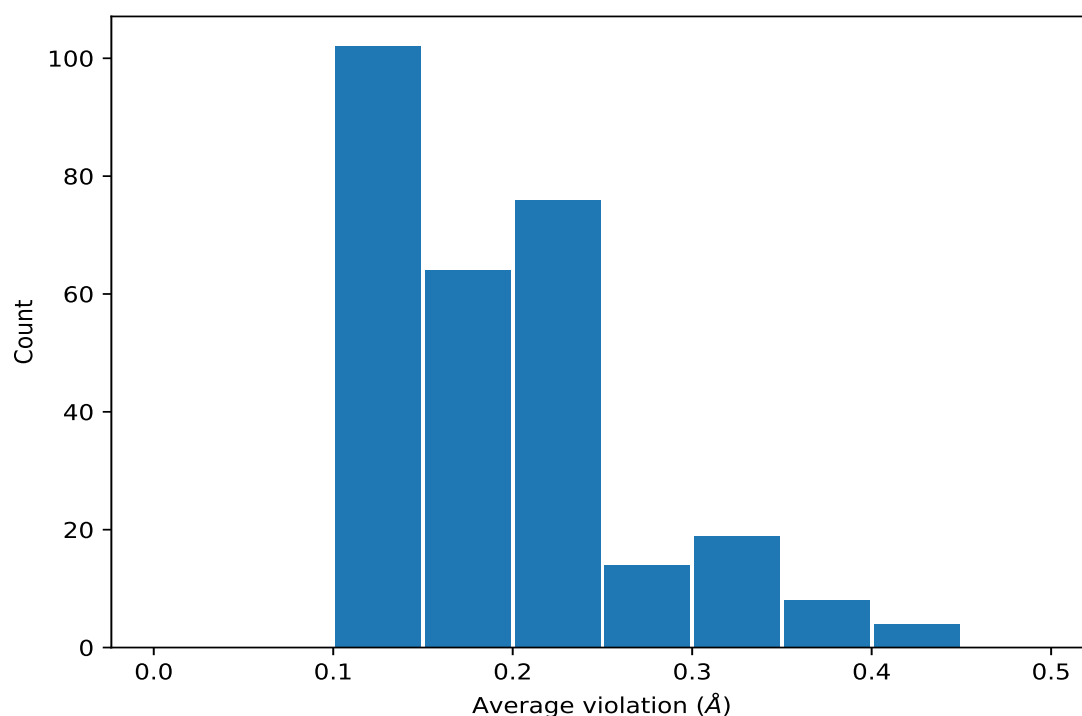
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	20	0.41	0.19	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	20	0.41	0.19	0.54
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	20	0.35	0.05	0.34
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	20	0.35	0.05	0.34
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	20	0.35	0.05	0.34
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	20	0.35	0.05	0.34
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	20	0.35	0.05	0.34
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	20	0.35	0.05	0.34
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	20	0.34	0.02	0.34
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	20	0.34	0.02	0.34
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	20	0.34	0.02	0.34
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	20	0.34	0.02	0.34
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	20	0.34	0.02	0.34
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	20	0.34	0.02	0.34
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	20	0.33	0.03	0.34
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	20	0.33	0.03	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	20	0.33	0.03	0.34
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	20	0.32	0.05	0.33
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	20	0.32	0.05	0.33
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	20	0.32	0.05	0.33
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	20	0.28	0.15	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	20	0.28	0.15	0.41
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	20	0.28	0.03	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	20	0.28	0.03	0.29
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	20	0.27	0.03	0.27
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	20	0.27	0.03	0.27
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	20	0.26	0.02	0.27
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	20	0.26	0.02	0.27
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	20	0.26	0.04	0.26
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	20	0.26	0.04	0.26
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	20	0.25	0.05	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	20	0.25	0.05	0.29
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	20	0.25	0.05	0.28
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	20	0.25	0.05	0.28
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	20	0.24	0.02	0.24
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	20	0.24	0.02	0.24
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	20	0.24	0.01	0.24
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	20	0.24	0.01	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	20	0.24	0.03	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	20	0.24	0.03	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	20	0.24	0.03	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	20	0.23	0.03	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	20	0.23	0.03	0.24
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	20	0.23	0.03	0.24
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	20	0.23	0.04	0.22
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	20	0.23	0.04	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	20	0.22	0.01	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	20	0.22	0.0	0.22
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	20	0.22	0.04	0.22
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	20	0.22	0.04	0.22
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	20	0.22	0.04	0.22
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	20	0.22	0.03	0.22
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	20	0.22	0.03	0.22
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	20	0.21	0.02	0.21
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	20	0.21	0.02	0.21
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	20	0.21	0.02	0.21
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	20	0.21	0.02	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	20	0.21	0.01	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	20	0.21	0.01	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	20	0.21	0.01	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	20	0.21	0.01	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	20	0.21	0.01	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	20	0.21	0.01	0.21
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	20	0.21	0.03	0.21
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	20	0.21	0.03	0.21
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	20	0.21	0.03	0.21
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	20	0.21	0.03	0.21
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	20	0.21	0.03	0.21
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	20	0.2	0.03	0.2
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	20	0.2	0.03	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	20	0.2	0.02	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	20	0.2	0.02	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	20	0.2	0.02	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	20	0.2	0.02	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	20	0.2	0.02	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	20	0.2	0.02	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	20	0.2	0.02	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	20	0.2	0.02	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	20	0.2	0.02	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	20	0.2	0.02	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	20	0.2	0.02	0.21
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	20	0.2	0.02	0.19
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	20	0.2	0.02	0.19
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	20	0.2	0.02	0.2
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	20	0.2	0.02	0.2
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	20	0.19	0.03	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	20	0.19	0.03	0.19
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	20	0.19	0.13	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	20	0.19	0.13	0.12
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	20	0.19	0.05	0.18
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	20	0.19	0.05	0.18
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	20	0.19	0.05	0.18
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	20	0.19	0.05	0.18
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	20	0.19	0.05	0.18
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	20	0.19	0.05	0.18
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	20	0.19	0.01	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	20	0.19	0.02	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	20	0.19	0.0	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	20	0.19	0.0	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	20	0.19	0.0	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	20	0.19	0.0	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	20	0.19	0.0	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	20	0.19	0.0	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	20	0.19	0.0	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	20	0.19	0.0	0.19
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	20	0.19	0.02	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	20	0.19	0.02	0.2
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	20	0.19	0.03	0.18
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	20	0.19	0.03	0.18
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	20	0.19	0.02	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	20	0.19	0.02	0.17
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	20	0.19	0.02	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	20	0.19	0.02	0.18
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	20	0.18	0.02	0.16
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	20	0.18	0.02	0.16
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	20	0.17	0.01	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	20	0.17	0.01	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	20	0.17	0.01	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	20	0.17	0.01	0.17
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	20	0.15	0.0	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	20	0.15	0.0	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	20	0.15	0.0	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	20	0.15	0.0	0.15
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	20	0.15	0.13	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	20	0.15	0.13	0.11
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	20	0.14	0.0	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	20	0.14	0.0	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	20	0.13	0.02	0.13
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	20	0.13	0.02	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	20	0.13	0.02	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	20	0.13	0.02	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	20	0.13	0.02	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	20	0.13	0.02	0.13
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	19	0.4	0.17	0.52
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	19	0.4	0.17	0.52
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	19	0.22	0.03	0.22
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	19	0.22	0.03	0.22
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	19	0.22	0.03	0.22
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	19	0.2	0.01	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	19	0.2	0.01	0.21
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	19	0.2	0.04	0.19
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	19	0.2	0.04	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	19	0.2	0.04	0.19
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	19	0.2	0.04	0.19
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	19	0.2	0.04	0.19
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	19	0.2	0.04	0.19
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	19	0.19	0.04	0.18
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	19	0.19	0.04	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	19	0.19	0.03	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	19	0.19	0.03	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	19	0.17	0.01	0.17
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	19	0.17	0.01	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	19	0.17	0.01	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	19	0.17	0.01	0.17
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	19	0.13	0.02	0.12
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	19	0.13	0.02	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	19	0.13	0.02	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	19	0.13	0.02	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	19	0.13	0.02	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	19	0.13	0.02	0.12
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	19	0.12	0.02	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	19	0.12	0.02	0.11
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	17	0.16	0.04	0.18
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	17	0.16	0.04	0.18
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	17	0.13	0.02	0.12
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	17	0.13	0.02	0.12
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	16	0.16	0.03	0.16
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	16	0.16	0.03	0.16
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	16	0.15	0.03	0.14
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	16	0.15	0.03	0.14
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	16	0.15	0.03	0.14
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	16	0.15	0.03	0.14
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	16	0.15	0.03	0.14
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	16	0.15	0.03	0.14
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	16	0.15	0.03	0.13
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	16	0.15	0.03	0.13
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	16	0.15	0.03	0.13
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	16	0.15	0.03	0.13
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	16	0.15	0.03	0.13
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	16	0.15	0.03	0.13
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	16	0.13	0.02	0.12
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	16	0.11	0.0	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	16	0.11	0.0	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	16	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	16	0.11	0.0	0.11
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	15	0.13	0.02	0.12
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	15	0.12	0.01	0.12
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	14	0.14	0.03	0.14
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	14	0.14	0.03	0.14
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	14	0.13	0.03	0.12
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	14	0.13	0.03	0.12
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	14	0.13	0.03	0.12
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	14	0.12	0.01	0.12
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	13	0.39	0.01	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	13	0.39	0.01	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	13	0.39	0.01	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	13	0.39	0.01	0.39
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	13	0.15	0.02	0.15
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	13	0.14	0.03	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	13	0.13	0.01	0.13
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	13	0.13	0.01	0.13
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	13	0.11	0.01	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	13	0.11	0.01	0.11
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	12	0.38	0.01	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	12	0.38	0.01	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	12	0.38	0.01	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	12	0.38	0.01	0.39
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	12	0.17	0.04	0.18
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	12	0.17	0.04	0.18
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	12	0.16	0.04	0.18
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	12	0.16	0.04	0.18
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	12	0.12	0.01	0.13
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	12	0.12	0.01	0.13
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	12	0.12	0.01	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	12	0.12	0.01	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	12	0.12	0.01	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	12	0.12	0.01	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	12	0.12	0.01	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	12	0.12	0.01	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	12	0.12	0.01	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	12	0.12	0.01	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	12	0.12	0.01	0.12
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	12	0.11	0.01	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	12	0.11	0.0	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	12	0.11	0.0	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	12	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	12	0.11	0.0	0.11
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	11	0.19	0.05	0.19
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	11	0.19	0.05	0.19
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	11	0.14	0.02	0.14
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	11	0.14	0.02	0.14
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	11	0.12	0.0	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	11	0.12	0.0	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	11	0.12	0.0	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	11	0.12	0.0	0.12
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	11	0.11	0.01	0.11
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	11	0.11	0.01	0.11
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	11	0.11	0.01	0.11
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	10	0.19	0.05	0.22
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	10	0.19	0.05	0.22
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	10	0.16	0.04	0.18
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	10	0.16	0.04	0.18
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	9	0.19	0.05	0.21
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	9	0.19	0.05	0.21
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	9	0.12	0.01	0.12
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	9	0.12	0.01	0.12
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	8	0.22	0.04	0.2
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	8	0.22	0.04	0.2
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	8	0.22	0.04	0.2
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	8	0.22	0.04	0.2
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	8	0.21	0.06	0.19
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	8	0.21	0.06	0.19
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	8	0.15	0.03	0.15
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	8	0.15	0.03	0.15
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	7	0.2	0.02	0.2
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	7	0.2	0.02	0.2
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	7	0.2	0.02	0.2
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	7	0.2	0.02	0.2
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	7	0.18	0.04	0.19
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	7	0.18	0.04	0.19
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	7	0.16	0.02	0.15
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	7	0.16	0.02	0.15
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	5	0.12	0.0	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	5	0.12	0.0	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	5	0.12	0.0	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	5	0.12	0.0	0.12
(1,77)	1:49:B:LYS:HG2	1:50:B:CYS:H	4	0.18	0.01	0.18
(1,77)	1:49:B:LYS:HG3	1:50:B:CYS:H	4	0.18	0.01	0.18

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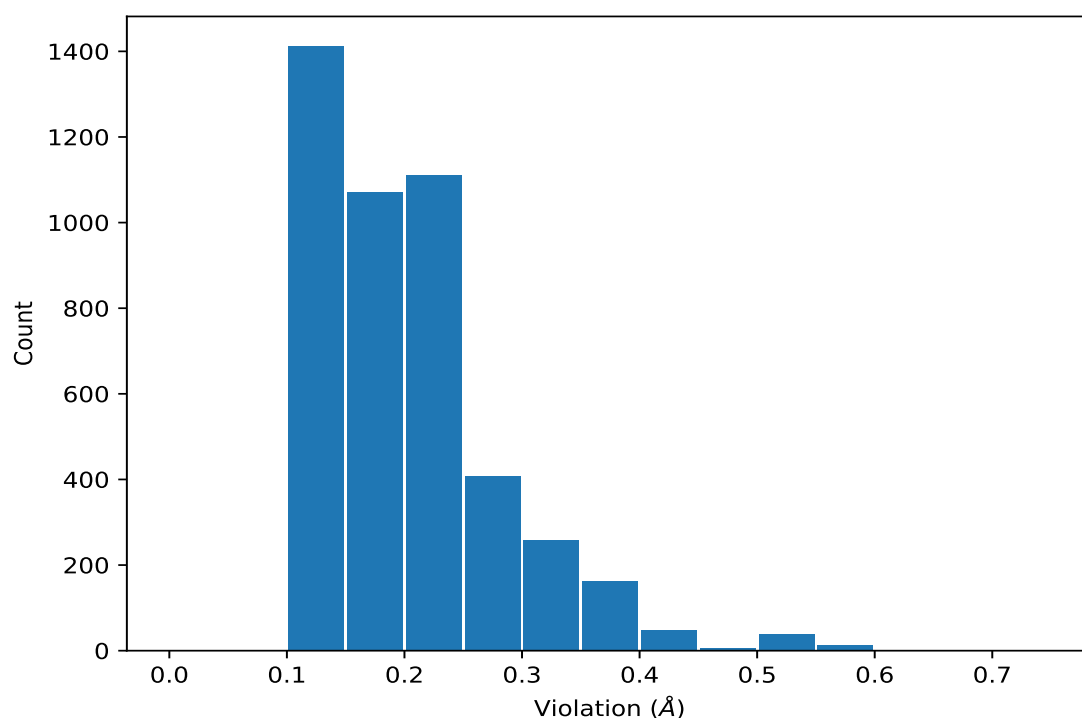
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,56)	1:41:B:ILE:HD11	1:42:B:TYR:H	4	0.12	0.01	0.12
(1,56)	1:41:B:ILE:HD12	1:42:B:TYR:H	4	0.12	0.01	0.12
(1,56)	1:41:B:ILE:HD13	1:42:B:TYR:H	4	0.12	0.01	0.12
(1,249)	1:36:B:LYS:H	1:35:B:LYS:H	3	0.31	0.0	0.31
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE21	3	0.22	0.0	0.22
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE22	3	0.22	0.0	0.22
(1,34)	1:17:A:LYS:HG2	1:18:A:CYS:H	3	0.15	0.01	0.16
(1,34)	1:17:A:LYS:HG3	1:18:A:CYS:H	3	0.15	0.01	0.16
(1,297)	1:19:A:GLN:HE21	1:10:A:TYR:H	3	0.15	0.01	0.16
(1,297)	1:19:A:GLN:HE22	1:10:A:TYR:H	3	0.15	0.01	0.16
(1,160)	1:21:A:MET:HB2	1:21:A:MET:H	3	0.14	0.01	0.13
(1,160)	1:21:A:MET:HB3	1:21:A:MET:H	3	0.14	0.01	0.13
(1,13)	1:9:A:ILE:HD11	1:10:A:TYR:H	3	0.12	0.01	0.12
(1,13)	1:9:A:ILE:HD12	1:10:A:TYR:H	3	0.12	0.01	0.12
(1,13)	1:9:A:ILE:HD13	1:10:A:TYR:H	3	0.12	0.01	0.12
(1,39)	1:19:A:GLN:HE21	1:20:A:ARG:H	3	0.12	0.0	0.12
(1,39)	1:19:A:GLN:HE22	1:20:A:ARG:H	3	0.12	0.0	0.12
(1,234)	1:53:B:MET:HB2	1:53:B:MET:H	2	0.24	0.04	0.24
(1,234)	1:53:B:MET:HB3	1:53:B:MET:H	2	0.24	0.04	0.24

