



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 6B5W / pdb_00006b5w
BMRB ID : 30187
Title : Benenodin-1-dC5, state 2
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Deposited on : 2017-09-29

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

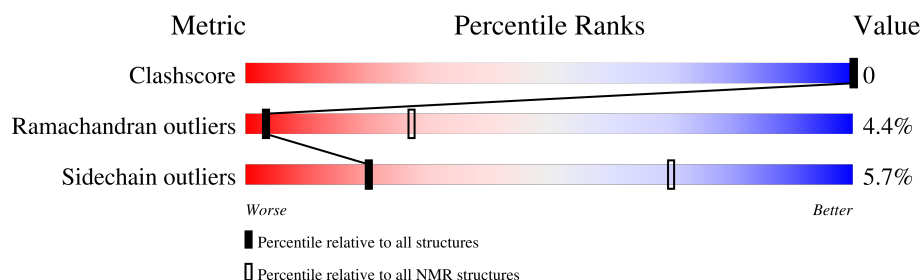
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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	19	 89% 5% 5%

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:1-A:18 (18)	0.86	18

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 282 atoms, of which 141 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Benenodin-1.

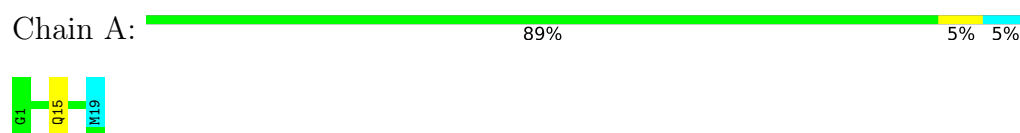
Mol	Chain	Residues	Atoms						Trace
1	A	19	Total	C	H	N	O	S	0
			282	88	141	25	27	1	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Benenodin-1

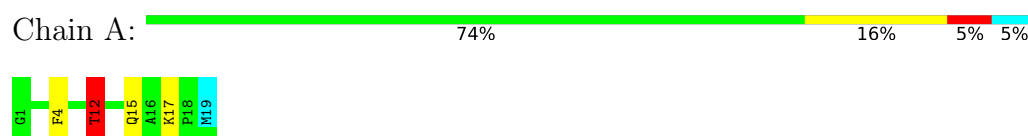


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

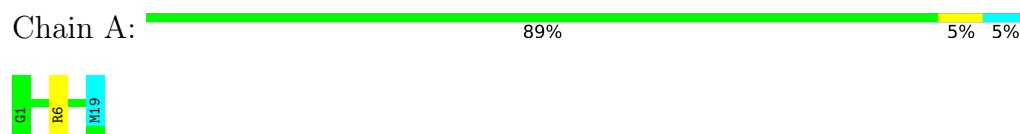
4.2.1 Score per residue for model 1

- Molecule 1: Benenodin-1



4.2.2 Score per residue for model 2

- Molecule 1: Benenodin-1



4.2.3 Score per residue for model 3

- Molecule 1: Benenodin-1

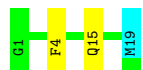
Chain A:  74% 5% 16% 5%



4.2.4 Score per residue for model 4

- Molecule 1: Benenodin-1

Chain A:  84% 11% 5%



4.2.5 Score per residue for model 5

- Molecule 1: Benenodin-1

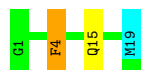
Chain A:  84% 11% 5%



4.2.6 Score per residue for model 6

- Molecule 1: Benenodin-1

Chain A:  84% 5% 5% 5%



4.2.7 Score per residue for model 7

- Molecule 1: Benenodin-1

Chain A:  84% 11% 5%



4.2.8 Score per residue for model 8

- Molecule 1: Benenodin-1

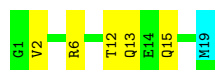
Chain A:  84% 11% 5%



4.2.9 Score per residue for model 9

- Molecule 1: Benenodin-1

Chain A:  68% 26% 5%



4.2.10 Score per residue for model 10

- Molecule 1: Benenodin-1

Chain A:  79% 11% 5% 5%



4.2.11 Score per residue for model 11

- Molecule 1: Benenodin-1

Chain A:  89% 5% 5%



4.2.12 Score per residue for model 12

- Molecule 1: Benenodin-1

Chain A:  79% 11% 5% 5%



4.2.13 Score per residue for model 13

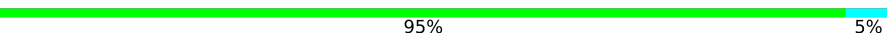
- Molecule 1: Benenodin-1

Chain A:  79% 16% 5%



4.2.14 Score per residue for model 14

- Molecule 1: Benenodin-1

Chain A:  95% 5%



4.2.15 Score per residue for model 15

- Molecule 1: Benenodin-1

Chain A:  89% 5% 5%



4.2.16 Score per residue for model 16

- Molecule 1: Benenodin-1

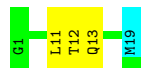
Chain A:  89% 5% 5%



4.2.17 Score per residue for model 17

- Molecule 1: Benenodin-1

Chain A:  79% 16% 5%



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Benenodin-1

Chain A:  79% 16% 5%



4.2.19 Score per residue for model 19

- Molecule 1: Benenodin-1

Chain A:  79% 16% 5%



4.2.20 Score per residue for model 20

- Molecule 1: Benenodin-1

Chain A:  79% 16% 5%



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure calculation	2.0
GROMACS	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	130
Number of shifts mapped to atoms	130
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.54±0.01	0±0/135 (0.0± 0.0%)	1.75±0.10	1±2/182 (0.7± 0.9%)
All	All	0.54	0/2700 (0.0%)	1.76	26/3640 (0.7%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.4
All	All	0	5

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	13	GLN	OE1-CD-NE2	-7.28	115.32	122.60	13	4
1	A	17	LYS	CA-C-N	6.51	126.47	120.21	1	1
1	A	17	LYS	C-N-CA	6.51	126.47	120.21	1	1
1	A	15	GLN	OE1-CD-NE2	-6.04	116.56	122.60	6	8
1	A	4	PHE	CA-CB-CG	5.47	119.27	113.80	8	2
1	A	6	ARG	CD-NE-CZ	5.41	131.97	124.40	15	2
1	A	9	SER	CA-C-N	5.27	127.39	120.60	3	1
1	A	9	SER	C-N-CA	5.27	127.39	120.60	3	1
1	A	5	GLY	CA-C-N	5.25	129.63	122.07	3	1
1	A	5	GLY	C-N-CA	5.25	129.63	122.07	3	1
1	A	9	SER	N-CA-C	5.21	119.12	112.87	3	1
1	A	7	PRO	N-CA-CB	5.04	107.56	103.32	16	1
1	A	14	GLU	CA-C-N	5.04	131.16	121.54	3	1
1	A	14	GLU	C-N-CA	5.04	131.16	121.54	3	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	6	ARG	Sidechain	2
1	A	12	THR	Peptide	1
1	A	14	GLU	Peptide	1
1	A	17	LYS	Peptide	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	2640	2640	2634	-

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 -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	17/19 (89%)	14±1 (81±7%)	2±1 (15±7%)	1±1 (4±5%)	3	27
All	All	340/380 (89%)	275 (81%)	50 (15%)	15 (4%)	3	27