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)
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	18	0.71
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	18	0.71
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	9	0.55
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	9	0.55
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	12	0.55
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	12	0.55
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	20	0.55
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	20	0.55
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	5	0.55
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	5	0.55
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	9	0.55
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	9	0.55
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	16	0.55
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	16	0.55
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	5	0.54
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	5	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	13	0.54
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	13	0.54
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	14	0.54
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	14	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	1	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	1	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	3	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	3	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	6	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	6	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	7	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	7	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	10	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	10	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	13	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	13	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	18	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	18	0.54
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	20	0.54
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	20	0.54
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	1	0.53
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	1	0.53
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	2	0.53
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	2	0.53
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	2	0.53
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	2	0.53
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	17	0.53
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	17	0.53
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	3	0.52
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	3	0.52
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	11	0.52
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	11	0.52
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	18	0.52
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	18	0.52
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	15	0.51
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	15	0.51
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	16	0.49
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	16	0.49
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	16	0.49
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	16	0.49
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	16	0.49
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	16	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	2	0.42
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	2	0.42
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	19	0.42
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	19	0.42
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	15	0.41
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	15	0.41
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	15	0.41
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	15	0.41
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	15	0.41
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	15	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	4	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	4	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	6	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	6	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	10	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	10	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	11	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	11	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	12	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	12	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	13	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	13	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	15	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	15	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	17	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	17	0.41
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	18	0.41
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	18	0.41
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	3	0.41
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	3	0.41
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	7	0.41
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	7	0.41
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	10	0.41
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	10	0.41
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	13	0.41
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	13	0.41
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	20	0.41
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	20	0.41
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	5	0.4
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	5	0.4
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	5	0.4
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	5	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	5	0.4
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	5	0.4
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	6	0.4
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	6	0.4
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	6	0.4
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	6	0.4
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	1	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	1	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	1	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	1	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	2	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	2	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	2	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	2	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	5	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	5	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	5	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	5	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	9	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	9	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	9	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	9	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	11	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	11	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	11	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	11	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	13	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	13	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	13	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	13	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	14	0.39
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	14	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	14	0.39
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	14	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	1	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	1	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	1	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	1	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	2	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	2	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	2	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	2	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	3	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	3	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	3	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	3	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	7	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	7	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	7	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	7	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	9	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	9	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	9	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	9	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	10	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	10	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	10	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	10	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	13	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	13	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	13	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	13	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	17	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	17	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	17	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	17	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	18	0.39
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	18	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	18	0.39
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	18	0.39
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	9	0.38
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	9	0.38
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	9	0.38
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	9	0.38
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	9	0.38
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	9	0.38
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	20	0.38
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	20	0.38
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	20	0.38
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	20	0.38
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	20	0.38
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	20	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	3	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	3	0.38
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	3	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	12	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	12	0.38
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	12	0.38
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	12	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	18	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	18	0.38
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	18	0.38
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	18	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	20	0.38
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	20	0.38
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	20	0.38
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	20	0.38
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	5	0.38
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	5	0.38
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	5	0.38
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	5	0.38
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	16	0.38
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	16	0.38
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	16	0.38
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	16	0.38
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE21	20	0.38
(1,339)	1:10:A:TYR:HD1	1:19:A:GLN:HE22	20	0.38
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE21	20	0.38
(1,339)	1:10:A:TYR:HD2	1:19:A:GLN:HE22	20	0.38
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	1	0.37
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	1	0.37
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	1	0.37
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	1	0.37
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	1	0.37
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	1	0.37
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	3	0.37
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	3	0.37
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	3	0.37
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	3	0.37
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	3	0.37
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	3	0.37
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	13	0.37
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	13	0.37
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	13	0.37
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	13	0.37
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	13	0.37
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	13	0.37
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	13	0.37
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	13	0.37
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	13	0.37
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	13	0.37
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	13	0.37
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	16	0.37
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	16	0.37
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	5	0.37
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	5	0.37
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	5	0.37
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	16	0.37
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	16	0.37
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	16	0.37
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	9	0.36
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	9	0.36
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	9	0.36
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	9	0.36
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	9	0.36
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	9	0.36
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	9	0.36
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	9	0.36
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	9	0.36
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	11	0.36
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	11	0.36
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	11	0.36
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	13	0.36
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	13	0.36
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	13	0.36
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	20	0.36
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	20	0.36
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	20	0.36
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE21	15	0.36
(1,358)	1:42:B:TYR:HD1	1:51:B:GLN:HE22	15	0.36
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE21	15	0.36
(1,358)	1:42:B:TYR:HD2	1:51:B:GLN:HE22	15	0.36
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	13	0.36
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	13	0.36
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	13	0.36
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	16	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	16	0.36
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	8	0.35
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	8	0.35
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	8	0.35
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	8	0.35
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	8	0.35
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	8	0.35
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	11	0.35
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	11	0.35
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	11	0.35
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	11	0.35
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	11	0.35
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	11	0.35
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	20	0.35
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	20	0.35
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	20	0.35
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	20	0.35
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	20	0.35
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	20	0.35
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	2	0.35
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	2	0.35
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	2	0.35
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	2	0.35
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	2	0.35
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	2	0.35
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	5	0.35
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	5	0.35
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	5	0.35
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	5	0.35
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	5	0.35
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	5	0.35
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	6	0.35
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	6	0.35
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	6	0.35
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	6	0.35
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	6	0.35
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	6	0.35
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	12	0.35
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	12	0.35
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	12	0.35
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	12	0.35
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	12	0.35
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	17	0.35
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	17	0.35
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	17	0.35
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	17	0.35
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	17	0.35
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	17	0.35
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	1	0.35
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	1	0.35
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	1	0.35
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	2	0.35
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	2	0.35
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	2	0.35
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	3	0.35
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	3	0.35
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	3	0.35
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	5	0.35
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	5	0.35
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	5	0.35
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	3	0.35
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	3	0.35
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	3	0.35
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	7	0.35
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	7	0.35
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	7	0.35
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	18	0.35
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	18	0.35
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	18	0.35
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	20	0.35
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	20	0.35
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	20	0.35
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	2	0.34
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	2	0.34
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	2	0.34
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	2	0.34
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	2	0.34
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	2	0.34
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	12	0.34
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	12	0.34
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	12	0.34
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	12	0.34
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	12	0.34
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	14	0.34
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	14	0.34
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	14	0.34
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	14	0.34
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	14	0.34
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	14	0.34
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	7	0.34
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	7	0.34
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	7	0.34
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	7	0.34
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	7	0.34
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	7	0.34
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	8	0.34
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	8	0.34
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	8	0.34
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	8	0.34
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	8	0.34
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	8	0.34
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	10	0.34
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	10	0.34
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	10	0.34
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	10	0.34
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	10	0.34
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	10	0.34
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	16	0.34
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	16	0.34
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	16	0.34
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	16	0.34
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	16	0.34
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	16	0.34
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	18	0.34
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	18	0.34
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	18	0.34
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	18	0.34
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	18	0.34
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	18	0.34
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	15	0.34
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	15	0.34
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	15	0.34
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	1	0.34
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	1	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	1	0.34
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	2	0.34
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	2	0.34
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	2	0.34
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	6	0.34
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	6	0.34
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	6	0.34
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	9	0.34
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	9	0.34
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	9	0.34
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	10	0.34
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	10	0.34
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	10	0.34
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	17	0.34
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	17	0.34
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	17	0.34
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	7	0.33
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	7	0.33
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	7	0.33
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	7	0.33
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	7	0.33
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	7	0.33
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	10	0.33
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	10	0.33
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	10	0.33
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	10	0.33
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	10	0.33
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	10	0.33
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	3	0.33
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	3	0.33
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	3	0.33
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	3	0.33
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	3	0.33
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	3	0.33
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	14	0.33
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	14	0.33
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	14	0.33
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	14	0.33
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	14	0.33
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	14	0.33
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	19	0.33
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	19	0.33
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	19	0.33
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	19	0.33
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	19	0.33
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	12	0.33
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	12	0.33
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	12	0.33
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	14	0.33
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	14	0.33
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	14	0.33
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	18	0.33
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	18	0.33
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	18	0.33
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	16	0.33
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	16	0.33
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	16	0.33
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	16	0.33
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	1	0.32
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	1	0.32
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	1	0.32
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	1	0.32
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	1	0.32
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	1	0.32
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	4	0.32
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	4	0.32
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	4	0.32
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	4	0.32
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	4	0.32
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	4	0.32
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	11	0.32
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	11	0.32
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	11	0.32
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	11	0.32
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	11	0.32
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	11	0.32
(1,385)	1:6:A:VAL:HG11	1:20:A:ARG:HE	15	0.32
(1,385)	1:6:A:VAL:HG12	1:20:A:ARG:HE	15	0.32
(1,385)	1:6:A:VAL:HG13	1:20:A:ARG:HE	15	0.32
(1,385)	1:6:A:VAL:HG21	1:20:A:ARG:HE	15	0.32
(1,385)	1:6:A:VAL:HG22	1:20:A:ARG:HE	15	0.32
(1,385)	1:6:A:VAL:HG23	1:20:A:ARG:HE	15	0.32
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	8	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	8	0.32
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	8	0.32
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	12	0.32
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	12	0.32
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	12	0.32
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	4	0.31
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	4	0.31
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	4	0.31
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	4	0.31
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	4	0.31
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	4	0.31
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	6	0.31
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	6	0.31
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	6	0.31
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	6	0.31
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	6	0.31
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	6	0.31
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	17	0.31
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	17	0.31
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	17	0.31
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	17	0.31
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	17	0.31
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	17	0.31
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	8	0.31
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	8	0.31
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	8	0.31
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	19	0.31
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	19	0.31
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	19	0.31
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	18	0.31
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	18	0.31
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	14	0.31
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	14	0.31
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	14	0.31
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	15	0.31
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	15	0.31
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	15	0.31
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	18	0.31
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	18	0.31
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	18	0.31
(1,249)	1:36:B:LYS:H	1:35:B:LYS:H	8	0.31
(1,249)	1:36:B:LYS:H	1:35:B:LYS:H	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:36:B:LYS:H	1:35:B:LYS:H	20	0.31
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	17	0.31
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	17	0.31
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	11	0.31
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	11	0.31
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	19	0.31
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	19	0.31
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	6	0.3
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	6	0.3
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	6	0.3
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	7	0.3
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	7	0.3
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	7	0.3
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	10	0.3
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	10	0.3
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	10	0.3
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	3	0.3
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	3	0.3
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	4	0.3
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	4	0.3
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	4	0.3
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	12	0.3
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	12	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	9	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	9	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	12	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	12	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	14	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	14	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	20	0.3
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	20	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	5	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	5	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	9	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	9	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	10	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	10	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	14	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	14	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	16	0.3
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	16	0.3
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	1	0.3
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	1	0.3
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	18	0.29
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	18	0.29
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	18	0.29
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	18	0.29
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	18	0.29
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	18	0.29
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	4	0.29
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	4	0.29
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	4	0.29
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	17	0.29
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	17	0.29
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	17	0.29
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	1	0.29
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	1	0.29
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	7	0.29
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	7	0.29
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	16	0.29
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	16	0.29
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	3	0.29
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	3	0.29
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	5	0.29
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	5	0.29
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	1	0.29
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	1	0.29
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	2	0.29
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	2	0.29
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	3	0.29
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	3	0.29
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	5	0.29
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	5	0.29
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	13	0.29
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	13	0.29
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	18	0.29
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	18	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	2	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	2	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	6	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	6	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	13	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	17	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	17	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	18	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	18	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	20	0.29
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	20	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	1	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	1	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	2	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	2	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	3	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	3	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	6	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	6	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	7	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	7	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	9	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	9	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	13	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	13	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	16	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	16	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	17	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	17	0.29
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	18	0.29
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	18	0.29
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	18	0.29
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	18	0.29
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	3	0.29
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	3	0.29
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	3	0.29
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	7	0.29
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	7	0.29
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	7	0.29
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	10	0.28
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	10	0.28
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	15	0.28
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	15	0.28
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	19	0.28
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	19	0.28
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	19	0.28
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	19	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	19	0.28
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	1	0.28
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	1	0.28
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	7	0.28
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	7	0.28
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	14	0.28
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	14	0.28
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	15	0.28
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	15	0.28
(1,234)	1:53:B:MET:HB2	1:53:B:MET:H	15	0.28
(1,234)	1:53:B:MET:HB3	1:53:B:MET:H	15	0.28
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	2	0.28
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	2	0.28
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	13	0.28
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	13	0.28
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	9	0.28
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	9	0.28
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	11	0.28
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	11	0.28
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	12	0.28
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	12	0.28
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	14	0.28
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	14	0.28
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	15	0.28
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	15	0.28
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	20	0.28
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	20	0.28
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	5	0.28
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	5	0.28
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	10	0.28
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	10	0.28
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	20	0.28
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	20	0.28
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	13	0.28
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	13	0.28
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	15	0.28
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	15	0.28
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	13	0.28
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	13	0.28
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	4	0.27
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	4	0.27
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	4	0.27
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	4	0.27
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	4	0.27
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	6	0.27
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	6	0.27
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	6	0.27
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	6	0.27
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	6	0.27
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	6	0.27
(1,388)	1:38:B:VAL:HG11	1:52:B:ARG:HE	19	0.27
(1,388)	1:38:B:VAL:HG12	1:52:B:ARG:HE	19	0.27
(1,388)	1:38:B:VAL:HG13	1:52:B:ARG:HE	19	0.27
(1,388)	1:38:B:VAL:HG21	1:52:B:ARG:HE	19	0.27
(1,388)	1:38:B:VAL:HG22	1:52:B:ARG:HE	19	0.27
(1,388)	1:38:B:VAL:HG23	1:52:B:ARG:HE	19	0.27
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	4	0.27
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	4	0.27
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	4	0.27
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	4	0.27
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	4	0.27
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	4	0.27
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	2	0.27
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	2	0.27
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	4	0.27
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	4	0.27
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	6	0.27
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	6	0.27
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	8	0.27
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	8	0.27
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	13	0.27
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	13	0.27
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	17	0.27
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	17	0.27
(1,344)	1:8:A:ILE:HD11	1:21:A:MET:H	11	0.27
(1,344)	1:8:A:ILE:HD12	1:21:A:MET:H	11	0.27
(1,344)	1:8:A:ILE:HD13	1:21:A:MET:H	11	0.27
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	2	0.27
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	2	0.27
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	4	0.27
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	4	0.27
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	11	0.27
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	18	0.27
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	18	0.27
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	19	0.27
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	19	0.27
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	20	0.27
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	20	0.27
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	11	0.27
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	11	0.27
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	10	0.27
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	10	0.27
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	15	0.27
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	15	0.27
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	15	0.27
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	19	0.27
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	19	0.27
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	19	0.27
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	1	0.27
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	1	0.27
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	3	0.27
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	3	0.27
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	7	0.27
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	7	0.27
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	12	0.27
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	12	0.27
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	7	0.26
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	7	0.26
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	7	0.26
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	7	0.26
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	7	0.26
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	7	0.26
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	8	0.26
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	8	0.26
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	8	0.26
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	8	0.26
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	8	0.26
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	8	0.26
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	10	0.26
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	10	0.26
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	10	0.26
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	10	0.26
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	10	0.26
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	10	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	17	0.26
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	17	0.26
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	17	0.26
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	17	0.26
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	17	0.26
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	17	0.26
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	8	0.26
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	8	0.26
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	8	0.26
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	8	0.26
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	8	0.26
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	8	0.26
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	11	0.26
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	11	0.26
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	11	0.26
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	11	0.26
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	11	0.26
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	11	0.26
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	19	0.26
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	19	0.26
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	19	0.26
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	19	0.26
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	19	0.26
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	19	0.26
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	8	0.26
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	8	0.26
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	5	0.26
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	5	0.26
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	11	0.26
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	11	0.26
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	8	0.26
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	8	0.26
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	13	0.26
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	13	0.26
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	16	0.26
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	16	0.26
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	16	0.26
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	16	0.26
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	1	0.26
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	1	0.26
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	5	0.26
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	9	0.26
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	9	0.26
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	14	0.26
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	14	0.26
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	15	0.26
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	15	0.26
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	12	0.25
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	12	0.25
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	12	0.25
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	12	0.25
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	12	0.25
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	12	0.25
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	14	0.25
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	14	0.25
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	14	0.25
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	14	0.25
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	14	0.25
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	14	0.25
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	15	0.25
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	15	0.25
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	15	0.25
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	15	0.25
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	15	0.25
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	15	0.25
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	15	0.25
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	15	0.25
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	15	0.25
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	15	0.25
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	8	0.25
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	8	0.25
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	16	0.25
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	16	0.25
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	9	0.25
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	9	0.25
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	12	0.25
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	12	0.25
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	14	0.25
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	14	0.25
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	15	0.25
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	15	0.25
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	6	0.25
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	17	0.25
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	17	0.25
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	1	0.25
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	1	0.25
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	1	0.25
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	2	0.25
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	2	0.25
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	2	0.25
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	4	0.25
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	4	0.25
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	4	0.25
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	7	0.25
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	7	0.25
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	7	0.25
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	10	0.25
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	10	0.25
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	10	0.25
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	11	0.25
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	11	0.25
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	11	0.25
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	16	0.25
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	16	0.25
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	16	0.25
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	2	0.25
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	2	0.25
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	2	0.25
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	4	0.25
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	4	0.25
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	4	0.25
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	7	0.25
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	7	0.25
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	7	0.25
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	11	0.25
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	11	0.25
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	11	0.25
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	17	0.25
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	17	0.25
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	17	0.25
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	16	0.25
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	3	0.25
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	3	0.25
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	18	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	18	0.25
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	6	0.25
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	6	0.25
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	7	0.25
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	7	0.25
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	8	0.25
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	8	0.25
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	9	0.25
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	9	0.25
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	15	0.25
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	15	0.25
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	19	0.25
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	19	0.25
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	9	0.25
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	9	0.25
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	9	0.25
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	12	0.25
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	12	0.25
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	12	0.25
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	14	0.25
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	14	0.25
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	14	0.25
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	1	0.25
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	1	0.25
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	8	0.25
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	8	0.25
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	11	0.25
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	11	0.25
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	20	0.25
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	20	0.25
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	9	0.25
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	9	0.25
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	9	0.25
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	5	0.25
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	5	0.25
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	9	0.25
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	9	0.25
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	9	0.24
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	9	0.24
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	18	0.24
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	18	0.24
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	5	0.24
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	10	0.24
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	10	0.24
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	10	0.24
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	10	0.24
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	15	0.24
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	15	0.24
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	20	0.24
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	20	0.24
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	3	0.24
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	3	0.24
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	8	0.24
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	8	0.24
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	12	0.24
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	12	0.24
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	15	0.24
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	15	0.24
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	8	0.24
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	8	0.24
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	5	0.24
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	5	0.24
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	10	0.24
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	10	0.24
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	16	0.24
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	16	0.24
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	19	0.24
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	19	0.24
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	4	0.24
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	4	0.24
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	8	0.24
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	8	0.24
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	10	0.24
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	10	0.24
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	4	0.24
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	4	0.24
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	12	0.24
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	12	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	3	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	3	0.24
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	3	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	5	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	5	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	6	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	6	0.24
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	6	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	13	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	13	0.24
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	13	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	17	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	17	0.24
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	17	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	18	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	18	0.24
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	18	0.24
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	19	0.24
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	19	0.24
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	19	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	1	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	1	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	1	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	6	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	6	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	6	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	12	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	12	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	12	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	13	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	13	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	13	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	14	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	14	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	14	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	15	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	15	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	15	0.24
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	19	0.24
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	19	0.24
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	19	0.24
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	9	0.24
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	9	0.24
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	1	0.24
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	1	0.24
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	2	0.24
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	3	0.24
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	3	0.24
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	16	0.24
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	16	0.24
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	17	0.24
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	17	0.24
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	18	0.24
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	18	0.24
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	5	0.24
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	5	0.24
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	5	0.24
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	5	0.24
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	5	0.24
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	3	0.24
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	3	0.24
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	5	0.24
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	5	0.24
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	10	0.24
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	10	0.24
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	19	0.24
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	19	0.24
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	5	0.24
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	5	0.24
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	5	0.24
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	10	0.24
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	10	0.24
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	10	0.24
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	16	0.23
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	16	0.23
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	20	0.23
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	20	0.23
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	6	0.23
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	6	0.23
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	6	0.23
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	8	0.23
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	8	0.23
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	8	0.23
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	17	0.23
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	17	0.23
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	17	0.23
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	19	0.23
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	19	0.23
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	8	0.23
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	8	0.23
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	9	0.23
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	9	0.23
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	4	0.23
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	4	0.23
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	19	0.23
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	19	0.23
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	4	0.23
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	4	0.23
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	5	0.23
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	5	0.23
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	7	0.23
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	7	0.23
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	18	0.23
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	18	0.23
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	20	0.23
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	20	0.23
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	4	0.23
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	4	0.23
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	4	0.23
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	4	0.23
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	14	0.23
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	14	0.23
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	20	0.23
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	20	0.23
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	9	0.23
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	9	0.23
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	8	0.23
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	8	0.23
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	6	0.23
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	6	0.23
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	14	0.23
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	14	0.23
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	8	0.23
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	8	0.23
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	8	0.23
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	8	0.23
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	8	0.23
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	3	0.23
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	3	0.23
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	9	0.23
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	9	0.23
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	9	0.23
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	20	0.23
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	20	0.23
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	20	0.23
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	4	0.23
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	6	0.23
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	7	0.23
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	8	0.23
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	10	0.23
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	17	0.23
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	19	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	3	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	4	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	7	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	8	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	11	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	12	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	14	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	15	0.23
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	19	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	4	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	4	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	6	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	6	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	7	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	7	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	10	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	10	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	19	0.23
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	19	0.23
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	20	0.23
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	20	0.23
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	4	0.23
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	4	0.23
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	11	0.23
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	11	0.23
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	12	0.23
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	13	0.23
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	13	0.23
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	14	0.23
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	14	0.23
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	3	0.23
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	3	0.23
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	3	0.23
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	8	0.23
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	8	0.23
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	8	0.23
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	20	0.23
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	20	0.23
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	20	0.23
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	4	0.23
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	4	0.23
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	8	0.23
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	8	0.23
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	15	0.23
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	15	0.23
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	15	0.23
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	15	0.23
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	16	0.23
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	16	0.23
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	2	0.23
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	2	0.23
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	4	0.23
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	4	0.23
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	6	0.23
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	6	0.23
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	7	0.23
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	7	0.23
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	17	0.23
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	17	0.23
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	8	0.23
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	8	0.23
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	8	0.23
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	1	0.23
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	1	0.23
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	3	0.23
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	3	0.23
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	9	0.23
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	17	0.23
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	17	0.23
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	17	0.23
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	17	0.23
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	17	0.23
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	17	0.23
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	18	0.23
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	18	0.23
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	11	0.23
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	11	0.23
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	11	0.23
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	11	0.23
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	11	0.23
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	11	0.23
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	18	0.23
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	18	0.23
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	18	0.23
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	18	0.23
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	18	0.23
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	18	0.23
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	19	0.23
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	19	0.23
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	19	0.23
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	19	0.23
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	19	0.23
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	19	0.23
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	20	0.22
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	20	0.22
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	4	0.22
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	4	0.22
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	4	0.22
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	7	0.22
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	7	0.22
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	7	0.22
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	10	0.22
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	10	0.22
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	10	0.22
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	16	0.22
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	16	0.22
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	16	0.22
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	8	0.22
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	16	0.22
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	4	0.22
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	4	0.22
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	4	0.22
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	9	0.22
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	9	0.22
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	9	0.22
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	12	0.22
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	12	0.22
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	12	0.22
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	14	0.22
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	14	0.22
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	14	0.22
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	19	0.22
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	19	0.22
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	19	0.22
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	18	0.22
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	6	0.22
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	6	0.22
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	7	0.22
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	7	0.22
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	8	0.22
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	8	0.22
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	2	0.22
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	2	0.22
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	6	0.22
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	6	0.22
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	18	0.22
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	18	0.22
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	19	0.22
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	19	0.22
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	12	0.22
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	12	0.22
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	14	0.22
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	14	0.22
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	1	0.22
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	1	0.22
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	7	0.22
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	7	0.22
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	8	0.22
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	8	0.22
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	15	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	15	0.22
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	19	0.22
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	19	0.22
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	12	0.22
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	12	0.22
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	7	0.22
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	7	0.22
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	18	0.22
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	5	0.22
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	5	0.22
(1,333)	1:9:A:ILE:HG12	1:19:A:GLN:H	10	0.22
(1,333)	1:9:A:ILE:HG13	1:19:A:GLN:H	10	0.22
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	3	0.22
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	3	0.22
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	12	0.22
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	12	0.22
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	11	0.22
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	11	0.22
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	8	0.22
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	8	0.22
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	8	0.22
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	8	0.22
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	10	0.22
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	10	0.22
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	10	0.22
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	10	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	7	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	7	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	15	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	15	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	17	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	17	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	19	0.22
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	19	0.22
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	12	0.22
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	12	0.22
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	12	0.22
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	12	0.22
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	8	0.22
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	8	0.22
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	11	0.22
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	8	0.22
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	8	0.22
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	10	0.22
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	10	0.22
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	10	0.22
(1,262)	1:52:B:ARG:H	1:51:B:GLN:HE21	17	0.22
(1,262)	1:52:B:ARG:H	1:51:B:GLN:HE22	17	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	1	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	2	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	3	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	5	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	9	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	11	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	12	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	13	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	14	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	15	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	18	0.22
(1,251)	1:41:B:ILE:H	1:42:B:TYR:H	20	0.22
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE21	11	0.22
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE22	11	0.22
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE21	14	0.22
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE22	14	0.22
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE21	19	0.22
(1,248)	1:20:A:ARG:H	1:19:A:GLN:HE22	19	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	1	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	2	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	5	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	6	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	9	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	10	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	13	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	16	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	17	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	18	0.22
(1,237)	1:9:A:ILE:H	1:10:A:TYR:H	20	0.22
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	8	0.22
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	8	0.22
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	15	0.22
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	15	0.22
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	1	0.22
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	1	0.22
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	11	0.22
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	11	0.22
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	11	0.22
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE21	12	0.22
(1,147)	1:19:A:GLN:HA	1:19:A:GLN:HE22	12	0.22
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	8	0.22
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	8	0.22
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	13	0.22
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	13	0.22
(1,127)	1:12:A:ASN:HD21	1:12:A:ASN:H	16	0.22
(1,127)	1:12:A:ASN:HD22	1:12:A:ASN:H	16	0.22
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	15	0.22
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	15	0.22
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	15	0.22
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	18	0.22
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	18	0.22
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	18	0.22
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	20	0.22
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	20	0.22
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	20	0.22
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	7	0.22
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	7	0.22
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	11	0.22
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	11	0.22
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	17	0.22
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	17	0.22
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	20	0.22
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	20	0.22
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	1	0.22
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	1	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	1	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	1	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	1	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	1	0.22
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	3	0.22
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	3	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	3	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	3	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	3	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	3	0.22
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	7	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	7	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	7	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	7	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	7	0.22
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	18	0.22
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	18	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	18	0.22
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	18	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	18	0.22
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	18	0.22
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	4	0.22
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	4	0.22
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	6	0.22
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	6	0.22
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	8	0.22
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	8	0.22
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	10	0.22
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	10	0.22
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	16	0.22
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	16	0.22
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	20	0.22
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	20	0.22
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	12	0.22
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	12	0.22
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	12	0.22
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	12	0.22
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	12	0.22
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	12	0.22
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	14	0.22
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	14	0.22
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	14	0.22
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	14	0.22
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	14	0.22
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	14	0.22
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	16	0.22
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	16	0.22
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	16	0.22
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	16	0.22
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	16	0.22
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	16	0.22
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	5	0.21
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	8	0.21
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	8	0.21
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	10	0.21
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	10	0.21
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	12	0.21
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	12	0.21
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	14	0.21
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	14	0.21
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	1	0.21
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	1	0.21
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	1	0.21
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	2	0.21
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	2	0.21
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	2	0.21
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	5	0.21
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	5	0.21
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	5	0.21
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	11	0.21
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	11	0.21
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	11	0.21
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	13	0.21
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	13	0.21
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	13	0.21
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	20	0.21
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	20	0.21
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	20	0.21
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	4	0.21
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	6	0.21
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	7	0.21
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	10	0.21
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	17	0.21
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	19	0.21
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	12	0.21
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	12	0.21
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	14	0.21
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	14	0.21
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	20	0.21
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	20	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	2	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	2	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	7	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	7	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	7	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	10	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	10	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	10	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	11	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	11	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	11	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	13	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	13	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	13	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	17	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	17	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	17	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	18	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	18	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	18	0.21
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	20	0.21
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	20	0.21
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	20	0.21
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	4	0.21
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	11	0.21
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	12	0.21
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	14	0.21
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	1	0.21
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	1	0.21
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	3	0.21
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	3	0.21
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	9	0.21
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	9	0.21
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	11	0.21
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	11	0.21
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	12	0.21
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	12	0.21
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	14	0.21
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	14	0.21
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	17	0.21
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	17	0.21
(1,352)	1:41:B:ILE:HG12	1:51:B:GLN:H	9	0.21
(1,352)	1:41:B:ILE:HG13	1:51:B:GLN:H	9	0.21
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	4	0.21
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	10	0.21
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	10	0.21
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	11	0.21
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	11	0.21
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	11	0.21
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	11	0.21
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	17	0.21
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	17	0.21
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	9	0.21
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	9	0.21
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	12	0.21
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	12	0.21
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	14	0.21
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	14	0.21
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	14	0.21
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	14	0.21
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	1	0.21
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	1	0.21
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	3	0.21
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	3	0.21
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	11	0.21
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	11	0.21
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	19	0.21
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	19	0.21
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	9	0.21
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	9	0.21
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	9	0.21
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	1	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	1	0.21
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	2	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	2	0.21
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	6	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	6	0.21
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	7	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	7	0.21
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	11	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	11	0.21
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	14	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	14	0.21
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	19	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	20	0.21
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	20	0.21
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	6	0.21
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	6	0.21
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	17	0.21
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	17	0.21
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	4	0.21
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	4	0.21
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	4	0.21
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	4	0.21
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	5	0.21
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	5	0.21
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	4	0.21
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	4	0.21
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	4	0.21
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	4	0.21
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	8	0.21
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	8	0.21
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	8	0.21
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	8	0.21
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	15	0.21
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	15	0.21
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	19	0.21
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	19	0.21
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	20	0.21
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	20	0.21
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	15	0.21
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	15	0.21
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	15	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	1	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	1	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	3	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	3	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	5	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	5	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	7	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	7	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	8	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	8	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	9	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	9	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	14	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	14	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	16	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	16	0.21
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	20	0.21
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	20	0.21
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	12	0.21
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	12	0.21
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	15	0.21
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	15	0.21
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	11	0.21
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	11	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	1	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	1	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	2	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	2	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	4	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	4	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	5	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	5	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	6	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	6	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	8	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	8	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	9	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	9	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	11	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	11	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	12	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	12	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	14	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	14	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	15	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	15	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	16	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	16	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	17	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	17	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	18	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	18	0.21
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	19	0.21
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	19	0.21
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	12	0.21
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	14	0.21
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	14	0.21
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	13	0.21
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	13	0.21
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	13	0.21
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	18	0.21
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	18	0.21
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	18	0.21
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	9	0.21
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	9	0.21
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	2	0.21
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	2	0.21
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	2	0.21
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	13	0.21
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	13	0.21
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	13	0.21
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	17	0.21
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	17	0.21
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	17	0.21
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	19	0.21
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	19	0.21
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	19	0.21
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	2	0.21
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	2	0.21
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	4	0.21
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	4	0.21
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	6	0.21
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	6	0.21
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	8	0.21
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	8	0.21
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	10	0.21
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	10	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	2	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	2	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	2	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	2	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	2	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	2	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	4	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	4	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	4	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	4	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	4	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	6	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	6	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	6	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	6	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	6	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	6	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	8	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	8	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	8	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	8	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	8	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	8	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	13	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	13	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	13	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	13	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	13	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	13	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	20	0.21
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	20	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	20	0.21
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	20	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	20	0.21
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	20	0.21
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	2	0.21
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	2	0.21
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	5	0.21
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	5	0.21
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	11	0.21
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	11	0.21
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	17	0.21
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	17	0.21
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	19	0.21
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	19	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	2	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	2	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	2	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	2	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	2	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	3	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	3	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	3	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	3	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	3	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	3	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	4	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	4	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	4	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	4	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	4	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	4	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	6	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	6	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	6	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	6	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	6	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	6	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	13	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	13	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	13	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	13	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	13	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	13	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	15	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	15	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	15	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	15	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	15	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	15	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	20	0.21
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	20	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	20	0.21