All 7 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	12	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	15	GLN	3
1	A	11	LEU	2
1	A	5	GLY	1
1	A	2	VAL	1
1	A	18	PRO	1
1	A	14	GLU	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	14/15 (93%)	13±1 (94±5%)	1±1 (6±5%)	20	70
All	All	280/300 (93%)	264 (94%)	16 (6%)	20	70

All 4 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	4	PHE	6
1	A	6	ARG	6
1	A	15	GLN	3
1	A	12	THR	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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 51% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ben1_state2_coordinates.txt*

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	130
Number of shifts mapped to atoms	130
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 51%, i.e. 117 atoms were assigned a chemical shift out of a possible 231. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	32/89 (36%)	32/37 (86%)	0/36 (0%)	0/16 (0%)
Sidechain	81/132 (61%)	81/85 (95%)	0/41 (0%)	0/6 (0%)
Aromatic	4/10 (40%)	4/5 (80%)	0/5 (0%)	0/0 (—%)
Overall	117/231 (51%)	117/127 (92%)	0/82 (0%)	0/22 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 126 atoms were assigned a chemical shift out of a possible 246. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	34/94 (36%)	34/39 (87%)	0/38 (0%)	0/17 (0%)
Sidechain	88/142 (62%)	88/92 (96%)	0/44 (0%)	0/6 (0%)
Aromatic	4/10 (40%)	4/5 (80%)	0/5 (0%)	0/0 (—%)
Overall	126/246 (51%)	126/136 (93%)	0/87 (0%)	0/23 (0%)

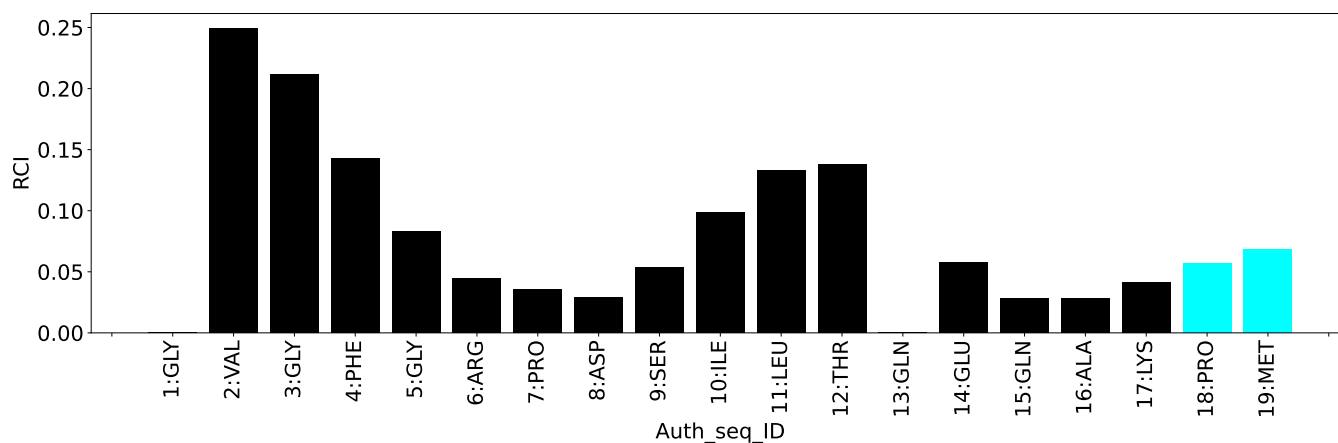
7.1.4 Statistically unusual chemical shifts [i](#)

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:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	245
Intra-residue ($ i-j =0$)	130
Sequential ($ i-j =1$)	60
Medium range ($ i-j >1$ and $ i-j <5$)	11
Long range ($ i-j \geq 5$)	44
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.9
Number of long range restraints per residue ¹	2.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.2	0.2
0.2-0.5 (Medium)	10.3	0.5
>0.5 (Large)	19.4	4.48

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

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis ⓘ

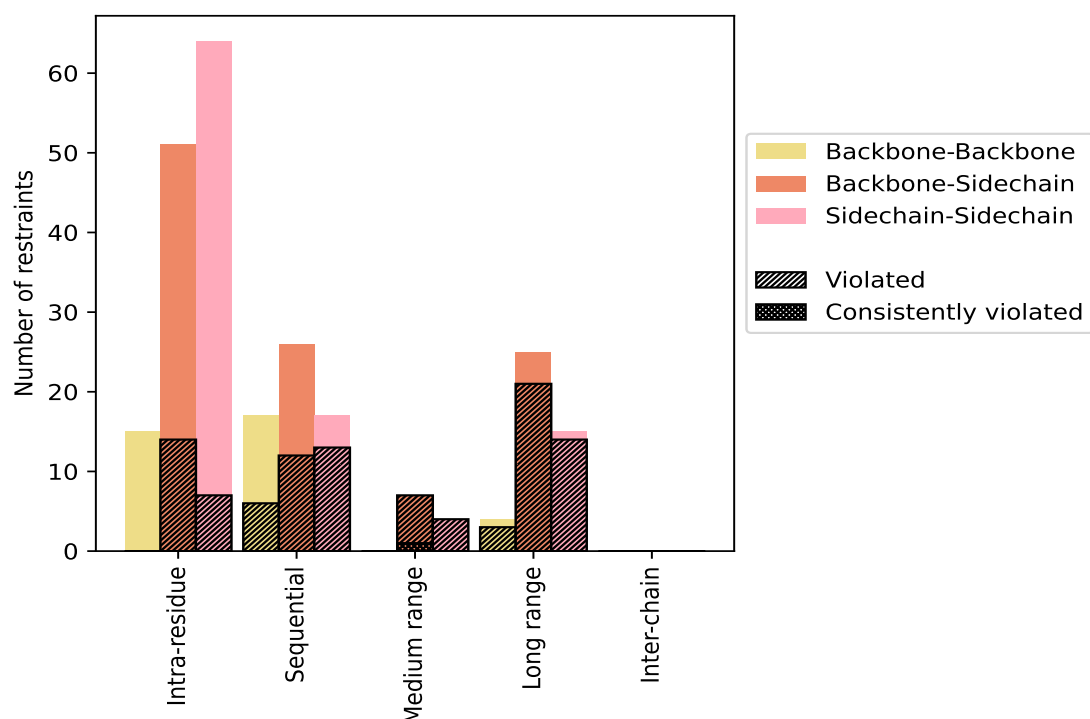
9.1 Summary of distance violations ⓘ

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)	130	53.1	21	16.2	8.6	0	0.0	0.0
Backbone-Backbone	15	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	51	20.8	14	27.5	5.7	0	0.0	0.0
Sidechain-Sidechain	64	26.1	7	10.9	2.9	0	0.0	0.0
Sequential (i-j =1)	60	24.5	31	51.7	12.7	0	0.0	0.0
Backbone-Backbone	17	6.9	6	35.3	2.4	0	0.0	0.0
Backbone-Sidechain	26	10.6	12	46.2	4.9	0	0.0	0.0
Sidechain-Sidechain	17	6.9	13	76.5	5.3	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	11	4.5	11	100.0	4.5	1	9.1	0.4
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	7	2.9	7	100.0	2.9	1	14.3	0.4
Sidechain-Sidechain	4	1.6	4	100.0	1.6	0	0.0	0.0
Long range (i-j ≥5)	44	18.0	38	86.4	15.5	0	0.0	0.0
Backbone-Backbone	4	1.6	3	75.0	1.2	0	0.0	0.0
Backbone-Sidechain	25	10.2	21	84.0	8.6	0	0.0	0.0
Sidechain-Sidechain	15	6.1	14	93.3	5.7	0	0.0	0.0
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	245	100.0	101	41.2	41.2	1	0.4	0.4
Backbone-Backbone	36	14.7	9	25.0	3.7	0	0.0	0.0
Backbone-Sidechain	109	44.5	54	49.5	22.0	1	0.9	0.4
Sidechain-Sidechain	100	40.8	38	38.0	15.5	0	0.0	0.0

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	5	9	6	14	0	34	0.67	2.37	0.57	0.46
2	2	5	6	17	0	30	0.67	1.35	0.39	0.6
3	5	9	4	17	0	35	0.77	2.49	0.55	0.73
4	5	5	5	15	0	30	1.07	4.26	0.97	0.72
5	5	7	4	21	0	37	0.78	2.01	0.51	0.67
6	7	4	3	18	0	32	0.89	2.56	0.61	0.75
7	2	12	7	16	0	37	0.72	2.4	0.6	0.57
8	5	6	7	12	0	30	0.76	2.71	0.7	0.5
9	5	11	4	20	0	40	0.78	2.31	0.62	0.52
10	8	9	2	19	0	38	0.9	3.41	0.8	0.66

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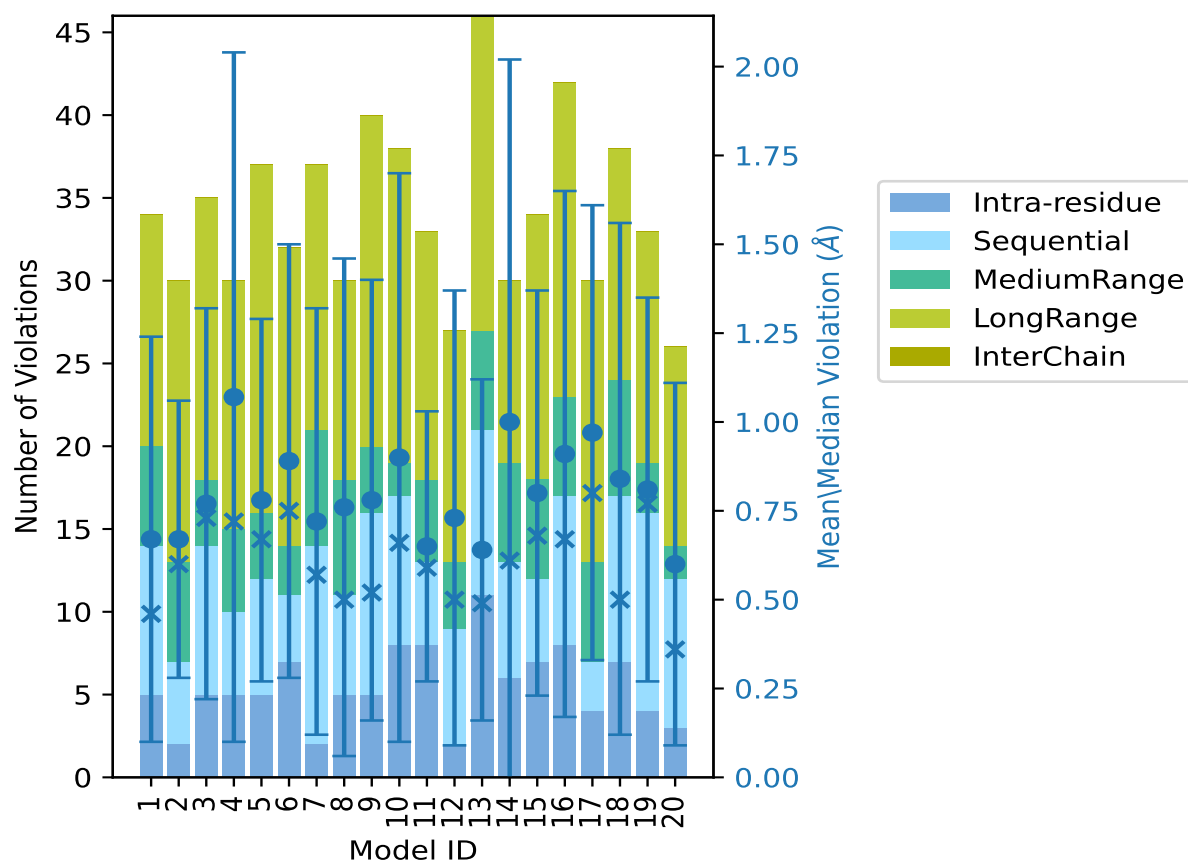
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	8	5	5	15	0	33	0.65	1.35	0.38	0.59
12	2	7	4	14	0	27	0.73	2.39	0.64	0.5
13	11	10	6	19	0	46	0.64	2.52	0.48	0.49
14	6	7	6	11	0	30	1.0	4.48	1.02	0.61
15	7	5	6	16	0	34	0.8	2.65	0.57	0.68
16	8	9	6	19	0	42	0.91	3.31	0.74	0.67
17	4	3	6	17	0	30	0.97	2.15	0.64	0.8
18	7	10	7	14	0	38	0.84	2.99	0.72	0.5
19	4	12	3	14	0	33	0.81	2.29	0.54	0.77
20	3	9	2	12	0	26	0.6	1.8	0.51	0.36

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

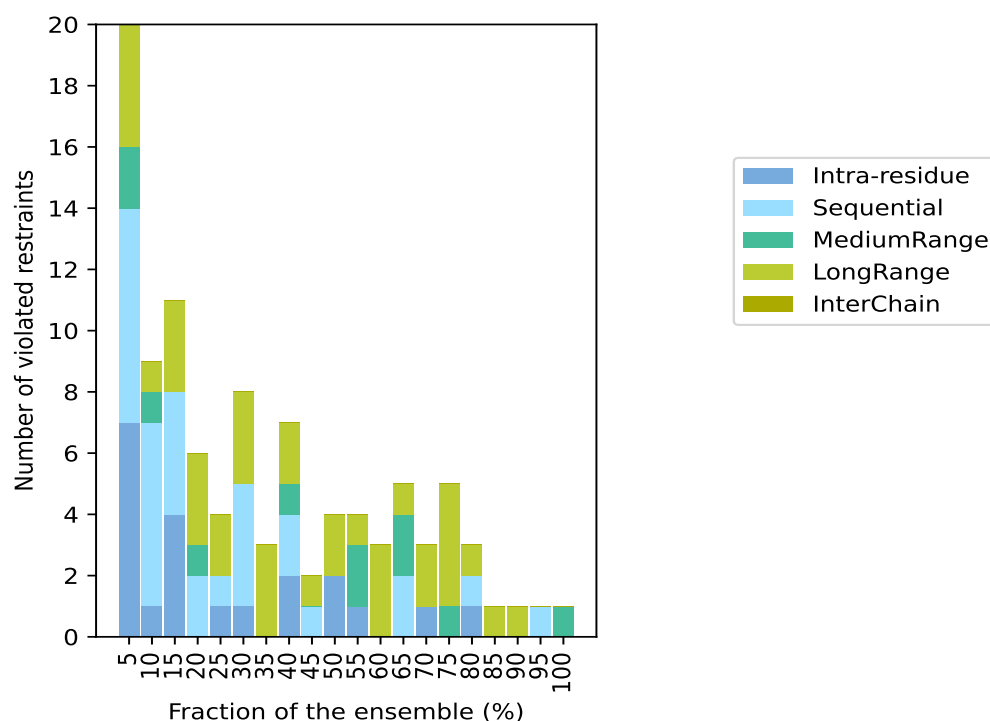
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 144(IR:109, SQ:29, MR:0, LR:6, IC:0) restraints are not violated in the ensemble.