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	20	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	20	0.21
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	20	0.21
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	6	0.2
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	6	0.2
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	6	0.2
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	6	0.2
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	6	0.2
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	9	0.2
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	9	0.2
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	9	0.2
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	9	0.2
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	9	0.2
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	9	0.2
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	19	0.2
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	19	0.2
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	19	0.2
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	19	0.2
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	19	0.2
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	19	0.2
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	1	0.2
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	1	0.2
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	7	0.2
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	7	0.2
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	18	0.2
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	18	0.2
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	19	0.2
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	19	0.2
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	3	0.2
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	3	0.2
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	3	0.2
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	15	0.2
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	15	0.2
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	15	0.2
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	18	0.2
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	18	0.2
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	18	0.2
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	14	0.2
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	14	0.2
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	11	0.2
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	11	0.2
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	1	0.2
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	1	0.2
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	1	0.2
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	3	0.2
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	3	0.2
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	3	0.2
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	6	0.2
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	6	0.2
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	19	0.2
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	17	0.2
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	17	0.2
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	13	0.2
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	13	0.2
(1,360)	1:42:B:TYR:HE1	1:52:B:ARG:HE	20	0.2
(1,360)	1:42:B:TYR:HE2	1:52:B:ARG:HE	20	0.2
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	2	0.2
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	2	0.2
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	5	0.2
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	5	0.2
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	13	0.2
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	13	0.2
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	2	0.2
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	2	0.2
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	6	0.2
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	6	0.2
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	8	0.2
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	8	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	2	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	2	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	5	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	5	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	6	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	6	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	9	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	9	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	10	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	10	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	13	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	13	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	16	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	16	0.2
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	17	0.2
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	17	0.2
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	4	0.2
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	4	0.2
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	10	0.2
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	10	0.2
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	13	0.2
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	15	0.2
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	15	0.2
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	17	0.2
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	17	0.2
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	2	0.2
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	2	0.2
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	6	0.2
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	6	0.2
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	6	0.2
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	6	0.2
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	7	0.2
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	7	0.2
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	7	0.2
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	7	0.2
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	11	0.2
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	11	0.2
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	18	0.2
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	18	0.2
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	14	0.2
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	14	0.2
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	14	0.2
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	14	0.2
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	15	0.2
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	15	0.2
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	15	0.2
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	15	0.2
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	6	0.2
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	6	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	1	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	1	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	3	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	3	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	5	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	5	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	7	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	7	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	8	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	8	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	9	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	9	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	14	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	14	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	16	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	16	0.2
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	20	0.2
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	20	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	1	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	1	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	2	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	2	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	4	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	4	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	5	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	5	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	6	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	6	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	8	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	8	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	9	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	9	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	12	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	12	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	14	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	14	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	15	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	15	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	16	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	16	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	17	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	17	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	18	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	18	0.2
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	19	0.2
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	19	0.2
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	11	0.2
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	11	0.2
(1,234)	1:53:B:MET:HB2	1:53:B:MET:H	5	0.2
(1,234)	1:53:B:MET:HB3	1:53:B:MET:H	5	0.2
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	4	0.2
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	4	0.2
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	7	0.2
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	7	0.2
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	19	0.2
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	5	0.2
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	5	0.2
(1,201)	1:44:B:ASN:HD21	1:44:B:ASN:H	20	0.2
(1,201)	1:44:B:ASN:HD22	1:44:B:ASN:H	20	0.2
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	2	0.2
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	2	0.2
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	2	0.2
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	10	0.2
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	10	0.2
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	10	0.2
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	17	0.2
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	17	0.2
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	17	0.2
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	4	0.2
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	4	0.2
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	15	0.2
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	15	0.2
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	12	0.2
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	12	0.2
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	12	0.2
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	14	0.2
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	14	0.2
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	14	0.2
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	12	0.2
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	12	0.2
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	14	0.2
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	14	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	10	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	10	0.2
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	10	0.2
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	10	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	10	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	10	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	11	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	11	0.2
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	11	0.2
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	11	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	11	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	11	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	15	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	15	0.2
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	15	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	15	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	15	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	19	0.2
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	19	0.2
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	19	0.2
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	19	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	19	0.2
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	19	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	4	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	4	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	7	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	7	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	17	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	17	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	19	0.2
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	19	0.2
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	11	0.2
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	11	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	1	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	1	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	1	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	1	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	1	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	1	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	5	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	5	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	5	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	5	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	5	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	5	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	7	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	7	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	7	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	7	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	7	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	7	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	8	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	8	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	8	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	8	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	8	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	17	0.2
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	17	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	17	0.2
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	17	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	17	0.2
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	17	0.2
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	4	0.2
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	4	0.2
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	11	0.2
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	11	0.2
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	19	0.2
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	19	0.2
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	4	0.19
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	4	0.19
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	4	0.19
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	4	0.19
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	4	0.19
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	4	0.19
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	8	0.19
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	8	0.19
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	8	0.19
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	8	0.19
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	8	0.19
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	8	0.19
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	10	0.19
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	10	0.19
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	10	0.19
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	10	0.19
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	10	0.19
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	10	0.19
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	12	0.19
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	12	0.19
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	12	0.19
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	12	0.19
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	12	0.19
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	12	0.19
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	14	0.19
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	14	0.19
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	14	0.19
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	14	0.19
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	14	0.19
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	16	0.19
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	16	0.19
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	16	0.19
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	16	0.19
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	16	0.19
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	16	0.19
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	4	0.19
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	4	0.19
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	4	0.19
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	4	0.19
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	4	0.19
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	4	0.19
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	8	0.19
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	8	0.19
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	8	0.19
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	8	0.19
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	8	0.19
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	8	0.19
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	12	0.19
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	12	0.19
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	12	0.19
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	12	0.19
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	12	0.19
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	12	0.19
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	15	0.19
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	15	0.19
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	15	0.19
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	15	0.19
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	15	0.19
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	15	0.19
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	5	0.19
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	5	0.19
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	5	0.19
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	5	0.19
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	5	0.19
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	5	0.19
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	9	0.19
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	9	0.19
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	9	0.19
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	9	0.19
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	9	0.19
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	10	0.19
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	10	0.19
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	10	0.19
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	10	0.19
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	10	0.19
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	10	0.19
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	9	0.19
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	9	0.19
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	17	0.19
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	17	0.19
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	2	0.19
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	2	0.19
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	3	0.19
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	3	0.19
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	6	0.19
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	6	0.19
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	15	0.19
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	15	0.19
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	17	0.19
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	17	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	2	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	5	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	9	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	11	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	15	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	16	0.19
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	18	0.19
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	12	0.19
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	12	0.19
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	16	0.19
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	16	0.19
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	1	0.19
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	1	0.19
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	3	0.19
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	3	0.19
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	19	0.19
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	19	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	1	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	2	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	6	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	9	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	10	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	15	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	17	0.19
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	20	0.19
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	6	0.19
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	6	0.19
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	17	0.19
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	17	0.19
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	6	0.19
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	6	0.19
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	13	0.19
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	13	0.19
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	4	0.19
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	4	0.19
(1,341)	1:10:A:TYR:HE1	1:20:A:ARG:HE	18	0.19
(1,341)	1:10:A:TYR:HE2	1:20:A:ARG:HE	18	0.19
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	9	0.19
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	9	0.19
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	16	0.19
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	16	0.19
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	13	0.19
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	13	0.19
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	18	0.19
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	18	0.19
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	4	0.19
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	4	0.19
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	15	0.19
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	15	0.19
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	19	0.19
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	19	0.19
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	19	0.19
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	19	0.19
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	1	0.19
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	1	0.19
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	2	0.19
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	2	0.19
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	3	0.19
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	3	0.19
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	18	0.19
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	18	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	6	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	7	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	7	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	9	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	9	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	17	0.19
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	17	0.19
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	4	0.19
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	4	0.19
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	10	0.19
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	10	0.19
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	19	0.19
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	19	0.19
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	4	0.19
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	4	0.19
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	6	0.19
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	6	0.19
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	7	0.19
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	7	0.19
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	10	0.19
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	10	0.19
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	19	0.19
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	19	0.19
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	20	0.19
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	20	0.19
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	20	0.19
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	4	0.19
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	4	0.19
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	4	0.19
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	4	0.19
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	8	0.19
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	8	0.19
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	15	0.19
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	15	0.19
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	16	0.19
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	16	0.19
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	16	0.19
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	2	0.19
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	2	0.19
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	10	0.19
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	10	0.19
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	17	0.19
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	19	0.19
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	19	0.19
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	6	0.19
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	6	0.19
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	8	0.19
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	8	0.19
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	10	0.19
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	10	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	1	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	1	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	3	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	3	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	8	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	8	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	18	0.19
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	18	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	1	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	1	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	1	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	1	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	2	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	2	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	2	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	2	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	3	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	3	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	3	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	3	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	4	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	4	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	4	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	4	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	5	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	5	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	5	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	5	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	6	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	6	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	6	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	6	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	7	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	7	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	7	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	8	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	8	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	8	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	8	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	9	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	9	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	9	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	9	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	10	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	10	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	10	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	10	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	11	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	11	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	11	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	11	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	12	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	12	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	12	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	12	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	13	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	13	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	13	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	13	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	14	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	14	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	14	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	14	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	15	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	15	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	15	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	15	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	16	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	16	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	16	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	16	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	17	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	17	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	17	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	18	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	18	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	18	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	18	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	19	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	19	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	19	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	19	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE1	20	0.19
(1,196)	1:42:B:TYR:HD1	1:42:B:TYR:HE2	20	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE1	20	0.19
(1,196)	1:42:B:TYR:HD2	1:42:B:TYR:HE2	20	0.19
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	7	0.19
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	7	0.19
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	7	0.19
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	8	0.19
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	8	0.19
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	12	0.19
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	12	0.19
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	12	0.19
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	12	0.19
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	14	0.19
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	14	0.19
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	20	0.19
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	20	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	1	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	1	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	1	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	1	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	2	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	2	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	2	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	2	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	3	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	3	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	3	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	3	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	4	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	4	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	4	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	5	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	5	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	5	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	5	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	6	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	6	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	6	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	6	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	7	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	7	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	7	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	7	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	8	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	8	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	8	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	8	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	9	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	9	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	9	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	9	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	10	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	10	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	10	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	10	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	11	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	11	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	11	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	11	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	12	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	12	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	12	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	12	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	13	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	13	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	13	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	13	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	14	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	14	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	14	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	14	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	15	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	15	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	15	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	16	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	16	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	16	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	16	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	17	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	17	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	17	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	17	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	18	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	18	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	18	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	18	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	19	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	19	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	19	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	19	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE1	20	0.19
(1,122)	1:10:A:TYR:HD1	1:10:A:TYR:HE2	20	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE1	20	0.19
(1,122)	1:10:A:TYR:HD2	1:10:A:TYR:HE2	20	0.19
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	6	0.19
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	6	0.19
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	6	0.19
(1,77)	1:49:B:LYS:HG2	1:50:B:CYS:H	9	0.19
(1,77)	1:49:B:LYS:HG3	1:50:B:CYS:H	9	0.19
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	11	0.19
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	11	0.19
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	5	0.19
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	5	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	5	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	5	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	5	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	5	0.19
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	9	0.19
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	9	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	9	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	9	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	9	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	9	0.19
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	12	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	12	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	12	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	12	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	12	0.19
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	14	0.19
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	14	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	14	0.19
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	14	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	14	0.19
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	14	0.19
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	6	0.19
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	6	0.19
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	15	0.19
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	15	0.19
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	20	0.19
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	20	0.19
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	2	0.19
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	2	0.19
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	10	0.19
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	10	0.19
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	17	0.19
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	17	0.19
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	19	0.19
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	19	0.19
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	9	0.19
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	9	0.19
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	9	0.19
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	9	0.19
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	9	0.19
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	9	0.19
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE1	10	0.19
(1,20)	1:9:A:ILE:HD11	1:10:A:TYR:HE2	10	0.19
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE1	10	0.19
(1,20)	1:9:A:ILE:HD12	1:10:A:TYR:HE2	10	0.19
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE1	10	0.19
(1,20)	1:9:A:ILE:HD13	1:10:A:TYR:HE2	10	0.19
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	8	0.19
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	8	0.19
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	7	0.18
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	7	0.18
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	7	0.18
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	7	0.18
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	7	0.18
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	17	0.18
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	17	0.18
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	17	0.18
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	17	0.18
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	17	0.18
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	17	0.18
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	19	0.18
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	19	0.18
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	19	0.18
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	19	0.18
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	19	0.18
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	19	0.18
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	5	0.18
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	5	0.18
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	5	0.18
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	5	0.18
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	5	0.18
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	5	0.18
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	20	0.18
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	20	0.18
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	20	0.18
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	20	0.18
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	20	0.18
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	20	0.18
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	11	0.18
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	11	0.18
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	11	0.18
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	11	0.18
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	11	0.18
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	11	0.18
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	14	0.18
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	14	0.18
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	14	0.18
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	14	0.18
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	14	0.18
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	14	0.18
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	17	0.18
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	17	0.18
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	17	0.18
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	17	0.18
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	17	0.18
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	6	0.18
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	6	0.18
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	12	0.18
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	12	0.18
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	14	0.18
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	14	0.18
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	13	0.18
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	13	0.18
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	1	0.18
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	3	0.18
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	13	0.18
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	5	0.18
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	5	0.18
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	19	0.18
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	19	0.18
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	2	0.18
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	2	0.18
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	10	0.18
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	10	0.18
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	13	0.18
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	13	0.18
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	18	0.18
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	18	0.18
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	3	0.18
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	5	0.18
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	7	0.18
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	13	0.18
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	12	0.18
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	12	0.18
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	1	0.18
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	1	0.18
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	18	0.18
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	18	0.18
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	19	0.18
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	19	0.18
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	10	0.18
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	10	0.18
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	17	0.18
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	19	0.18
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	19	0.18
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	19	0.18
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	19	0.18
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	5	0.18
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	5	0.18
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	20	0.18
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	20	0.18
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	5	0.18
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	5	0.18
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	14	0.18
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	14	0.18
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	19	0.18
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	19	0.18
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD1	17	0.18
(1,318)	1:51:B:GLN:HB2	1:42:B:TYR:HD2	17	0.18
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD1	17	0.18
(1,318)	1:51:B:GLN:HB3	1:42:B:TYR:HD2	17	0.18
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	13	0.18
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	13	0.18
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	11	0.18
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	11	0.18
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	11	0.18
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	11	0.18
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	11	0.18
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	11	0.18
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	1	0.18
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	1	0.18
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	2	0.18
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	2	0.18
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	3	0.18
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	3	0.18
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	7	0.18
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	7	0.18
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	8	0.18
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	8	0.18
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	14	0.18
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	14	0.18
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	14	0.18
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	12	0.18
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	12	0.18
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	5	0.18
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	5	0.18
(1,274)	1:15:A:THR:HG21	1:14:A:ALA:H	8	0.18
(1,274)	1:15:A:THR:HG22	1:14:A:ALA:H	8	0.18
(1,274)	1:15:A:THR:HG23	1:14:A:ALA:H	8	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	1	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	1	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	2	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	2	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	3	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	3	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	7	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	7	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	9	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	9	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	11	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	11	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	12	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	12	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	13	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	13	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	17	0.18
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	17	0.18
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	5	0.18
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	5	0.18
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	6	0.18
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	6	0.18
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	13	0.18
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	13	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	7	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	7	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	10	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	10	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	13	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	13	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	15	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	15	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	17	0.18
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	17	0.18
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	4	0.18
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	4	0.18
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:40:B:ILE:HD11	1:40:B:ILE:H	6	0.18
(1,180)	1:40:B:ILE:HD12	1:40:B:ILE:H	6	0.18
(1,180)	1:40:B:ILE:HD13	1:40:B:ILE:H	6	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	1	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	1	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	3	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	3	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	11	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	11	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	13	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	13	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	19	0.18
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	19	0.18
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	4	0.18
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	4	0.18
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	4	0.18
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	11	0.18