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

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

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

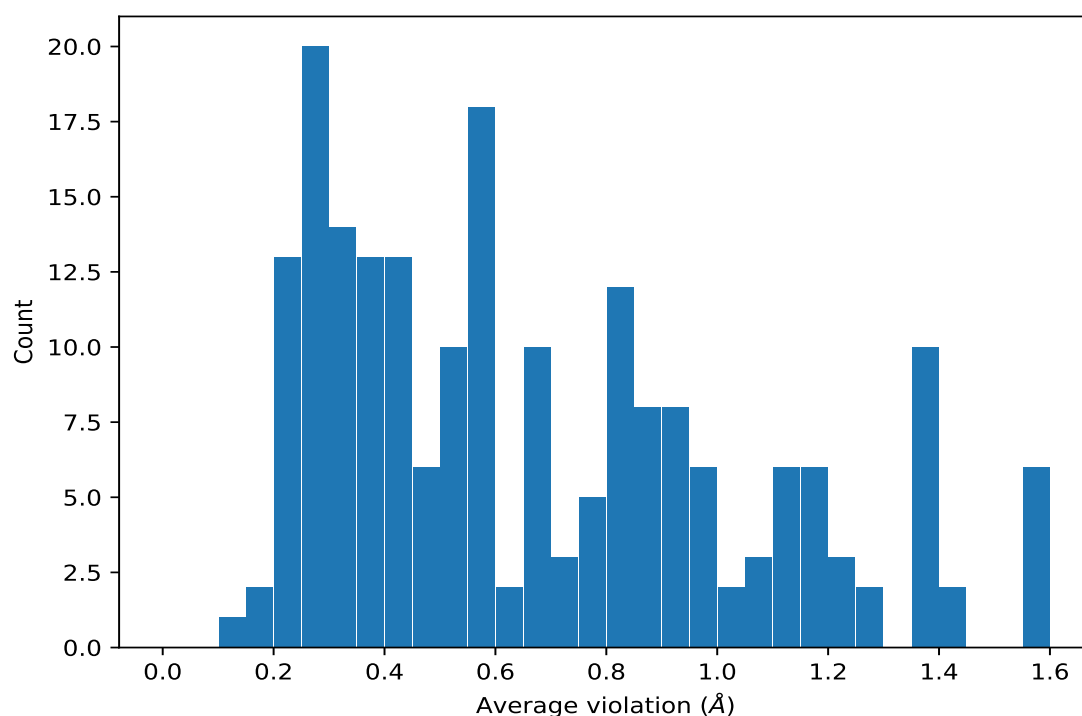
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	20	1.55	0.68	1.37
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	20	1.55	0.68	1.37
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	20	1.55	0.68	1.37
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	20	1.55	0.68	1.37
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	20	1.55	0.68	1.37
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	20	1.55	0.68	1.37
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	19	1.28	0.72	1.36
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	19	1.28	0.72	1.36
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	17	1.45	0.31	1.44
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	17	1.45	0.31	1.44
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	16	1.14	0.57	1.0
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	16	1.14	0.57	1.0
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	16	1.14	0.57	1.0
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	16	1.14	0.57	1.0
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	16	0.83	0.42	0.8
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	16	0.83	0.42	0.8

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	16	0.26	0.13	0.22
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	15	1.38	0.71	1.47
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	15	1.37	1.07	1.02
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	15	1.37	1.07	1.02
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	15	1.37	1.07	1.02
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	15	1.37	1.07	1.02
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	15	0.85	0.57	0.55
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	15	0.6	0.22	0.52
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	15	0.6	0.22	0.52
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	15	0.6	0.22	0.52
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	15	0.47	0.36	0.37
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	14	0.79	0.49	0.7
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	14	0.56	0.05	0.56
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	14	0.27	0.13	0.23
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	14	0.27	0.13	0.23
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	14	0.27	0.13	0.23
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	13	1.36	0.67	1.16
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	13	0.84	0.52	0.71
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	13	0.84	0.52	0.71
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	13	0.83	0.25	0.78
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	13	0.78	0.4	0.82
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	13	0.78	0.4	0.82
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	13	0.78	0.4	0.82
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	13	0.48	0.24	0.39
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	13	0.48	0.24	0.39
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	13	0.48	0.24	0.39
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	12	1.22	0.88	1.09
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	12	1.21	0.73	1.2
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	12	1.21	0.73	1.2
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	12	0.7	0.44	0.62
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	12	0.7	0.44	0.62
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	11	1.38	0.7	1.12
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	11	1.38	0.7	1.12
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	11	0.86	0.62	0.85
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	11	0.86	0.62	0.85
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	11	0.86	0.62	0.85
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	11	0.86	0.62	0.85
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	11	0.86	0.62	0.85
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	11	0.86	0.62	0.85
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	11	0.42	0.29	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	11	0.42	0.29	0.37
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	11	0.42	0.29	0.37
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	11	0.36	0.12	0.39
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	11	0.36	0.12	0.39
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	11	0.36	0.12	0.39
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	10	1.02	0.35	1.0
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	10	1.02	0.35	1.0
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	10	0.89	0.67	0.73
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	10	0.89	0.67	0.73
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	10	0.71	0.26	0.78
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	10	0.71	0.26	0.78
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	10	0.34	0.09	0.33
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	10	0.34	0.09	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	10	0.34	0.09	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	10	0.34	0.09	0.33
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	9	0.84	0.68	0.62
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	9	0.84	0.68	0.62
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	9	0.73	0.15	0.78
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	8	0.97	0.74	0.92
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	8	0.97	0.74	0.92
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	8	0.97	0.74	0.92
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	8	0.97	0.74	0.92
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	8	0.97	0.74	0.92
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	8	0.97	0.74	0.92
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	8	0.8	0.16	0.78
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	8	0.8	0.67	0.57
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	8	0.8	0.67	0.57
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	8	0.51	0.16	0.48
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	8	0.28	0.09	0.28
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	8	0.28	0.09	0.28
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	8	0.27	0.1	0.27
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	8	0.27	0.1	0.27
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	8	0.27	0.1	0.27
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	8	0.16	0.07	0.12
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	7	0.79	0.52	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	7	0.53	0.31	0.46
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	7	0.48	0.37	0.37
(1,25)	1:6:A:ARG:HH11	1:18:A:PRO:HA	6	1.14	0.71	0.9
(1,25)	1:6:A:ARG:HH12	1:18:A:PRO:HA	6	1.14	0.71	0.9
(1,80)	1:6:A:ARG:HD2	1:18:A:PRO:HB2	6	0.95	0.52	1.12
(1,80)	1:6:A:ARG:HD3	1:18:A:PRO:HB2	6	0.95	0.52	1.12
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB1	6	0.68	0.29	0.74
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB2	6	0.68	0.29	0.74
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB3	6	0.68	0.29	0.74
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB1	6	0.68	0.29	0.74
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB2	6	0.68	0.29	0.74
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB3	6	0.68	0.29	0.74
(1,138)	1:17:A:LYS:HG3	1:18:A:PRO:HD2	6	0.53	0.3	0.48
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG2	6	0.52	0.36	0.43
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG3	6	0.52	0.36	0.43
(1,133)	1:17:A:LYS:HG2	1:18:A:PRO:HD2	6	0.36	0.23	0.22
(1,233)	1:17:A:LYS:HG3	1:17:A:LYS:HD3	6	0.28	0.21	0.16
(1,6)	1:4:A:PHE:HE1	1:5:A:GLY:H	6	0.25	0.12	0.23
(1,6)	1:4:A:PHE:HE2	1:5:A:GLY:H	6	0.25	0.12	0.23
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH11	5	0.7	0.28	0.69
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH12	5	0.7	0.28	0.69
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE2	5	0.64	0.33	0.5
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE3	5	0.64	0.33	0.5
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB1	5	0.59	0.14	0.52
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB2	5	0.59	0.14	0.52
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB3	5	0.59	0.14	0.52
(1,146)	1:9:A:SER:HB3	1:10:A:ILE:HG12	5	0.41	0.26	0.38
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB1	4	1.05	0.52	1.29
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB2	4	1.05	0.52	1.29
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB3	4	1.05	0.52	1.29
(1,139)	1:4:A:PHE:H	1:17:A:LYS:HG3	4	0.84	0.85	0.37
(1,94)	1:14:A:GLU:HB2	1:15:A:GLN:HE21	4	0.57	0.42	0.5
(1,94)	1:14:A:GLU:HB3	1:15:A:GLN:HE21	4	0.57	0.42	0.5
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG2	4	0.57	0.18	0.56
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG3	4	0.57	0.18	0.56
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG2	4	0.57	0.18	0.56
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG3	4	0.57	0.18	0.56
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG2	4	0.57	0.18	0.56
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG3	4	0.57	0.18	0.56
(1,210)	1:7:A:PRO:HB2	1:9:A:SER:HA	4	0.49	0.24	0.46
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE1	3	1.16	0.04	1.15
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE2	3	1.16	0.04	1.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE3	3	1.16	0.04	1.15
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE1	3	1.16	0.04	1.15
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE2	3	1.16	0.04	1.15
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE3	3	1.16	0.04	1.15
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB1	3	0.92	0.28	0.89
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB2	3	0.92	0.28	0.89
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB3	3	0.92	0.28	0.89
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB1	3	0.92	0.28	0.89
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB2	3	0.92	0.28	0.89
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB3	3	0.92	0.28	0.89
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD11	3	0.6	0.1	0.65
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD12	3	0.6	0.1	0.65
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD13	3	0.6	0.1	0.65
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE2	3	0.52	0.25	0.37
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE3	3	0.52	0.25	0.37
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE2	3	0.52	0.25	0.37
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE3	3	0.52	0.25	0.37
(1,31)	1:6:A:ARG:H	1:18:A:PRO:HD3	3	0.51	0.38	0.28
(1,107)	1:1:A:GLY:HA2	1:2:A:VAL:HB	3	0.38	0.04	0.4
(1,97)	1:14:A:GLU:HB2	1:15:A:GLN:H	3	0.31	0.05	0.29
(1,97)	1:14:A:GLU:HB3	1:15:A:GLN:H	3	0.31	0.05	0.29
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH11	3	0.31	0.09	0.29
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH12	3	0.31	0.09	0.29
(1,102)	1:19:A:MET:H	1:19:A:MET:HE1	3	0.3	0.09	0.25
(1,102)	1:19:A:MET:H	1:19:A:MET:HE2	3	0.3	0.09	0.25
(1,102)	1:19:A:MET:H	1:19:A:MET:HE3	3	0.3	0.09	0.25
(1,103)	1:2:A:VAL:H	1:2:A:VAL:HB	3	0.3	0.01	0.29
(1,46)	1:18:A:PRO:HD2	1:19:A:MET:H	3	0.19	0.04	0.21
(1,70)	1:1:A:GLY:HA2	1:13:A:GLN:HG2	2	1.4	0.22	1.4
(1,70)	1:1:A:GLY:HA2	1:13:A:GLN:HG3	2	1.4	0.22	1.4
(1,182)	1:2:A:VAL:HG11	1:4:A:PHE:H	2	0.36	0.21	0.36
(1,182)	1:2:A:VAL:HG12	1:4:A:PHE:H	2	0.36	0.21	0.36
(1,182)	1:2:A:VAL:HG13	1:4:A:PHE:H	2	0.36	0.21	0.36
(1,182)	1:2:A:VAL:HG21	1:4:A:PHE:H	2	0.36	0.21	0.36
(1,182)	1:2:A:VAL:HG22	1:4:A:PHE:H	2	0.36	0.21	0.36
(1,182)	1:2:A:VAL:HG23	1:4:A:PHE:H	2	0.36	0.21	0.36
(1,32)	1:3:A:GLY:HA2	1:4:A:PHE:HD1	2	0.36	0.04	0.36
(1,32)	1:3:A:GLY:HA2	1:4:A:PHE:HD2	2	0.36	0.04	0.36
(1,181)	1:2:A:VAL:HG11	1:3:A:GLY:H	2	0.33	0.02	0.33
(1,181)	1:2:A:VAL:HG12	1:3:A:GLY:H	2	0.33	0.02	0.33
(1,181)	1:2:A:VAL:HG13	1:3:A:GLY:H	2	0.33	0.02	0.33
(1,181)	1:2:A:VAL:HG21	1:3:A:GLY:H	2	0.33	0.02	0.33