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	11	0.18
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	11	0.18
(1,106)	1:8:A:ILE:HD11	1:8:A:ILE:H	16	0.18
(1,106)	1:8:A:ILE:HD12	1:8:A:ILE:H	16	0.18
(1,106)	1:8:A:ILE:HD13	1:8:A:ILE:H	16	0.18
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	16	0.18
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	16	0.18
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	19	0.18
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	19	0.18
(1,77)	1:49:B:LYS:HG2	1:50:B:CYS:H	20	0.18
(1,77)	1:49:B:LYS:HG3	1:50:B:CYS:H	20	0.18
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	2	0.18
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	2	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	1	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	1	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	2	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	2	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	3	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	3	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	7	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	7	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	9	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	9	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	11	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	12	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	12	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	13	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	13	0.18
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	17	0.18
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	17	0.18
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	8	0.18
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	8	0.18
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	10	0.18
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	10	0.18
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	1	0.18
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	1	0.18
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	3	0.18
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	3	0.18
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	7	0.18
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	7	0.18
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	12	0.18
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	12	0.18
(1,42)	1:20:A:ARG:HD2	1:21:A:MET:H	14	0.18
(1,42)	1:20:A:ARG:HD3	1:21:A:MET:H	14	0.18
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	5	0.18
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	5	0.18
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	6	0.18
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	6	0.18
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	13	0.18
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	13	0.18
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	15	0.18
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	15	0.18
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	11	0.17
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	11	0.17
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	11	0.17
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	11	0.17
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	11	0.17
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	11	0.17
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	13	0.17
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	13	0.17
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	13	0.17
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	13	0.17
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	13	0.17
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	13	0.17
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	19	0.17
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	19	0.17
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	19	0.17
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	19	0.17
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	19	0.17
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	6	0.17
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	6	0.17
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	6	0.17
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	6	0.17
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	6	0.17
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	6	0.17
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	13	0.17
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	13	0.17
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	13	0.17
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	13	0.17
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	13	0.17
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	13	0.17
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	19	0.17
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	19	0.17
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	4	0.17
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	4	0.17
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	11	0.17
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	11	0.17
(1,379)	1:44:B:ASN:HD21	1:46:B:ALA:H	16	0.17
(1,379)	1:44:B:ASN:HD22	1:46:B:ALA:H	16	0.17
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	12	0.17
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	14	0.17
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	4	0.17
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	4	0.17
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	6	0.17
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	6	0.17
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	7	0.17
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	7	0.17
(1,369)	1:12:A:ASN:HD21	1:14:A:ALA:H	17	0.17
(1,369)	1:12:A:ASN:HD22	1:14:A:ALA:H	17	0.17
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	3	0.17
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	15	0.17
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	14	0.17
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	14	0.17
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	9	0.17
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	3	0.17
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	3	0.17
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	20	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	20	0.17
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	11	0.17
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	11	0.17
(1,330)	1:11:A:CYS:HB2	1:18:A:CYS:H	8	0.17
(1,330)	1:11:A:CYS:HB3	1:18:A:CYS:H	8	0.17
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	8	0.17
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	8	0.17
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	10	0.17
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	10	0.17
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	12	0.17
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	12	0.17
(1,313)	1:51:B:GLN:HE21	1:42:B:TYR:H	17	0.17
(1,313)	1:51:B:GLN:HE22	1:42:B:TYR:H	17	0.17
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD1	19	0.17
(1,302)	1:19:A:GLN:HB2	1:10:A:TYR:HD2	19	0.17
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD1	19	0.17
(1,302)	1:19:A:GLN:HB3	1:10:A:TYR:HD2	19	0.17
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	10	0.17
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	10	0.17
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	13	0.17
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	13	0.17
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	12	0.17
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	12	0.17
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	12	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	2	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	2	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	4	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	4	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	6	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	6	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	10	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	10	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	11	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	11	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	12	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	12	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	13	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	13	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	17	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	17	0.17
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	18	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	19	0.17
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	19	0.17
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	3	0.17
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	3	0.17
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	7	0.17
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	7	0.17
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	10	0.17
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	10	0.17
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	13	0.17
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	13	0.17
(1,263)	1:5:A:PRO:HB2	1:4:A:LYS:H	20	0.17
(1,263)	1:5:A:PRO:HB3	1:4:A:LYS:H	20	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	4	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	4	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	14	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	14	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	18	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	18	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	19	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	19	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	20	0.17
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	20	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	1	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	1	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	3	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	3	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	4	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	4	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	9	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	9	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	16	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	16	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	18	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	18	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	20	0.17
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	20	0.17
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	17	0.17
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	17	0.17
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	2	0.17
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	2	0.17
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	6	0.17
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	19	0.17
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	19	0.17
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	11	0.17
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	11	0.17
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	14	0.17
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	14	0.17
(1,145)	1:19:A:GLN:HB2	1:19:A:GLN:H	19	0.17
(1,145)	1:19:A:GLN:HB3	1:19:A:GLN:H	19	0.17
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	2	0.17
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	2	0.17
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	10	0.17
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	10	0.17
(1,77)	1:49:B:LYS:HG2	1:50:B:CYS:H	12	0.17
(1,77)	1:49:B:LYS:HG3	1:50:B:CYS:H	12	0.17
(1,77)	1:49:B:LYS:HG2	1:50:B:CYS:H	14	0.17
(1,77)	1:49:B:LYS:HG3	1:50:B:CYS:H	14	0.17
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	14	0.17
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	14	0.17
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	16	0.17
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	16	0.17
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	20	0.17
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	20	0.17
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	4	0.17
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	4	0.17
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	14	0.17
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	14	0.17
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	18	0.17
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	18	0.17
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	19	0.17
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	19	0.17
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	20	0.17
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	20	0.17
(1,62)	1:41:B:ILE:HB	1:42:B:TYR:HE1	16	0.17
(1,62)	1:41:B:ILE:HB	1:42:B:TYR:HE2	16	0.17
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	17	0.17
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	17	0.17
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	1	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	1	0.17
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	3	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	3	0.17
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	4	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	9	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	9	0.17
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	16	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	16	0.17
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	18	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	18	0.17
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	20	0.17
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	20	0.17
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	12	0.17
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	12	0.17
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	2	0.16
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	2	0.16
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	2	0.16
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	2	0.16
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	2	0.16
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	2	0.16
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	2	0.16
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	2	0.16
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	2	0.16
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	2	0.16
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	2	0.16
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	2	0.16
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	16	0.16
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	16	0.16
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	16	0.16
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	16	0.16
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	16	0.16
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	16	0.16
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	18	0.16
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	18	0.16
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	18	0.16
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	18	0.16
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	18	0.16
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	18	0.16
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	20	0.16
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	20	0.16
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	20	0.16
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	20	0.16
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	20	0.16
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	20	0.16
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	20	0.16
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	12	0.16
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	12	0.16
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	12	0.16
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	14	0.16
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	14	0.16
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	14	0.16
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	8	0.16
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	8	0.16
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	8	0.16
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	15	0.16
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	15	0.16
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	15	0.16
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	16	0.16
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	16	0.16
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	16	0.16
(1,367)	1:15:A:THR:HB	1:13:A:ALA:H	16	0.16
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	1	0.16
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	11	0.16
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	18	0.16
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	20	0.16
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	20	0.16
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	12	0.16
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	14	0.16
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	4	0.16
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	4	0.16
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	7	0.16
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	7	0.16
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	15	0.16
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	15	0.16
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	15	0.16
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	15	0.16
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	1	0.16
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	7	0.16
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	5	0.16
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	3	0.16
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	3	0.16
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	4	0.16
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	4	0.16
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	9	0.16
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	9	0.16
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	14	0.16
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	15	0.16
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	15	0.16
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	11	0.16
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	11	0.16
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	16	0.16
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	16	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	9	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	9	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	12	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	12	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	14	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	14	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD1	20	0.16
(1,316)	1:51:B:GLN:HA	1:42:B:TYR:HD2	20	0.16
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	2	0.16
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	2	0.16
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	17	0.16
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	17	0.16
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	19	0.16
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	19	0.16
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	18	0.16
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	18	0.16
(1,297)	1:19:A:GLN:HE21	1:10:A:TYR:H	11	0.16
(1,297)	1:19:A:GLN:HE22	1:10:A:TYR:H	11	0.16
(1,297)	1:19:A:GLN:HE21	1:10:A:TYR:H	19	0.16
(1,297)	1:19:A:GLN:HE22	1:10:A:TYR:H	19	0.16
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	6	0.16
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	6	0.16
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	10	0.16
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	10	0.16
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	13	0.16
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	13	0.16
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	17	0.16
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	17	0.16
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	18	0.16
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	18	0.16
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	19	0.16
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	19	0.16
(1,279)	1:37:B:PRO:HB2	1:36:B:LYS:H	15	0.16
(1,279)	1:37:B:PRO:HB3	1:36:B:LYS:H	15	0.16
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	7	0.16
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	10	0.16
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	10	0.16
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	13	0.16
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	13	0.16
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	5	0.16
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	5	0.16
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	6	0.16
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	6	0.16
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	10	0.16
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	10	0.16
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	7	0.16
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	7	0.16
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	14	0.16
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	14	0.16
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	15	0.16
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	15	0.16
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	16	0.16
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	16	0.16
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	6	0.16
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	6	0.16
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	7	0.16
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	7	0.16
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	17	0.16
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	17	0.16
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	9	0.16
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	9	0.16
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	1	0.16
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	1	0.16
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	5	0.16
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	5	0.16
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	6	0.16
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	6	0.16
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	10	0.16
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	10	0.16
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	20	0.16
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	20	0.16
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	20	0.16
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	20	0.16
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	20	0.16
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	20	0.16
(1,34)	1:17:A:LYS:HG2	1:18:A:CYS:H	5	0.16
(1,34)	1:17:A:LYS:HG3	1:18:A:CYS:H	5	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:17:A:LYS:HG2	1:18:A:CYS:H	16	0.16
(1,34)	1:17:A:LYS:HG3	1:18:A:CYS:H	16	0.16
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	5	0.16
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	5	0.16
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	16	0.16
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	16	0.16
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	14	0.16
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	14	0.16
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	7	0.16
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	7	0.16
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	14	0.16
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	14	0.16
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	15	0.16
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	15	0.16
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	5	0.16
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	5	0.16
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	5	0.16
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	5	0.16
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	5	0.16
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	5	0.16
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	16	0.16
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	16	0.16
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	16	0.16
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	16	0.16
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	16	0.16
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	16	0.16
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	18	0.16
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	18	0.16
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	18	0.16
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	18	0.16
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	18	0.16
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	18	0.16
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	14	0.16
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	14	0.16
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	1	0.15
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	1	0.15
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	1	0.15
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	1	0.15
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	1	0.15
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	1	0.15
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	15	0.15
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	15	0.15
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	15	0.15
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	15	0.15
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	15	0.15
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	9	0.15
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	9	0.15
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	12	0.15
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	12	0.15
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	14	0.15
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	14	0.15
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	20	0.15
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	20	0.15
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	5	0.15
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	5	0.15
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	16	0.15
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	16	0.15
(1,368)	1:15:A:THR:HG21	1:13:A:ALA:H	5	0.15
(1,368)	1:15:A:THR:HG22	1:13:A:ALA:H	5	0.15
(1,368)	1:15:A:THR:HG23	1:13:A:ALA:H	5	0.15
(1,363)	1:40:B:ILE:HD11	1:53:B:MET:H	16	0.15
(1,363)	1:40:B:ILE:HD12	1:53:B:MET:H	16	0.15
(1,363)	1:40:B:ILE:HD13	1:53:B:MET:H	16	0.15
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	2	0.15
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	9	0.15
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	13	0.15
(1,349)	1:43:B:CYS:HB2	1:50:B:CYS:H	9	0.15
(1,349)	1:43:B:CYS:HB3	1:50:B:CYS:H	9	0.15
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	11	0.15
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	11	0.15
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	11	0.15
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	19	0.15
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	19	0.15
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	19	0.15
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	20	0.15
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	20	0.15
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	20	0.15
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	3	0.15
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	8	0.15
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	10	0.15
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	1	0.15
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	1	0.15
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	7	0.15
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	9	0.15
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	9	0.15
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	2	0.15
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	2	0.15
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	17	0.15
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	17	0.15
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	6	0.15
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	6	0.15
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	5	0.15
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	5	0.15
(1,290)	1:47:B:THR:HG21	1:46:B:ALA:H	9	0.15
(1,290)	1:47:B:THR:HG22	1:46:B:ALA:H	9	0.15
(1,290)	1:47:B:THR:HG23	1:46:B:ALA:H	9	0.15
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	2	0.15
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	2	0.15
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	4	0.15
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	4	0.15
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	11	0.15
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	11	0.15
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	12	0.15
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	12	0.15
(1,281)	1:37:B:PRO:HG2	1:36:B:LYS:H	15	0.15
(1,281)	1:37:B:PRO:HG3	1:36:B:LYS:H	15	0.15
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	14	0.15
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	14	0.15
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	3	0.15
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	3	0.15
(1,265)	1:5:A:PRO:HG2	1:4:A:LYS:H	20	0.15
(1,265)	1:5:A:PRO:HG3	1:4:A:LYS:H	20	0.15
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	8	0.15
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	8	0.15
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD1	15	0.15
(1,253)	1:43:B:CYS:H	1:42:B:TYR:HD2	15	0.15
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	8	0.15
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	8	0.15
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD1	12	0.15
(1,239)	1:11:A:CYS:H	1:10:A:TYR:HD2	12	0.15
(1,235)	1:4:A:LYS:H	1:3:A:LYS:H	13	0.15
(1,219)	1:51:B:GLN:HB2	1:51:B:GLN:H	16	0.15
(1,219)	1:51:B:GLN:HB3	1:51:B:GLN:H	16	0.15
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	4	0.15
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD21	11	0.15
(1,202)	1:44:B:ASN:HA	1:44:B:ASN:HD22	11	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	1	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	1	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	2	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	2	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	3	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	3	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	4	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	4	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	5	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	5	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	6	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	6	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	7	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	7	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	8	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	8	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	9	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	9	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	10	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	10	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	11	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	11	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	12	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	12	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	13	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	13	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	14	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	14	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	15	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	15	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	16	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	16	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	17	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	17	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	18	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	18	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	19	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	19	0.15
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE1	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,193)	1:42:B:TYR:HA	1:42:B:TYR:HE2	20	0.15
(1,160)	1:21:A:MET:HB2	1:21:A:MET:H	3	0.15
(1,160)	1:21:A:MET:HB3	1:21:A:MET:H	3	0.15
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	18	0.15
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD21	4	0.15
(1,128)	1:12:A:ASN:HA	1:12:A:ASN:HD22	4	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	1	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	1	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	2	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	2	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	3	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	3	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	4	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	4	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	5	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	5	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	6	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	6	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	7	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	7	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	8	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	8	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	9	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	9	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	10	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	10	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	12	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	12	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	13	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	13	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	14	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	14	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	15	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	15	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	16	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	16	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	17	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	17	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	18	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	18	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	20	0.15
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:52:B:ARG:HD2	1:53:B:MET:H	18	0.15
(1,85)	1:52:B:ARG:HD3	1:53:B:MET:H	18	0.15
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	12	0.15
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	12	0.15
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	17	0.15
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	17	0.15
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	6	0.15
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	6	0.15
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	17	0.15
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	17	0.15
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	19	0.15
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	19	0.15
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	8	0.15
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	8	0.15
(1,64)	1:42:B:TYR:HD1	1:43:B:CYS:H	15	0.15
(1,64)	1:42:B:TYR:HD2	1:43:B:CYS:H	15	0.15
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	9	0.15
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	9	0.15
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	9	0.15
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	9	0.15
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	9	0.15
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	9	0.15
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	12	0.15
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	12	0.15
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	12	0.15
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	12	0.15
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	12	0.15
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	12	0.15
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	14	0.15
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	14	0.15
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	14	0.15
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	14	0.15
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	14	0.15
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	14	0.15
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	12	0.15
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	12	0.15
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	14	0.15
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	14	0.15
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	19	0.15
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	19	0.15
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	12	0.15
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	8	0.15
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	8	0.15
(1,21)	1:10:A:TYR:HD1	1:11:A:CYS:H	12	0.15
(1,21)	1:10:A:TYR:HD2	1:11:A:CYS:H	12	0.15
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	12	0.14
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	12	0.14
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	12	0.14
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	12	0.14
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	12	0.14
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	12	0.14
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	14	0.14
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	14	0.14
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	14	0.14
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	14	0.14
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	14	0.14
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	14	0.14
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	15	0.14
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	15	0.14
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	15	0.14
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	15	0.14
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	15	0.14
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	15	0.14
(1,389)	1:38:B:VAL:HG11	1:41:B:ILE:H	3	0.14
(1,389)	1:38:B:VAL:HG12	1:41:B:ILE:H	3	0.14
(1,389)	1:38:B:VAL:HG13	1:41:B:ILE:H	3	0.14
(1,389)	1:38:B:VAL:HG21	1:41:B:ILE:H	3	0.14
(1,389)	1:38:B:VAL:HG22	1:41:B:ILE:H	3	0.14
(1,389)	1:38:B:VAL:HG23	1:41:B:ILE:H	3	0.14
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	8	0.14
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	8	0.14
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	8	0.14
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	8	0.14
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	15	0.14
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	15	0.14
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	6	0.14
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	6	0.14
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	6	0.14
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	19	0.14
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	19	0.14
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	19	0.14
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	5	0.14
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	5	0.14
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	5	0.14
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	8	0.14
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	8	0.14
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	7	0.14
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	7	0.14
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	4	0.14
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	4	0.14
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	4	0.14
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	2	0.14
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	6	0.14
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	17	0.14
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	9	0.14
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	18	0.14
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	9	0.14
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	12	0.14
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	14	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	1	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	1	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	7	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	7	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	13	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	13	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	18	0.14
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	18	0.14
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	9	0.14
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	10	0.14
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	13	0.14
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	13	0.14
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	20	0.14
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	20	0.14
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD1	16	0.14
(1,300)	1:19:A:GLN:HA	1:10:A:TYR:HD2	16	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	1	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	3	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	4	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	5	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	6	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	7	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	8	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	9	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	11	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	12	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	13	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	14	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	16	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	17	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	18	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	19	0.14
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	20	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	1	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	2	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	3	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	4	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	5	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	6	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	7	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	8	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	9	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	10	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	11	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	12	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	13	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	14	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	15	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	16	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	17	0.14
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	19	0.14
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	11	0.14
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	11	0.14
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE1	19	0.14
(1,119)	1:10:A:TYR:HA	1:10:A:TYR:HE2	19	0.14
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	19	0.14
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	19	0.14
(1,75)	1:49:B:LYS:HB2	1:50:B:CYS:H	16	0.14
(1,75)	1:49:B:LYS:HB3	1:50:B:CYS:H	16	0.14
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	2	0.14
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	2	0.14
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	2	0.14
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	2	0.14
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	2	0.14
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	2	0.14
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	13	0.14
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	13	0.14
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	13	0.14
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	13	0.14
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	13	0.14
(1,34)	1:17:A:LYS:HG2	1:18:A:CYS:H	8	0.14
(1,34)	1:17:A:LYS:HG3	1:18:A:CYS:H	8	0.14
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	20	0.14
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	20	0.14
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	18	0.14
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	18	0.14
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	19	0.14
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	19	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	2	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	2	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	2	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	2	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	2	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	2	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	6	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	6	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	6	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	6	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	6	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	6	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	10	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	10	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	10	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	10	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	10	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	10	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	13	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	13	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	13	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	13	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	13	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	13	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	17	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	17	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	17	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	17	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	17	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	20	0.14
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	20	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	20	0.14
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	20	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	20	0.14
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	20	0.14
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	1	0.13
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	1	0.13
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	1	0.13
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	1	0.13
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	1	0.13
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	1	0.13
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	7	0.13
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	7	0.13
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	7	0.13
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	7	0.13
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	7	0.13
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	7	0.13
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	10	0.13
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	10	0.13
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	10	0.13
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	10	0.13
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	10	0.13
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	10	0.13
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	7	0.13
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	7	0.13
(1,378)	1:47:B:THR:HG21	1:45:B:ALA:H	9	0.13
(1,378)	1:47:B:THR:HG22	1:45:B:ALA:H	9	0.13
(1,378)	1:47:B:THR:HG23	1:45:B:ALA:H	9	0.13
(1,377)	1:47:B:THR:HB	1:45:B:ALA:H	20	0.13
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	11	0.13
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	11	0.13
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	4	0.13
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	4	0.13
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	4	0.13
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	8	0.13
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	8	0.13
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	8	0.13
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	12	0.13
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	12	0.13
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	14	0.13
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	14	0.13
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	14	0.13
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	17	0.13
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	17	0.13
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	17	0.13
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	20	0.13
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	20	0.13
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	20	0.13
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	16	0.13
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	5	0.13
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	15	0.13
(1,347)	1:42:B:TYR:HE1	1:50:B:CYS:H	10	0.13
(1,347)	1:42:B:TYR:HE2	1:50:B:CYS:H	10	0.13
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	18	0.13
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	18	0.13
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	18	0.13
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	5	0.13
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	13	0.13
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	6	0.13
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	16	0.13
(1,328)	1:10:A:TYR:HE1	1:18:A:CYS:H	12	0.13
(1,328)	1:10:A:TYR:HE2	1:18:A:CYS:H	12	0.13
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	20	0.13
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	20	0.13
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	4	0.13
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	10	0.13
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	3	0.13
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	3	0.13
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	6	0.13
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	6	0.13
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	19	0.13
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	19	0.13
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	4	0.13
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	5	0.13
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	6	0.13
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	8	0.13
(1,297)	1:19:A:GLN:HE21	1:10:A:TYR:H	14	0.13
(1,297)	1:19:A:GLN:HE22	1:10:A:TYR:H	14	0.13
(1,294)	1:51:B:GLN:HG2	1:50:B:CYS:H	17	0.13
(1,294)	1:51:B:GLN:HG3	1:50:B:CYS:H	17	0.13
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	19	0.13
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	4	0.13
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	4	0.13
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	8	0.13
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	2	0.13
(1,209)	1:47:B:THR:HA	1:47:B:THR:H	15	0.13
(1,160)	1:21:A:MET:HB2	1:21:A:MET:H	1	0.13
(1,160)	1:21:A:MET:HB3	1:21:A:MET:H	1	0.13
(1,160)	1:21:A:MET:HB2	1:21:A:MET:H	7	0.13
(1,160)	1:21:A:MET:HB3	1:21:A:MET:H	7	0.13
(1,135)	1:15:A:THR:HA	1:15:A:THR:H	20	0.13
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	6	0.13
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	6	0.13
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE1	16	0.13
(1,63)	1:41:B:ILE:HD11	1:42:B:TYR:HE2	16	0.13
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE1	16	0.13
(1,63)	1:41:B:ILE:HD12	1:42:B:TYR:HE2	16	0.13
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE1	16	0.13
(1,63)	1:41:B:ILE:HD13	1:42:B:TYR:HE2	16	0.13
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	2	0.13
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	2	0.13
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	2	0.13
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	2	0.13
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	9	0.13
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	9	0.13
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	9	0.13
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	9	0.13
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	11	0.13
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	11	0.13
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	11	0.13
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	11	0.13
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	1	0.13
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	1	0.13
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	1	0.13
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	1	0.13
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	1	0.13
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	1	0.13
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	11	0.13
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	11	0.13
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	11	0.13
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	11	0.13
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	11	0.13
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	17	0.13
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	17	0.13
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	17	0.13
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	17	0.13
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	17	0.13
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	17	0.13
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	18	0.13
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	18	0.13
(1,56)	1:41:B:ILE:HD11	1:42:B:TYR:H	9	0.13
(1,56)	1:41:B:ILE:HD12	1:42:B:TYR:H	9	0.13
(1,56)	1:41:B:ILE:HD13	1:42:B:TYR:H	9	0.13
(1,56)	1:41:B:ILE:HD11	1:42:B:TYR:H	12	0.13
(1,56)	1:41:B:ILE:HD12	1:42:B:TYR:H	12	0.13
(1,56)	1:41:B:ILE:HD13	1:42:B:TYR:H	12	0.13
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	2	0.13
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	2	0.13
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	2	0.13
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	2	0.13
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	19	0.13
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	19	0.13
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	19	0.13
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	19	0.13
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	15	0.13
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	15	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	5	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	5	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	5	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	5	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	10	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	10	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	10	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	10	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	16	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	16	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	16	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	16	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	18	0.13
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	18	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	18	0.13
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	18	0.13
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	9	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	9	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	9	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	9	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	9	0.13
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	11	0.13
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	11	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	11	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	11	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	11	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	11	0.13
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	19	0.13
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	19	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	19	0.13
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	19	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	19	0.13
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	19	0.13
(1,13)	1:9:A:ILE:HD11	1:10:A:TYR:H	5	0.13
(1,13)	1:9:A:ILE:HD12	1:10:A:TYR:H	5	0.13
(1,13)	1:9:A:ILE:HD13	1:10:A:TYR:H	5	0.13
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	13	0.13
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	13	0.13
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	13	0.13
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	13	0.13
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	5	0.12
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	5	0.12
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	5	0.12
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	5	0.12
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	5	0.12
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	5	0.12
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	9	0.12
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	9	0.12
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	9	0.12
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	9	0.12
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	9	0.12
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	9	0.12
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	11	0.12
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	11	0.12
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	11	0.12
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	11	0.12
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	11	0.12
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	5	0.12
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	5	0.12
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	5	0.12
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	5	0.12
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	5	0.12
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	5	0.12
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	17	0.12
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	17	0.12
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	17	0.12
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	17	0.12
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	17	0.12
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	17	0.12
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	7	0.12
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	7	0.12
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	7	0.12
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	7	0.12
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	7	0.12
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	7	0.12
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	13	0.12
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	13	0.12
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	18	0.12
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	18	0.12
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	9	0.12
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	9	0.12
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	10	0.12
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	10	0.12
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	13	0.12
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	13	0.12
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	11	0.12
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	11	0.12
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	9	0.12
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	9	0.12
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	9	0.12
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	12	0.12
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	14	0.12
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	4	0.12
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	8	0.12
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	10	0.12
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	13	0.12
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	5	0.12
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	5	0.12
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	11	0.12
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	13	0.12
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	13	0.12
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	6	0.12
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	6	0.12
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	6	0.12
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	8	0.12
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	8	0.12
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	8	0.12
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	10	0.12
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	16	0.12
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	4	0.12
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	13	0.12
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	15	0.12
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	6	0.12
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	6	0.12
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	7	0.12
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	7	0.12
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	13	0.12
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	13	0.12
(1,327)	1:10:A:TYR:HD1	1:18:A:CYS:H	17	0.12
(1,327)	1:10:A:TYR:HD2	1:18:A:CYS:H	17	0.12
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	5	0.12
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	6	0.12
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	8	0.12
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	13	0.12
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	20	0.12
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	4	0.12
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	4	0.12
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	11	0.12
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	11	0.12
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	13	0.12
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	17	0.12
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	1	0.12
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	1	0.12
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	4	0.12
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	4	0.12
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	9	0.12
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	9	0.12
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	6	0.12
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	9	0.12
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	14	0.12
(1,278)	1:19:A:GLN:HG2	1:18:A:CYS:H	11	0.12
(1,278)	1:19:A:GLN:HG3	1:18:A:CYS:H	11	0.12
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	5	0.12
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	8	0.12
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	18	0.12
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	6	0.12
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	7	0.12
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	8	0.12
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	10	0.12
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	16	0.12
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	17	0.12
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	11	0.12
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	15	0.12
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	19	0.12
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE21	16	0.12
(1,221)	1:51:B:GLN:HA	1:51:B:GLN:HE22	16	0.12
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	7	0.12
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	7	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	1	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	1	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	3	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	3	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	5	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	5	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	7	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	7	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	8	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	8	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	9	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	9	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	14	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	14	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	16	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	16	0.12
(1,166)	1:36:B:LYS:HB2	1:36:B:LYS:H	20	0.12
(1,166)	1:36:B:LYS:HB3	1:36:B:LYS:H	20	0.12
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	11	0.12
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	11	0.12
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	19	0.12
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	19	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	1	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	2	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	2	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	4	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	4	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	5	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	5	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	6	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	6	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	8	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	8	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	9	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	9	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	11	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	11	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	12	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	12	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	14	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	14	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	15	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	15	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	16	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	16	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	17	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	17	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	18	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	18	0.12
(1,92)	1:4:A:LYS:HB2	1:4:A:LYS:H	19	0.12
(1,92)	1:4:A:LYS:HB3	1:4:A:LYS:H	19	0.12
(1,82)	1:51:B:GLN:HE21	1:52:B:ARG:H	17	0.12
(1,82)	1:51:B:GLN:HE22	1:52:B:ARG:H	17	0.12
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	7	0.12
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	7	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	1	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	1	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	1	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	1	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	12	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	12	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	12	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	12	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	13	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	13	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	13	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	14	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	14	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	14	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	14	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	20	0.12
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	20	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	20	0.12
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	20	0.12
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	3	0.12
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	3	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	3	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	3	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	3	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	3	0.12
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	5	0.12
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	5	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	5	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	5	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	5	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	5	0.12
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	18	0.12
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	18	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	18	0.12
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	18	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	18	0.12
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	18	0.12
(1,56)	1:41:B:ILE:HD11	1:42:B:TYR:H	14	0.12
(1,56)	1:41:B:ILE:HD12	1:42:B:TYR:H	14	0.12
(1,56)	1:41:B:ILE:HD13	1:42:B:TYR:H	14	0.12
(1,56)	1:41:B:ILE:HD11	1:42:B:TYR:H	20	0.12
(1,56)	1:41:B:ILE:HD12	1:42:B:TYR:H	20	0.12
(1,56)	1:41:B:ILE:HD13	1:42:B:TYR:H	20	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	4	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	4	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	4	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	4	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	6	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	6	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	6	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	10	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	10	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	10	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	10	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	11	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	11	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	11	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	11	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	12	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	12	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	12	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	12	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	13	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	13	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	13	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	13	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	15	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	15	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	15	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	15	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	17	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	17	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	17	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	17	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD2	18	0.12
(1,47)	1:36:B:LYS:HG2	1:37:B:PRO:HD3	18	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD2	18	0.12
(1,47)	1:36:B:LYS:HG3	1:37:B:PRO:HD3	18	0.12
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	10	0.12
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	10	0.12
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	10	0.12
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	10	0.12
(1,39)	1:19:A:GLN:HE21	1:20:A:ARG:H	11	0.12
(1,39)	1:19:A:GLN:HE22	1:20:A:ARG:H	11	0.12
(1,39)	1:19:A:GLN:HE21	1:20:A:ARG:H	14	0.12
(1,39)	1:19:A:GLN:HE22	1:20:A:ARG:H	14	0.12
(1,39)	1:19:A:GLN:HE21	1:20:A:ARG:H	19	0.12
(1,39)	1:19:A:GLN:HE22	1:20:A:ARG:H	19	0.12
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	8	0.12
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	8	0.12
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	11	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	2	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	2	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	2	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	2	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	3	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	3	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	3	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	3	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	6	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	6	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	6	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	6	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	13	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	13	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	13	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	13	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	17	0.12
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	17	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	17	0.12
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	17	0.12
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	1	0.12
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	1	0.12
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	1	0.12
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	1	0.12
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	1	0.12
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	1	0.12
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	3	0.12
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	3	0.12
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	3	0.12
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	3	0.12
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	3	0.12
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	3	0.12
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	7	0.12
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	7	0.12
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	7	0.12
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	7	0.12
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	7	0.12
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	7	0.12
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	16	0.12
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	16	0.12
(1,13)	1:9:A:ILE:HD11	1:10:A:TYR:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:9:A:ILE:HD12	1:10:A:TYR:H	9	0.12
(1,13)	1:9:A:ILE:HD13	1:10:A:TYR:H	9	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	3	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	3	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	3	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	3	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	7	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	7	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	7	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	7	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	10	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	10	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	10	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	10	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD2	20	0.12
(1,4)	1:4:A:LYS:HG2	1:5:A:PRO:HD3	20	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD2	20	0.12
(1,4)	1:4:A:LYS:HG3	1:5:A:PRO:HD3	20	0.12
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	13	0.12
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	13	0.12
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	13	0.12
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	13	0.12
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	2	0.11
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	2	0.11
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	2	0.11
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	2	0.11
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	2	0.11
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	2	0.11
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	20	0.11
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	20	0.11
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	20	0.11
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	20	0.11
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	20	0.11
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	20	0.11
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	3	0.11
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	3	0.11
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	3	0.11
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	3	0.11
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	3	0.11
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	3	0.11
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	6	0.11
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	6	0.11
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	6	0.11
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	6	0.11
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	6	0.11
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	4	0.11
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	4	0.11
(1,383)	1:49:B:LYS:HG2	1:44:B:ASN:H	10	0.11
(1,383)	1:49:B:LYS:HG3	1:44:B:ASN:H	10	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	1	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	1	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	2	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	2	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	3	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	3	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	4	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	4	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	5	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	5	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	6	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	6	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	7	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	7	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	8	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	8	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	15	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	15	0.11
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	17	0.11
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	17	0.11
(1,373)	1:17:A:LYS:HG2	1:12:A:ASN:H	4	0.11
(1,373)	1:17:A:LYS:HG3	1:12:A:ASN:H	4	0.11
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	1	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	1	0.11
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	2	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	2	0.11
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	3	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	3	0.11
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	4	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	4	0.11
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	6	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	6	0.11
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	7	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	11	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	11	0.11
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	19	0.11
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	19	0.11
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	9	0.11
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	9	0.11
(1,364)	1:40:B:ILE:HG12	1:53:B:MET:H	13	0.11
(1,364)	1:40:B:ILE:HG13	1:53:B:MET:H	13	0.11
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	5	0.11
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	5	0.11
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	5	0.11
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	7	0.11
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	7	0.11
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	7	0.11
(1,357)	1:44:B:ASN:H	1:51:B:GLN:H	20	0.11
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	11	0.11
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	5	0.11
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	5	0.11
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	10	0.11
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	10	0.11
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	10	0.11
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	14	0.11
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	14	0.11
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	14	0.11
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	16	0.11
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	16	0.11
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	16	0.11
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	17	0.11
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	17	0.11
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	17	0.11
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	9	0.11
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	1	0.11
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	2	0.11
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	3	0.11
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	7	0.11
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	17	0.11
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	19	0.11
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	10	0.11
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	10	0.11
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE1	20	0.11
(1,321)	1:50:B:CYS:HA	1:42:B:TYR:HE2	20	0.11
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	15	0.11
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	16	0.11
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	18	0.11
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	20	0.11
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	10	0.11
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	10	0.11
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	16	0.11
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	16	0.11
(1,293)	1:51:B:GLN:HB2	1:50:B:CYS:H	17	0.11
(1,293)	1:51:B:GLN:HB3	1:50:B:CYS:H	17	0.11
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	4	0.11
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	8	0.11
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	10	0.11
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	11	0.11
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	19	0.11
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	20	0.11
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	11	0.11
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	11	0.11
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	14	0.11
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	14	0.11
(1,277)	1:19:A:GLN:HB2	1:18:A:CYS:H	19	0.11
(1,277)	1:19:A:GLN:HB3	1:18:A:CYS:H	19	0.11
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	4	0.11
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	10	0.11
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	15	0.11
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	17	0.11
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	12	0.11
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	14	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	1	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	1	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	3	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	3	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	4	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	4	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	6	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	6	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	8	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	8	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	10	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	10	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	17	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	18	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	18	0.11
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	19	0.11
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	19	0.11
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	4	0.11
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	4	0.11
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	12	0.11
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	12	0.11
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	14	0.11
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	14	0.11
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	15	0.11
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	15	0.11
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	1	0.11
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	1	0.11
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	4	0.11
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	4	0.11
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	8	0.11
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	8	0.11
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	10	0.11
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	10	0.11
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	11	0.11
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	11	0.11
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	15	0.11
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	15	0.11
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	18	0.11
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	18	0.11
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	3	0.11
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	3	0.11
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	3	0.11
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	3	0.11
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	5	0.11
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	5	0.11
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	5	0.11
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	5	0.11
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	15	0.11
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	15	0.11
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	15	0.11
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	15	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	4	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	4	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	4	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	4	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	4	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	6	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	6	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	6	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	6	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	6	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	6	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	7	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	7	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	7	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	7	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	7	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	7	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	15	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	15	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	15	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	15	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	15	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	15	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	19	0.11
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	19	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	19	0.11
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	19	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	19	0.11
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	19	0.11
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	1	0.11
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	1	0.11
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	2	0.11
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	2	0.11
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	3	0.11
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	3	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	1	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	1	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	1	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	1	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	3	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	3	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	3	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	3	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	5	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	5	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	5	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	7	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	7	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	7	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	7	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	8	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	8	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	8	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	8	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	9	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	9	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	9	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	9	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	14	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	14	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	14	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	14	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	15	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	15	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	15	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	15	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	16	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	16	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	16	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	16	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	20	0.11
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	20	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	20	0.11
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	20	0.11
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	3	0.11
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	3	0.11
(1,33)	1:17:A:LYS:HD2	1:18:A:CYS:H	4	0.11
(1,33)	1:17:A:LYS:HD3	1:18:A:CYS:H	4	0.11
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	6	0.11
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	6	0.11
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	1	0.11
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	1	0.11
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	1	0.11
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	1	0.11
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	7	0.11
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	7	0.11
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	7	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	4	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	4	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	4	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	4	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	4	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	4	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	8	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	8	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	8	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	8	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	8	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	8	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	14	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	14	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	14	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	14	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	14	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	14	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	15	0.11
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	15	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	15	0.11
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	15	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	15	0.11
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	15	0.11
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	2	0.11
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	2	0.11
(1,13)	1:9:A:ILE:HD11	1:10:A:TYR:H	10	0.11
(1,13)	1:9:A:ILE:HD12	1:10:A:TYR:H	10	0.11
(1,13)	1:9:A:ILE:HD13	1:10:A:TYR:H	10	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	1	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	1	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	1	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	1	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	2	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	2	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	2	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	2	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	4	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	4	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	4	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	5	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	5	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	5	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	5	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	6	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	6	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	6	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	6	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	8	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	8	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	8	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	8	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	9	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	9	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	9	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	9	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	11	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	11	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	11	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	11	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	12	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	12	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	12	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	12	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	14	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	14	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	14	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	14	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	15	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	15	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	15	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	15	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	16	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	16	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	16	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	16	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	17	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	17	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	17	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	17	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	18	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	18	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	18	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD2	19	0.11
(1,3)	1:4:A:LYS:HD2	1:5:A:PRO:HD3	19	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD2	19	0.11
(1,3)	1:4:A:LYS:HD3	1:5:A:PRO:HD3	19	0.11
(1,390)	1:38:B:VAL:HG11	1:42:B:TYR:H	18	0.1
(1,390)	1:38:B:VAL:HG12	1:42:B:TYR:H	18	0.1
(1,390)	1:38:B:VAL:HG13	1:42:B:TYR:H	18	0.1
(1,390)	1:38:B:VAL:HG21	1:42:B:TYR:H	18	0.1
(1,390)	1:38:B:VAL:HG22	1:42:B:TYR:H	18	0.1
(1,390)	1:38:B:VAL:HG23	1:42:B:TYR:H	18	0.1
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	9	0.1
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	9	0.1
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	9	0.1
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	9	0.1
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	9	0.1
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	9	0.1
(1,387)	1:6:A:VAL:HG11	1:10:A:TYR:H	20	0.1
(1,387)	1:6:A:VAL:HG12	1:10:A:TYR:H	20	0.1
(1,387)	1:6:A:VAL:HG13	1:10:A:TYR:H	20	0.1
(1,387)	1:6:A:VAL:HG21	1:10:A:TYR:H	20	0.1
(1,387)	1:6:A:VAL:HG22	1:10:A:TYR:H	20	0.1
(1,387)	1:6:A:VAL:HG23	1:10:A:TYR:H	20	0.1
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	1	0.1
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	1	0.1
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	1	0.1
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	1	0.1
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	1	0.1
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	1	0.1
(1,386)	1:6:A:VAL:HG11	1:9:A:ILE:H	3	0.1
(1,386)	1:6:A:VAL:HG12	1:9:A:ILE:H	3	0.1
(1,386)	1:6:A:VAL:HG13	1:9:A:ILE:H	3	0.1
(1,386)	1:6:A:VAL:HG21	1:9:A:ILE:H	3	0.1
(1,386)	1:6:A:VAL:HG22	1:9:A:ILE:H	3	0.1
(1,386)	1:6:A:VAL:HG23	1:9:A:ILE:H	3	0.1
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	10	0.1
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	10	0.1
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	11	0.1
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	11	0.1
(1,380)	1:44:B:ASN:HB2	1:47:B:THR:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,380)	1:44:B:ASN:HB3	1:47:B:THR:H	19	0.1
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	12	0.1
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	12	0.1
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	14	0.1
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	14	0.1
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	17	0.1
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	17	0.1
(1,370)	1:12:A:ASN:HB2	1:15:A:THR:H	20	0.1
(1,370)	1:12:A:ASN:HB3	1:15:A:THR:H	20	0.1
(1,359)	1:41:B:ILE:HD11	1:52:B:ARG:HE	10	0.1
(1,359)	1:41:B:ILE:HD12	1:52:B:ARG:HE	10	0.1
(1,359)	1:41:B:ILE:HD13	1:52:B:ARG:HE	10	0.1
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	2	0.1
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	6	0.1
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	7	0.1
(1,348)	1:43:B:CYS:HA	1:50:B:CYS:H	19	0.1
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	2	0.1
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	2	0.1
(1,346)	1:42:B:TYR:HD1	1:50:B:CYS:H	16	0.1
(1,346)	1:42:B:TYR:HD2	1:50:B:CYS:H	16	0.1
(1,345)	1:8:A:ILE:HG12	1:21:A:MET:H	13	0.1
(1,345)	1:8:A:ILE:HG13	1:21:A:MET:H	13	0.1
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	2	0.1
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	2	0.1
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	2	0.1
(1,340)	1:9:A:ILE:HD11	1:20:A:ARG:HE	5	0.1
(1,340)	1:9:A:ILE:HD12	1:20:A:ARG:HE	5	0.1
(1,340)	1:9:A:ILE:HD13	1:20:A:ARG:HE	5	0.1
(1,338)	1:12:A:ASN:H	1:19:A:GLN:H	20	0.1
(1,329)	1:11:A:CYS:HA	1:18:A:CYS:H	20	0.1
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	2	0.1
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	7	0.1
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	11	0.1
(1,326)	1:50:B:CYS:HA	1:43:B:CYS:H	17	0.1
(1,310)	1:18:A:CYS:HA	1:11:A:CYS:H	7	0.1
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE1	3	0.1
(1,305)	1:18:A:CYS:HA	1:10:A:TYR:HE2	3	0.1
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	16	0.1
(1,288)	1:45:B:ALA:HA	1:44:B:ASN:H	17	0.1
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	9	0.1
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	14	0.1
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,272)	1:13:A:ALA:HA	1:12:A:ASN:H	19	0.1
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	9	0.1
(1,250)	1:41:B:ILE:H	1:40:B:ILE:H	13	0.1
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	9	0.1
(1,236)	1:9:A:ILE:H	1:8:A:ILE:H	13	0.1
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	2	0.1
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	2	0.1
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	11	0.1
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	11	0.1
(1,187)	1:42:B:TYR:HB2	1:42:B:TYR:H	13	0.1
(1,187)	1:42:B:TYR:HB3	1:42:B:TYR:H	13	0.1
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	2	0.1
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	2	0.1
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	6	0.1
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	6	0.1
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	16	0.1
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	16	0.1
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	18	0.1
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	18	0.1
(1,113)	1:10:A:TYR:HB2	1:10:A:TYR:H	20	0.1
(1,113)	1:10:A:TYR:HB3	1:10:A:TYR:H	20	0.1
(1,76)	1:49:B:LYS:HD2	1:50:B:CYS:H	3	0.1
(1,76)	1:49:B:LYS:HD3	1:50:B:CYS:H	3	0.1
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD1	18	0.1
(1,61)	1:41:B:ILE:HG12	1:42:B:TYR:HD2	18	0.1
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD1	18	0.1
(1,61)	1:41:B:ILE:HG13	1:42:B:TYR:HD2	18	0.1
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	8	0.1
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	8	0.1
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	8	0.1
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	8	0.1
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	8	0.1
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	8	0.1
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD1	10	0.1
(1,60)	1:41:B:ILE:HD11	1:42:B:TYR:HD2	10	0.1
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD1	10	0.1
(1,60)	1:41:B:ILE:HD12	1:42:B:TYR:HD2	10	0.1
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD1	10	0.1
(1,60)	1:41:B:ILE:HD13	1:42:B:TYR:HD2	10	0.1
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD1	11	0.1
(1,59)	1:41:B:ILE:HB	1:42:B:TYR:HD2	11	0.1
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD2	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:36:B:LYS:HD2	1:37:B:PRO:HD3	11	0.1
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD2	11	0.1
(1,46)	1:36:B:LYS:HD3	1:37:B:PRO:HD3	11	0.1
(1,32)	1:17:A:LYS:HB2	1:18:A:CYS:H	1	0.1
(1,32)	1:17:A:LYS:HB3	1:18:A:CYS:H	1	0.1
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD1	20	0.1
(1,18)	1:9:A:ILE:HG12	1:10:A:TYR:HD2	20	0.1
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD1	20	0.1
(1,18)	1:9:A:ILE:HG13	1:10:A:TYR:HD2	20	0.1
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD1	12	0.1
(1,17)	1:9:A:ILE:HD11	1:10:A:TYR:HD2	12	0.1
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD1	12	0.1
(1,17)	1:9:A:ILE:HD12	1:10:A:TYR:HD2	12	0.1
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD1	12	0.1
(1,17)	1:9:A:ILE:HD13	1:10:A:TYR:HD2	12	0.1
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD1	17	0.1
(1,16)	1:9:A:ILE:HB	1:10:A:TYR:HD2	17	0.1