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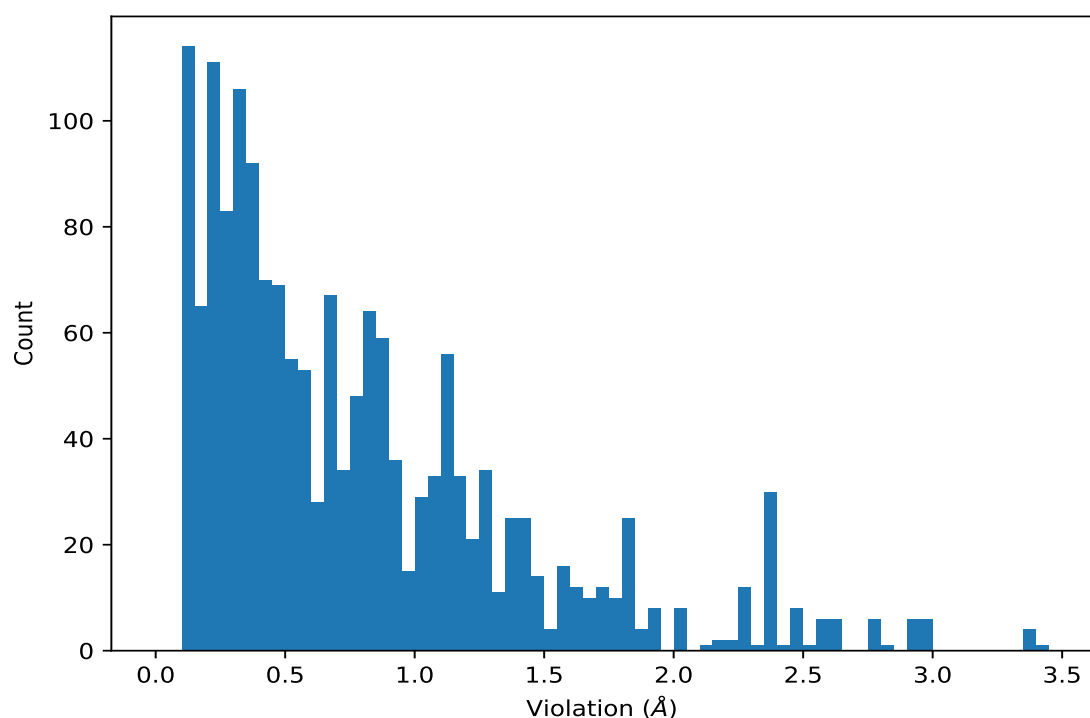
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,181)	1:2:A:VAL:HG22	1:3:A:GLY:H	2	0.33	0.02	0.33
(1,181)	1:2:A:VAL:HG23	1:3:A:GLY:H	2	0.33	0.02	0.33
(1,198)	1:4:A:PHE:HD1	1:5:A:GLY:HA3	2	0.26	0.16	0.26
(1,198)	1:4:A:PHE:HD2	1:5:A:GLY:HA3	2	0.26	0.16	0.26
(1,151)	1:5:A:GLY:H	1:6:A:ARG:HG2	2	0.25	0.09	0.25
(1,151)	1:5:A:GLY:H	1:6:A:ARG:HG3	2	0.25	0.09	0.25
(1,160)	1:10:A:ILE:HA	1:10:A:ILE:HG13	2	0.23	0.05	0.23
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG11	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG12	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG13	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG21	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG22	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG23	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG11	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG12	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG13	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG21	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG22	2	0.2	0.04	0.2
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG23	2	0.2	0.04	0.2
(1,1)	1:9:A:SER:H	1:10:A:ILE:H	2	0.14	0.02	0.14