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

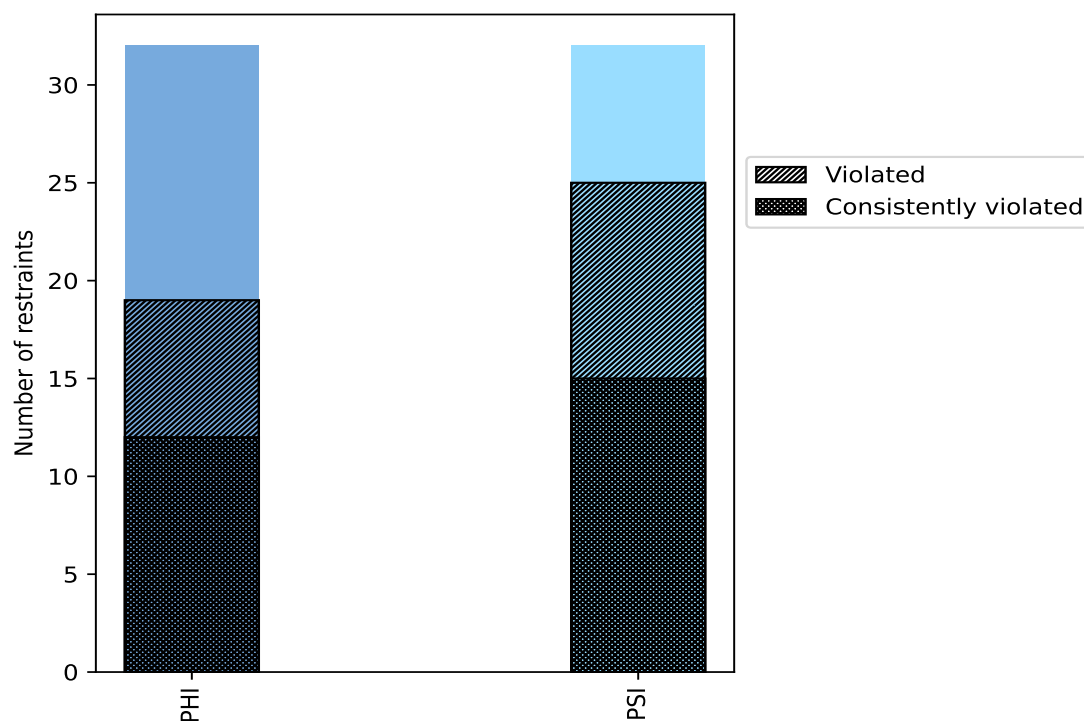
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	32	50.0	19	59.4	29.7	12	37.5	18.8
PSI	32	50.0	25	78.1	39.1	15	46.9	23.4
Total	64	100.0	44	68.8	68.8	27	42.2	42.2

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

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



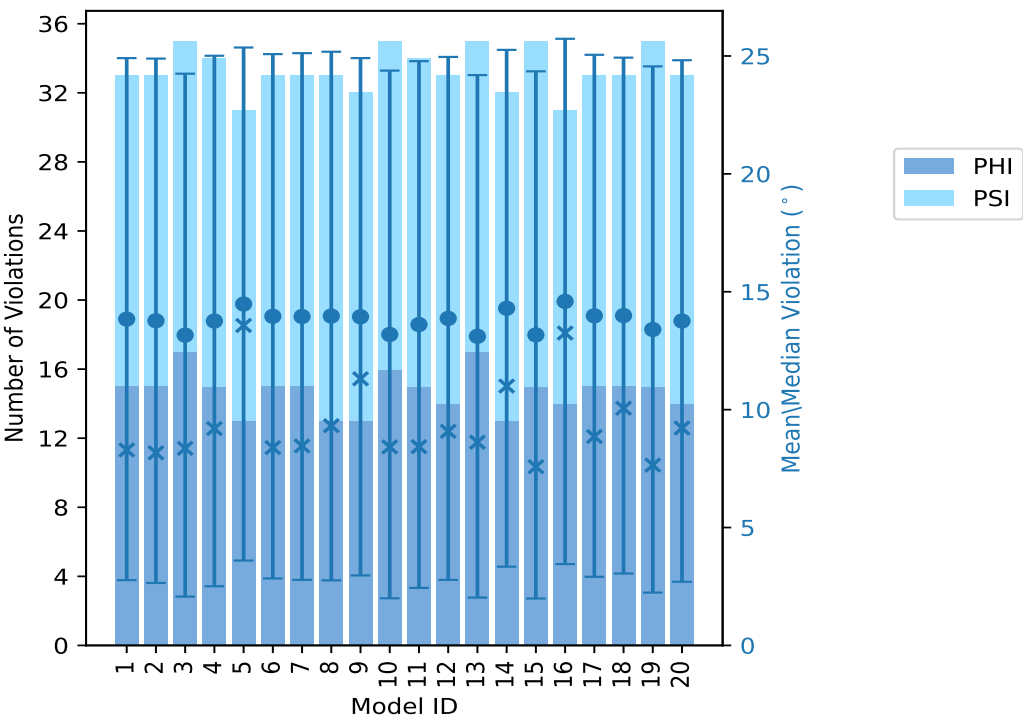
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	15	18	33	13.84	41.14	11.07	8.29
2	15	18	33	13.77	41.0	11.12	8.17
3	17	18	35	13.16	41.22	11.09	8.36
4	15	19	34	13.76	40.57	11.25	9.2
5	13	18	31	14.48	40.86	10.88	13.57
6	15	18	33	13.96	41.01	11.12	8.39
7	15	18	33	13.95	41.13	11.17	8.46
8	13	20	33	13.97	40.28	11.21	9.32
9	13	19	32	13.94	40.77	10.97	11.31
10	16	19	35	13.19	40.61	11.19	8.42
11	15	19	34	13.61	41.09	11.17	8.43
12	14	19	33	13.87	40.54	11.09	9.08
13	17	18	35	13.11	41.09	11.08	8.62
14	13	19	32	14.3	40.66	10.96	11.0
15	15	20	35	13.17	40.69	11.18	7.58
16	14	17	31	14.59	40.76	11.14	13.25
17	15	18	33	13.98	41.05	11.07	8.86
18	15	18	33	13.99	43.98	10.94	10.06
19	15	20	35	13.4	40.52	11.16	7.65
20	14	19	33	13.76	41.09	11.06	9.22

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

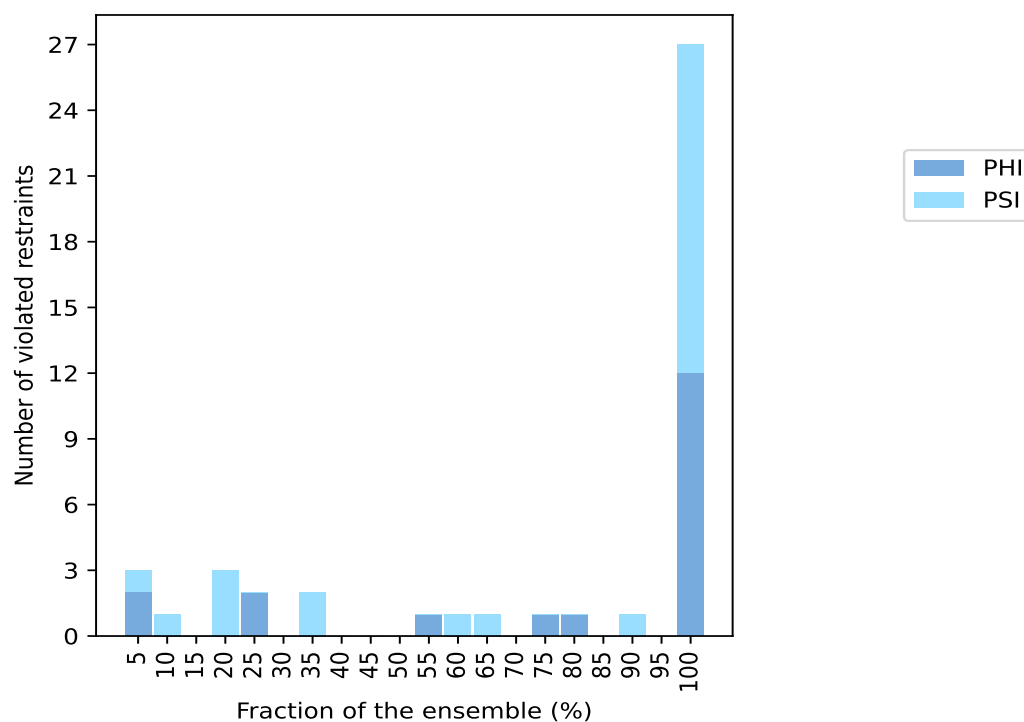
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
12	15	27	20	100.0

¹ Number of models with violations

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

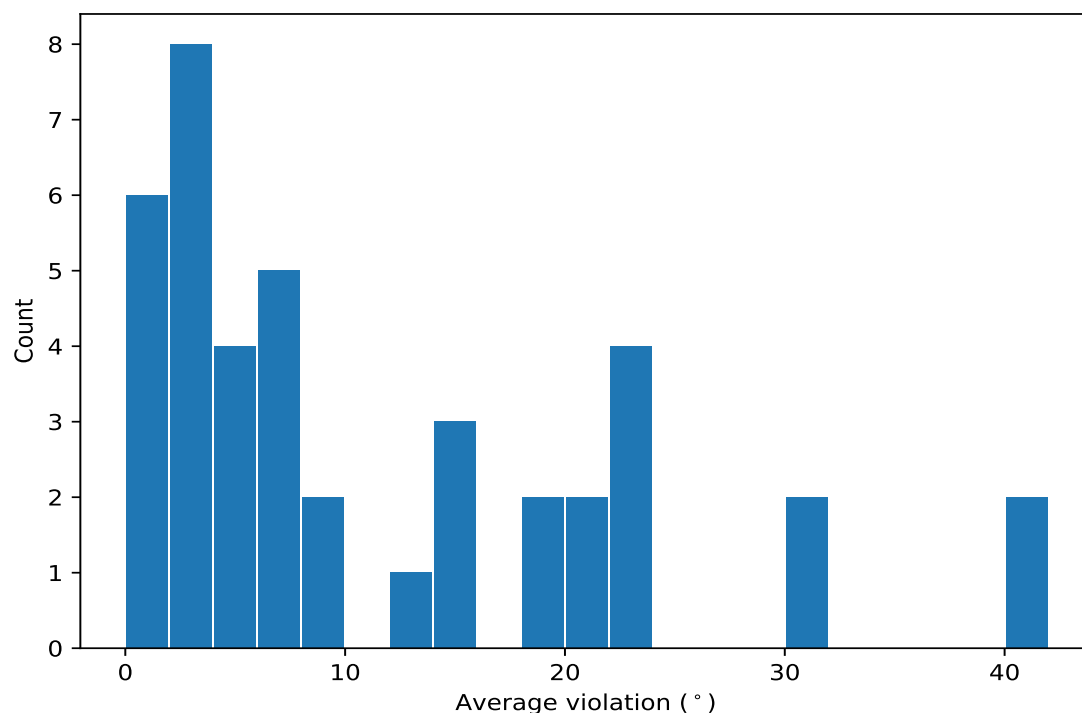


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	20	40.88	0.77	40.76
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	20	40.74	0.29	40.67
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	20	31.93	0.82	31.9
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	20	31.58	1.29	31.96
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	20	23.21	0.93	23.51
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	20	22.87	1.95	23.52
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	20	22.81	1.0	22.94
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	20	22.35	0.92	22.66
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	20	20.92	1.19	20.58
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	20	20.65	1.47	20.58
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	20	19.77	3.87	17.63
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	20	19.5	3.4	17.7
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	20	14.4	3.11	13.72
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	20	14.18	0.16	14.21
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	20	14.09	0.11	14.04
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	20	13.61	0.63	13.56
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	20	8.36	0.72	8.33
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	20	8.27	1.6	8.64
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	20	7.16	0.57	7.02
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	20	7.08	0.68	6.98

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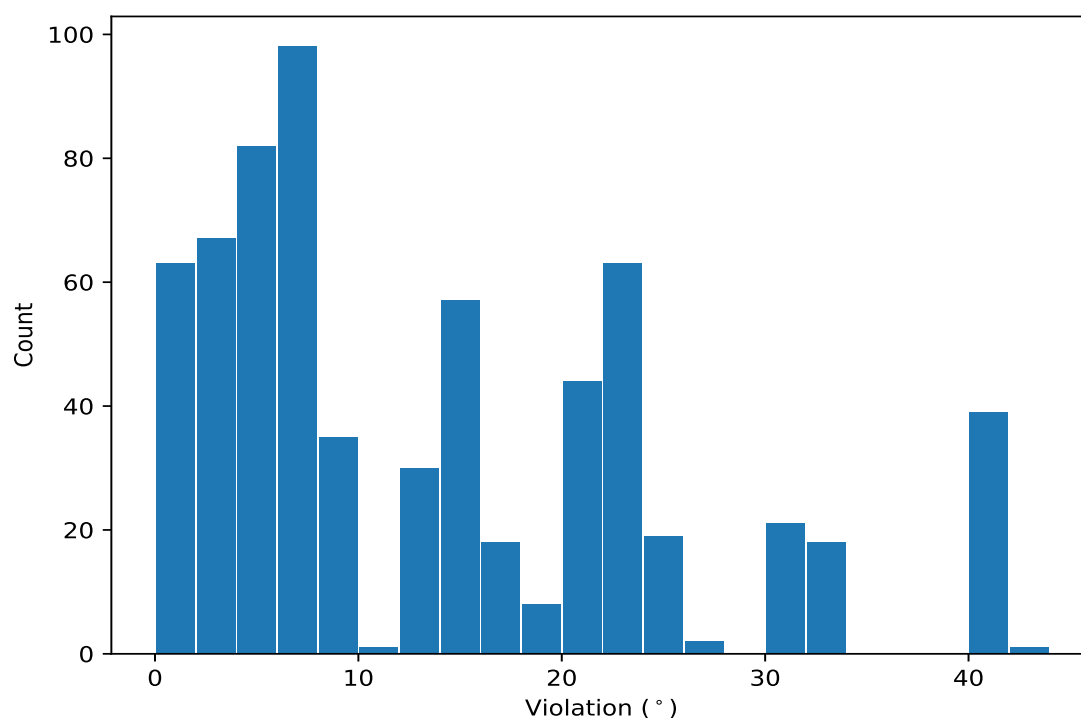
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	20	7.02	0.32	7.02
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	20	6.82	0.96	6.72
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	20	6.08	0.29	6.04
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	20	5.99	0.21	5.98
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	20	5.33	0.22	5.32
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	20	5.19	0.38	5.16
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	20	2.34	0.65	2.2
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	18	2.28	0.58	2.23
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	16	2.46	0.86	2.68
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	15	2.34	0.85	1.9
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	13	4.0	0.41	4.04
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	12	3.82	0.48	3.96
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	11	1.52	0.07	1.53
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	7	3.14	0.89	3.08
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	7	2.83	0.72	2.67
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	5	2.18	0.6	2.27
(1,5)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	5	1.56	0.05	1.58
(1,32)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:MET:N	4	1.41	0.37	1.4
(1,64)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:MET:N	4	1.24	0.2	1.16
(1,36)	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	1:36:B:LYS:N	4	1.1	0.06	1.1
(1,4)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:LYS:N	2	1.08	0.07	1.08