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	10	3.41
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	14	3.38
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	14	3.38
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	14	3.38
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	14	3.38
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	18	2.99
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	18	2.99
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	18	2.99
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	18	2.99
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	14	2.96
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	14	2.96
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	4	2.92
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	4	2.92
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	4	2.92
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	4	2.92
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	4	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	4	2.92
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	18	2.83
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	16	2.77
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	16	2.77
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	16	2.77
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	16	2.77
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	4	2.75
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	4	2.75
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	15	2.65
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	15	2.65
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	15	2.65
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	15	2.65
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	4	2.63
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	4	2.63
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	6	2.56
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	6	2.56
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	6	2.56
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	6	2.56
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	6	2.56
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	6	2.56
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	13	2.52
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	3	2.49
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	3	2.49
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	16	2.47
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	16	2.47
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	16	2.47
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	16	2.47
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	16	2.47
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	16	2.47
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	8	2.41
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	7	2.4
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	7	2.4
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	7	2.4
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	7	2.4
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	7	2.4
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	7	2.4
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	12	2.39
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	7	2.37
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	7	2.37
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	7	2.37
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	7	2.37
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	7	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	7	2.37
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	10	2.37
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	10	2.37
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	1	2.37
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	10	2.37
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	10	2.37
(1,25)	1:6:A:ARG:HH11	1:18:A:PRO:HA	10	2.37
(1,25)	1:6:A:ARG:HH12	1:18:A:PRO:HA	10	2.37
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	12	2.36
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	12	2.36
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	12	2.36
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	12	2.36
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	12	2.36
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	12	2.36
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	10	2.35
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	10	2.35
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	4	2.35
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	4	2.35
(1,139)	1:4:A:PHE:H	1:17:A:LYS:HG3	9	2.31
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	8	2.29
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	8	2.29
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	8	2.29
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	8	2.29
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	8	2.29
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	8	2.29
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	19	2.29
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	19	2.29
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	19	2.29
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	19	2.29
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	16	2.26
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	16	2.26
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	9	2.24
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	9	2.24
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	18	2.15
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	17	2.15
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	14	2.11
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	5	2.01
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	5	2.01
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	5	2.01
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	5	2.01
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	5	2.01
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	5	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	15	2.0
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	15	2.0
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	15	1.94
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	15	1.94
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	15	1.94
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	15	1.94
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	15	1.94
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	15	1.94
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	16	1.91
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	16	1.91
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	7	1.86
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	7	1.86
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	19	1.85
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	19	1.85
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	12	1.84
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	12	1.84
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	9	1.84
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	9	1.84
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	9	1.83
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	9	1.83
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	9	1.83
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	9	1.83
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	6	1.83
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	17	1.82
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	17	1.82
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	10	1.82
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	10	1.82
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	10	1.82
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	10	1.82
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	17	1.8
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	17	1.8
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	17	1.8
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	17	1.8
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	17	1.8
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	17	1.8
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	20	1.8
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	20	1.8
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	20	1.8
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	20	1.8
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	17	1.79
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	17	1.79
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	17	1.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	17	1.79
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	18	1.79
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	18	1.79
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	1	1.78
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	9	1.77
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	1	1.75
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	1	1.75
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	20	1.74
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	20	1.74
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	16	1.74
(1,25)	1:6:A:ARG:HH11	1:18:A:PRO:HA	17	1.73
(1,25)	1:6:A:ARG:HH12	1:18:A:PRO:HA	17	1.73
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	1	1.72
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	1	1.72
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	1	1.72
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	1	1.72
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	1	1.72
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	1	1.72
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	7	1.71
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	13	1.69
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	13	1.69
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	5	1.69
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	5	1.69
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	6	1.67
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	6	1.67
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	5	1.66
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	5	1.66
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	5	1.66
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	5	1.66
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	3	1.65
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	3	1.65
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	3	1.65
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	17	1.63
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	17	1.63
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	18	1.63
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	18	1.63
(1,70)	1:1:A:GLY:HA2	1:13:A:GLN:HG2	6	1.62
(1,70)	1:1:A:GLY:HA2	1:13:A:GLN:HG3	6	1.62
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	17	1.61
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	14	1.6
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	10	1.6
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	19	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	19	1.59
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	19	1.59
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	19	1.59
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	19	1.59
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	19	1.59
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	19	1.58
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	14	1.58
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	14	1.58
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	10	1.56
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	10	1.56
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	12	1.56
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	9	1.55
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	9	1.55
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	9	1.55
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	9	1.55
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	19	1.54
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	6	1.52
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	17	1.52
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	17	1.52
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	5	1.48
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	20	1.47
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	8	1.47
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	4	1.47
(1,80)	1:6:A:ARG:HD2	1:18:A:PRO:HB2	10	1.47
(1,80)	1:6:A:ARG:HD3	1:18:A:PRO:HB2	10	1.47
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	3	1.47
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	3	1.47
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	5	1.46
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	5	1.46
(1,80)	1:6:A:ARG:HD2	1:18:A:PRO:HB2	13	1.46
(1,80)	1:6:A:ARG:HD3	1:18:A:PRO:HB2	13	1.46
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	6	1.46
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	6	1.46
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	15	1.45
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	15	1.45
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	20	1.45
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	20	1.45
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB1	4	1.44
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB2	4	1.44
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB3	4	1.44
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB1	15	1.44
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB2	15	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB3	15	1.44
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	17	1.44
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	17	1.44
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	19	1.44
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	19	1.44
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	8	1.44
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	8	1.44
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	16	1.43
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	16	1.43
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	4	1.43
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	4	1.43
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	8	1.42
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	8	1.42
(1,206)	1:4:A:PHE:H	1:17:A:LYS:HE2	9	1.41
(1,206)	1:4:A:PHE:H	1:17:A:LYS:HE3	9	1.41
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	16	1.41
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	16	1.39
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	1	1.39
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	1	1.39
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	18	1.39
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	5	1.39
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	5	1.39
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	14	1.37
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	14	1.37
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	14	1.37
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	14	1.37
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	14	1.37
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	14	1.37
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	20	1.37
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	20	1.37
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	20	1.37
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	20	1.37
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	20	1.37
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	20	1.37
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	7	1.36
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	7	1.36
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	7	1.36
(1,80)	1:6:A:ARG:HD2	1:18:A:PRO:HB2	2	1.35
(1,80)	1:6:A:ARG:HD3	1:18:A:PRO:HB2	2	1.35
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	11	1.35
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	11	1.35
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	13	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	11	1.34
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	11	1.34
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	2	1.33
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	2	1.33
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	2	1.33
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	2	1.33
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	9	1.33
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	14	1.33
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	14	1.33
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	12	1.31
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	10	1.29
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	10	1.29
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	10	1.29
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	10	1.29
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	10	1.29
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	10	1.29
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	14	1.28
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	14	1.28
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	14	1.28
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	14	1.28
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	14	1.28
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	14	1.28
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB1	3	1.28
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB2	3	1.28
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB3	3	1.28
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB1	3	1.28
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB2	3	1.28
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB3	3	1.28
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	16	1.28
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	16	1.28
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	11	1.27
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	11	1.27
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	11	1.27
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	11	1.27
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	11	1.27
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	11	1.27
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	18	1.27
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	18	1.27
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG2	1	1.26
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG3	1	1.26
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE2	15	1.26
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE3	15	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	2	1.26
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	2	1.26
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	18	1.24
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	18	1.24
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	18	1.24
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	19	1.24
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	19	1.24
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	16	1.23
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	16	1.23
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	3	1.23
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	3	1.23
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE1	15	1.22
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE2	15	1.22
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE3	15	1.22
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE1	15	1.22
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE2	15	1.22
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE3	15	1.22
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	15	1.22
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	15	1.22
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	4	1.22
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	4	1.22
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	4	1.22
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	4	1.22
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	6	1.2
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	6	1.2
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	13	1.2
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	13	1.2
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	13	1.19
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	13	1.19
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	13	1.19
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	2	1.18
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	2	1.18
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	2	1.18
(1,70)	1:1:A:GLY:HA2	1:13:A:GLN:HG2	3	1.18
(1,70)	1:1:A:GLY:HA2	1:13:A:GLN:HG3	3	1.18
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	11	1.17
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	11	1.17
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	16	1.17
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	9	1.16
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	9	1.16
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	9	1.16
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	9	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	9	1.16
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	9	1.16
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	9	1.16
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	9	1.16
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	9	1.16
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	9	1.16
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	9	1.16
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	9	1.16
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	8	1.16
(1,94)	1:14:A:GLU:HB2	1:15:A:GLN:HE21	19	1.16
(1,94)	1:14:A:GLU:HB3	1:15:A:GLN:HE21	19	1.16
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	5	1.16
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	17	1.16
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	17	1.16
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE1	13	1.15
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE2	13	1.15
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE3	13	1.15
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE1	13	1.15
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE2	13	1.15
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE3	13	1.15
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	9	1.15
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	2	1.14
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	2	1.14
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	2	1.14
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	2	1.14
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	2	1.14
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	2	1.14
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB1	17	1.14
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB2	17	1.14
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB3	17	1.14
(1,138)	1:17:A:LYS:HG3	1:18:A:PRO:HD2	18	1.14
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE1	11	1.12
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE2	11	1.12
(1,219)	1:19:A:MET:HB2	1:19:A:MET:HE3	11	1.12
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE1	11	1.12
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE2	11	1.12
(1,219)	1:19:A:MET:HB3	1:19:A:MET:HE3	11	1.12
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	17	1.12
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	17	1.12
(1,184)	1:11:A:LEU:HD11	1:13:A:GLN:HG2	11	1.12
(1,184)	1:11:A:LEU:HD11	1:13:A:GLN:HG3	11	1.12
(1,184)	1:11:A:LEU:HD12	1:13:A:GLN:HG2	11	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	1:11:A:LEU:HD12	1:13:A:GLN:HG3	11	1.12
(1,184)	1:11:A:LEU:HD13	1:13:A:GLN:HG2	11	1.12
(1,184)	1:11:A:LEU:HD13	1:13:A:GLN:HG3	11	1.12
(1,184)	1:11:A:LEU:HD21	1:13:A:GLN:HG2	11	1.12
(1,184)	1:11:A:LEU:HD21	1:13:A:GLN:HG3	11	1.12
(1,184)	1:11:A:LEU:HD22	1:13:A:GLN:HG2	11	1.12
(1,184)	1:11:A:LEU:HD22	1:13:A:GLN:HG3	11	1.12
(1,184)	1:11:A:LEU:HD23	1:13:A:GLN:HG2	11	1.12
(1,184)	1:11:A:LEU:HD23	1:13:A:GLN:HG3	11	1.12
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	4	1.12
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	18	1.11
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	18	1.11
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	18	1.11
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	18	1.11
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	18	1.11
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	18	1.11
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	11	1.11
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	11	1.11
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	2	1.11
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	2	1.11
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	2	1.11
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	2	1.11
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	2	1.11
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	2	1.11
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	2	1.11
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	2	1.11
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	4	1.1
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	4	1.1
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	13	1.09
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	13	1.09
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	13	1.09
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	13	1.09
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	13	1.09
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	13	1.09
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB1	19	1.09
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB2	19	1.09
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB3	19	1.09
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB1	19	1.09
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB2	19	1.09
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB3	19	1.09
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	12	1.09
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	12	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,25)	1:6:A:ARG:HH11	1:18:A:PRO:HA	5	1.09
(1,25)	1:6:A:ARG:HH12	1:18:A:PRO:HA	5	1.09
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	6	1.08
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	6	1.08
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	6	1.08
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	6	1.08
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	3	1.08
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	3	1.08
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	11	1.07
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	11	1.07
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	11	1.07
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	11	1.07
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	11	1.07
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	11	1.07
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	7	1.07
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	16	1.05
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	16	1.05
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	19	1.05
(1,31)	1:6:A:ARG:H	1:18:A:PRO:HD3	17	1.05
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH11	18	1.04
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH12	18	1.04
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	5	1.04
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	5	1.04
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	16	1.03
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	16	1.03
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	16	1.03
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	16	1.03
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	6	1.02
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	6	1.02
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	11	1.02
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	11	1.02
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	11	1.02
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	11	1.02
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	7	1.01
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	7	1.01
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	19	1.01
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	19	1.01
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	19	1.01
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	10	1.01
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	10	1.01
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	16	1.01
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	14	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	14	1.0
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	5	1.0
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	5	1.0
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	5	1.0
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	3	1.0
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	1	1.0
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	12	0.98
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	12	0.98
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	12	0.98
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	12	0.98
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	16	0.97
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	16	0.97
(1,163)	1:9:A:SER:HB2	1:10:A:ILE:HG13	13	0.97
(1,163)	1:9:A:SER:HB3	1:10:A:ILE:HG13	13	0.97
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	2	0.97
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	2	0.97
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	1	0.96
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	1	0.96
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	8	0.96
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	8	0.96
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	8	0.96
(1,185)	1:11:A:LEU:HD11	1:13:A:GLN:HB2	11	0.95
(1,185)	1:11:A:LEU:HD11	1:13:A:GLN:HB3	11	0.95
(1,185)	1:11:A:LEU:HD12	1:13:A:GLN:HB2	11	0.95
(1,185)	1:11:A:LEU:HD12	1:13:A:GLN:HB3	11	0.95
(1,185)	1:11:A:LEU:HD13	1:13:A:GLN:HB2	11	0.95
(1,185)	1:11:A:LEU:HD13	1:13:A:GLN:HB3	11	0.95
(1,185)	1:11:A:LEU:HD21	1:13:A:GLN:HB2	11	0.95
(1,185)	1:11:A:LEU:HD21	1:13:A:GLN:HB3	11	0.95
(1,185)	1:11:A:LEU:HD22	1:13:A:GLN:HB2	11	0.95
(1,185)	1:11:A:LEU:HD22	1:13:A:GLN:HB3	11	0.95
(1,185)	1:11:A:LEU:HD23	1:13:A:GLN:HB2	11	0.95
(1,185)	1:11:A:LEU:HD23	1:13:A:GLN:HB3	11	0.95
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	12	0.94
(1,96)	1:4:A:PHE:HE1	1:15:A:GLN:HB3	7	0.94
(1,96)	1:4:A:PHE:HE2	1:15:A:GLN:HB3	7	0.94
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	5	0.93
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	5	0.93
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	5	0.93
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	10	0.93
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	10	0.93
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	5	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	11	0.92
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	11	0.92
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	11	0.92
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	11	0.92
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	8	0.92
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	8	0.92
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH11	19	0.92
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH12	19	0.92
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	5	0.92
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	5	0.92
(1,80)	1:6:A:ARG:HD2	1:18:A:PRO:HB2	1	0.9
(1,80)	1:6:A:ARG:HD3	1:18:A:PRO:HB2	1	0.9
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	13	0.9
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	13	0.9
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	4	0.9
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	13	0.89
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	13	0.89
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	13	0.89
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	13	0.89
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	13	0.89
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	13	0.89
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB1	14	0.89
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB2	14	0.89
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB3	14	0.89
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB1	14	0.89
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB2	14	0.89
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB3	14	0.89
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	14	0.89
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	14	0.89
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	14	0.89
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	15	0.89
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	2	0.89
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	2	0.89
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	2	0.89
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	2	0.89
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE2	16	0.88
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE3	16	0.88
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE2	16	0.88
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE3	16	0.88
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	8	0.88
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	8	0.88
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	8	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	8	0.88
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	8	0.88
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	8	0.88
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	1	0.87
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	1	0.87
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	1	0.87
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	1	0.87
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	1	0.87
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	1	0.87
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	19	0.87
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	19	0.87
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	19	0.87
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	2	0.87
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	2	0.87
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	2	0.87
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	2	0.87
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	2	0.87
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	2	0.87
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB1	10	0.87
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB2	10	0.87
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB3	10	0.87
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB1	10	0.87
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB2	10	0.87
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB3	10	0.87
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	19	0.87
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	19	0.87
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	7	0.87
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	4	0.87
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	13	0.87
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	13	0.87
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	15	0.86
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	4	0.86
(1,210)	1:7:A:PRO:HB2	1:9:A:SER:HA	7	0.85
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	9	0.85
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	9	0.85
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	9	0.85
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	3	0.85
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	3	0.85
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	3	0.85
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	3	0.85
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	3	0.85
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	3	0.85