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 (°)
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	18	43.98
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	3	41.22
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	1	41.14
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	7	41.13
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	11	41.09
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	13	41.09
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	20	41.09
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	13	41.07
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	17	41.05
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	1	41.02
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	3	41.02
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	18	41.01
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	6	41.01
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	2	41.0
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	2	40.97
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	5	40.86
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	20	40.83
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	9	40.77
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	16	40.76
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	15	40.69
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	16	40.69

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	14	40.66
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	10	40.61
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	7	40.6
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	4	40.57
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	4	40.57
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	11	40.57
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	12	40.54
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	9	40.53
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	19	40.52
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	5	40.5
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	17	40.49
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	10	40.48
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	14	40.47
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	19	40.45
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	12	40.41
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	8	40.28
(1,54)	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1:47:B:THR:N	6	40.26
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	8	40.2
(1,22)	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1:15:A:THR:N	15	40.14
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	20	33.79
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	12	33.22
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	14	33.12
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	16	32.86
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	7	32.53
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	13	32.49
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	11	32.44
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	9	32.42
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	15	32.39
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	1	32.36
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	5	32.34
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	10	32.32
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	3	32.29
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	13	32.23
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	6	32.2
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	2	32.16
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	17	32.11
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	3	32.01
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	2	31.97
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	8	31.96
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	18	31.95
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	1	31.85
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	5	31.7
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	15	31.58
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	16	31.5
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	9	31.47
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	20	31.47
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	4	31.42
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	4	31.4
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	17	31.32
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	19	31.24
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	19	31.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	11	31.08
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	14	31.03
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	10	30.94
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	7	30.92
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	6	30.85
(1,53)	1:45:B:ALA:C	1:46:B:ALA:N	1:46:B:ALA:CA	1:46:B:ALA:C	8	30.8
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	12	30.72
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	18	27.83
(1,21)	1:13:A:ALA:C	1:14:A:ALA:N	1:14:A:ALA:CA	1:14:A:ALA:C	18	26.51
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	10	25.17
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	16	25.06
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	7	25.02
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	4	24.67
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	4	24.61
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	19	24.57
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	15	24.42
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	11	24.4
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	12	24.37
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	17	24.29
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	20	24.22
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	8	24.2
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	15	24.18
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	10	24.16
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	6	24.13
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	2	24.13
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	16	24.11
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	6	24.09
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	8	24.03
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	6	23.95
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	8	23.92
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	6	23.88
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	19	23.84
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	14	23.81
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	11	23.77
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	7	23.72
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	11	23.67
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	17	23.65
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	14	23.65
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	2	23.64
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	12	23.63
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	9	23.58
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	5	23.57
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	10	23.55
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	17	23.55
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	19	23.54
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1	23.53
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	17	23.52
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1	23.52
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	11	23.51
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	15	23.48
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	4	23.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	4	23.44
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	19	23.4
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	6	23.38
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	4	23.37
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	16	23.34
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	9	23.34
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	2	23.32
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	8	23.31
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	3	23.31
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	7	23.29
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	12	23.29
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	19	23.29
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	20	23.28
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	16	23.25
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	3	23.22
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	5	23.22
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	4	23.2
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	18	23.17
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	7	23.16
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	19	23.1
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	11	23.09
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	20	23.04
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	2	23.01
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	13	23.0
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	13	22.99
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	10	22.98
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	14	22.93
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	3	22.91
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	14	22.91
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1	22.83
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	7	22.81
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	8	22.81
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	17	22.76
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	12	22.7
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	18	22.61
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	10	22.51
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1	22.39
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	13	22.16
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	5	22.14
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	15	22.14
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	12	21.98
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	8	21.92
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	13	21.89
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	3	21.86
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	15	21.8
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	5	21.77
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	14	21.75
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	14	21.61
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	9	21.54
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	9	21.48
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	5	21.48

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	15	21.4
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	16	21.35
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	12	21.29
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	9	21.26
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	16	21.18
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	18	21.11
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	15	21.05
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	3	21.02
(1,55)	1:46:B:ALA:C	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	20	21.01
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	13	20.94
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	5	20.92
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	1	20.91
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	3	20.9
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	9	20.83
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	13	20.79
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	18	20.71
(1,27)	1:17:A:LYS:C	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	8	20.69
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	10	20.67
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	7	20.63
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	1	20.6
(1,59)	1:49:B:LYS:C	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	20	20.56
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	20	20.56
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	2	20.47
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	2	20.37
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	12	20.24
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	17	20.21
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	19	20.13
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	16	20.12
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	7	20.1
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	11	20.1
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	6	20.08
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	6	20.06
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	10	20.03
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	17	19.95
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	11	19.93
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	8	19.89
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	14	19.87
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	19	19.8
(1,52)	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1:46:B:ALA:N	4	19.77
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	4	19.71
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	18	18.52
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	9	17.86
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	1	17.85
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	3	17.76
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	5	17.69
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	18	17.58
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	13	17.54
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	1	17.51
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	13	17.47
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	3	17.44
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	7	17.18

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	2	17.14
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	2	17.12
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	20	17.12
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	17	16.92
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	6	16.84
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	11	16.59
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	20	16.41
(1,20)	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1:14:A:ALA:N	18	16.12
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	10	15.92
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	16	15.78
(1,28)	1:18:A:CYS:N	1:18:A:CYS:CA	1:18:A:CYS:C	1:19:A:GLN:N	5	15.73
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	15	15.69
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	12	15.49
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	14	15.37
(1,60)	1:50:B:CYS:N	1:50:B:CYS:CA	1:50:B:CYS:C	1:51:B:GLN:N	9	15.35
(1,23)	1:14:A:ALA:C	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	18	15.16
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	9	14.59
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	18	14.55
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	7	14.51
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	15	14.43
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	1	14.41
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	3	14.39
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	4	14.36
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	13	14.36
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	5	14.34
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	6	14.34
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	10	14.33
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	11	14.31
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	3	14.3
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	11	14.29
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	17	14.28
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	10	14.27
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	2	14.26
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	13	14.26
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	20	14.26
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	12	14.25
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	12	14.23
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	19	14.22
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	7	14.21
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	18	14.2
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	10	14.17
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	5	14.16
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	15	14.12
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	19	14.12
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	8	14.09
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	14	14.09
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	16	14.07
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	8	14.06
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	9	14.05
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	8	14.04
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	20	14.04

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	1	14.03
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	14	14.03
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	14	14.02
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	16	14.02
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	5	14.02
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	3	14.01
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	7	14.01
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	6	14.01
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	11	14.01
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	9	14.0
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	15	14.0
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	2	14.0
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	4	14.0
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	12	14.0
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	20	13.99
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	18	13.98
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:PRO:N	17	13.96
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	19	13.92
(1,38)	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	1:37:B:PRO:N	1	13.91
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	2	13.86
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	17	13.74
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	3	13.73
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	1	13.7
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	13	13.67
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	6	13.65
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	9	13.59
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	5	13.57
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	2	13.53
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	13	13.5
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	4	13.41
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	6	13.41
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	4	13.4
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	16	13.34
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	8	13.29
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	16	13.25
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	15	13.18
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	19	13.16
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	17	13.03
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	10	13.02
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:ALA:N	7	12.91
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	11	12.8
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	12	12.76
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	14	12.65
(1,50)	1:44:B:ASN:N	1:44:B:ASN:CA	1:44:B:ASN:C	1:45:B:ALA:N	20	12.55
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	18	10.06
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	15	9.69
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	14	9.36
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	8	9.32
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	20	9.22
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	4	9.22
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	4	9.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	12	9.08
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	20	9.06
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	9	9.03
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	14	9.02
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	5	8.97
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	12	8.86
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	17	8.86
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	8	8.75
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	13	8.74
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	10	8.71
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	13	8.62
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	16	8.6
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	11	8.58
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	3	8.48
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	7	8.46
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	18	8.44
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	10	8.42
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	6	8.39
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	18	8.39
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	18	8.38
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	3	8.36
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1	8.29
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	11	8.28
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1	8.27
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	2	8.17
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	6	8.13
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	5	8.1
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1	8.1
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	17	8.08
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	2	7.99
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	3	7.91
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	19	7.86
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	7	7.79
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	2	7.77
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	13	7.72
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	2	7.71
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	20	7.68
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	19	7.65
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	13	7.63
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	15	7.58
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	18	7.58
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	17	7.57
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	3	7.57
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	11	7.51
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	6	7.51
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	6	7.51
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	14	7.47
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	16	7.43
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	19	7.43
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	16	7.43
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	12	7.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	17	7.35
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	14	7.35
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	19	7.34
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	7	7.33
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	7	7.32
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	9	7.32
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	5	7.29
(1,11)	1:8:A:ILE:C	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1	7.29
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	12	7.22
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	4	7.21
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	7	7.19
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	11	7.13
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	4	7.12
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	15	7.08
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	11	7.07
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	10	7.06
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	8	7.05
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	8	7.03
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	3	7.01
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	13	6.99
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	15	6.99
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	9	6.98
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	13	6.98
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	20	6.97
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	15	6.9
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	1	6.9
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	17	6.9
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	20	6.87
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	11	6.85
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	18	6.84
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	7	6.84
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	10	6.79
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	10	6.79
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	3	6.77
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	18	6.77
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	5	6.76
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	2	6.75
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	1	6.73
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	14	6.7
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	16	6.66
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	17	6.64
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	2	6.64
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	5	6.63
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	19	6.62
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	12	6.61
(1,24)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLY:N	9	6.56
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	10	6.54
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	4	6.51
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	4	6.48
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	7	6.48
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	15	6.45

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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	6	6.44
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	11	6.41
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	13	6.36
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	1	6.35
(1,56)	1:47:B:THR:N	1:47:B:THR:CA	1:47:B:THR:C	1:48:B:GLY:N	9	6.33
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	19	6.32
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	6	6.32
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	17	6.32
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	2	6.31
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	2	6.28
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	13	6.23
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	18	6.22
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	3	6.17
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	6	6.16
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	20	6.15
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	3	6.13
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	8	6.12
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	5	6.1
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	5	6.1
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	14	6.09
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	19	6.06
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	16	6.04
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	4	6.03
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	15	6.02
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	20	6.0
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	1	5.99
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	12	5.99
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	10	5.99
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	9	5.98
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	5	5.96
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	8	5.95
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	4	5.93
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	17	5.92
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	16	5.9
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	9	5.9
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	11	5.89
(1,29)	1:18:A:CYS:C	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	8	5.88
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	8	5.86
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	10	5.85
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	20	5.85
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	15	5.83
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	18	5.78
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	16	5.75
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	14	5.74
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	9	5.73
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	8	5.72
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	4	5.68
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	8	5.67
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	7	5.64
(1,51)	1:44:B:ASN:C	1:45:B:ALA:N	1:45:B:ALA:CA	1:45:B:ALA:C	6	5.63
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	12	5.62

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	15	5.6
(1,19)	1:12:A:ASN:C	1:13:A:ALA:N	1:13:A:ALA:CA	1:13:A:ALA:C	19	5.59
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	12	5.57
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	6	5.55
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	4	5.51
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	16	5.51
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	12	5.48
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	14	5.46
(1,61)	1:50:B:CYS:C	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	16	5.46
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	20	5.46
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	11	5.45
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	5	5.45
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	10	5.44
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	17	5.4
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	15	5.37
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	18	5.33
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	9	5.3
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	2	5.27
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	13	5.26
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	10	5.26
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	6	5.22
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	13	5.22
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	14	5.16
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	7	5.12
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	1	5.1
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	2	5.1
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	5	5.09
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	19	5.09
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	12	5.08
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	17	5.05
(1,46)	1:42:B:TYR:N	1:42:B:TYR:CA	1:42:B:TYR:C	1:43:B:CYS:N	3	5.04
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	19	4.93
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	11	4.89
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	14	4.89
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	18	4.85
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	20	4.83
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	1	4.78
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	9	4.71
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	3	4.69
(1,14)	1:10:A:TYR:N	1:10:A:TYR:CA	1:10:A:TYR:C	1:11:A:CYS:N	7	4.69
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	6	4.41
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	19	4.4
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	10	4.32
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	9	4.31
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	20	4.31
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	14	4.3
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	13	4.3
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	12	4.28
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	17	4.26
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	11	4.18
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	5	4.17

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	16	4.14
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	13	4.14
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	5	4.05
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	20	4.05
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	17	4.04
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	14	3.98
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	16	3.94
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	11	3.87
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	9	3.86
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	12	3.82
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	16	3.81
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	2	3.77
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	2	3.7
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	8	3.61
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	6	3.53
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	1	3.53
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	14	3.52
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	1	3.51
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	1	3.48
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	7	3.44
(1,12)	1:9:A:ILE:N	1:9:A:ILE:CA	1:9:A:ILE:C	1:10:A:TYR:N	3	3.36
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	17	3.3
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	19	3.3
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	15	3.27
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	3	3.26
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	19	3.22
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	3	3.19
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	19	3.16
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	11	3.15
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	10	3.12
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	15	3.08
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	16	3.02
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	19	3.01
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	4	3.0
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	14	2.97
(1,44)	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	1:42:B:TYR:N	18	2.91
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	6	2.82
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	7	2.82
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	15	2.77
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	4	2.7
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	10	2.69
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	7	2.68
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	10	2.67
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	12	2.67
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	6	2.64
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	4	2.62
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	1	2.61
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	3	2.61
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	9	2.61
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	18	2.55
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	4	2.55

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	15	2.53
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	18	2.52
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	8	2.51
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	7	2.5
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	20	2.42
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	7	2.41
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	13	2.4
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	11	2.37
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	19	2.37
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	18	2.36
(1,42)	1:40:B:ILE:N	1:40:B:ILE:CA	1:40:B:ILE:C	1:41:B:ILE:N	18	2.34
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	9	2.32
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	5	2.29
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	20	2.29
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	3	2.27
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	16	2.14
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	5	2.1
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	20	2.06
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	4	2.02
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	17	2.02
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	8	2.01
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	4	1.99
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	17	1.96
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	2	1.94
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	13	1.92
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	3	1.9
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	8	1.88
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	15	1.86
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	10	1.86
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	14	1.82
(1,32)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:MET:N	12	1.82
(1,43)	1:40:B:ILE:C	1:41:B:ILE:N	1:41:B:ILE:CA	1:41:B:ILE:C	16	1.76
(1,32)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:MET:N	14	1.74
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	2	1.72
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	5	1.72
(1,62)	1:51:B:GLN:N	1:51:B:GLN:CA	1:51:B:GLN:C	1:52:B:ARG:N	8	1.71
(1,30)	1:19:A:GLN:N	1:19:A:GLN:CA	1:19:A:GLN:C	1:20:A:ARG:N	12	1.71
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	12	1.69
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	6	1.68
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	3	1.65
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	1	1.64
(1,5)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	20	1.63
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	11	1.62
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	15	1.62
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	17	1.59
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	19	1.59
(1,48)	1:43:B:CYS:N	1:43:B:CYS:CA	1:43:B:CYS:C	1:44:B:ASN:N	9	1.58
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	2	1.58
(1,5)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	3	1.58
(1,5)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	7	1.58
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	13	1.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:MET:N	19	1.56
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	4	1.55
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	12	1.54
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	13	1.53
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	15	1.53
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	2	1.52
(1,5)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	13	1.51
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	11	1.5
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	18	1.49
(1,5)	1:3:A:LYS:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	10	1.49
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	7	1.47
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	6	1.44
(1,37)	1:35:B:LYS:C	1:36:B:LYS:N	1:36:B:LYS:CA	1:36:B:LYS:C	10	1.35
(1,25)	1:16:A:GLY:C	1:17:A:LYS:N	1:17:A:LYS:CA	1:17:A:LYS:C	17	1.33
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	1	1.3
(1,64)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:MET:N	8	1.26
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	13	1.25
(1,63)	1:51:B:GLN:C	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1	1.24
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	2	1.22
(1,57)	1:48:B:GLY:C	1:49:B:LYS:N	1:49:B:LYS:CA	1:49:B:LYS:C	11	1.21
(1,16)	1:11:A:CYS:N	1:11:A:CYS:CA	1:11:A:CYS:C	1:12:A:ASN:N	6	1.2
(1,36)	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	1:36:B:LYS:N	8	1.19
(1,3)	1:2:A:SER:C	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	13	1.18
(1,4)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:LYS:N	10	1.16
(1,36)	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	1:36:B:LYS:N	15	1.14
(1,31)	1:19:A:GLN:C	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	3	1.11
(1,32)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:MET:N	19	1.07
(1,64)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:MET:N	4	1.06
(1,64)	1:52:B:ARG:N	1:52:B:ARG:CA	1:52:B:ARG:C	1:53:B:MET:N	10	1.06
(1,36)	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	1:36:B:LYS:N	9	1.06
(1,36)	1:35:B:LYS:N	1:35:B:LYS:CA	1:35:B:LYS:C	1:36:B:LYS:N	20	1.03
(1,32)	1:20:A:ARG:N	1:20:A:ARG:CA	1:20:A:ARG:C	1:21:A:MET:N	11	1.01
(1,4)	1:3:A:LYS:N	1:3:A:LYS:CA	1:3:A:LYS:C	1:4:A:LYS:N	15	1.01