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB1	16	0.85
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB2	16	0.85
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB3	16	0.85
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	6	0.85
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	6	0.85
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	6	0.85
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	6	0.85
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	7	0.84
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	7	0.84
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	7	0.84
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	7	0.84
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	5	0.84
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	5	0.84
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	6	0.84
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	6	0.84
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	14	0.84
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	10	0.84
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	12	0.84
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	12	0.84
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	7	0.84
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	10	0.83
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	10	0.83
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	6	0.82
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	6	0.82
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	6	0.82
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	1	0.82
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	1	0.82
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	1	0.82
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG2	1	0.82
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG3	1	0.82
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG2	1	0.82
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG3	1	0.82
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG2	1	0.82
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG3	1	0.82
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	2	0.82
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	15	0.82
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	18	0.82
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	18	0.82
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	17	0.81
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	16	0.81
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	2	0.8
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	2	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	2	0.8
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB1	18	0.8
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB2	18	0.8
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB3	18	0.8
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB1	18	0.8
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB2	18	0.8
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB3	18	0.8
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	5	0.8
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	5	0.8
(1,133)	1:17:A:LYS:HG2	1:18:A:PRO:HD2	20	0.8
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	13	0.8
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	17	0.8
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	3	0.79
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	3	0.79
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	3	0.79
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	3	0.79
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	3	0.79
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	3	0.79
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	6	0.79
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	6	0.79
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	3	0.79
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	3	0.79
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	3	0.79
(1,161)	1:9:A:SER:H	1:10:A:ILE:HG13	10	0.79
(1,146)	1:9:A:SER:HB3	1:10:A:ILE:HG12	3	0.79
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	15	0.79
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	20	0.79
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	20	0.79
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	15	0.78
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	15	0.78
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	19	0.78
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	19	0.78
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	13	0.78
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	9	0.78
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	16	0.78
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	6	0.78
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	6	0.78
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	19	0.78
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	3	0.77
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	3	0.77
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	18	0.77
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	18	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	18	0.77
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	18	0.77
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	18	0.77
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	18	0.77
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	19	0.77
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	19	0.77
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	18	0.77
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	11	0.77
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	15	0.76
(1,94)	1:14:A:GLU:HB2	1:15:A:GLN:HE21	1	0.76
(1,94)	1:14:A:GLU:HB3	1:15:A:GLN:HE21	1	0.76
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	17	0.75
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	17	0.75
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	17	0.75
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	10	0.75
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	10	0.75
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	10	0.75
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	5	0.75
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	3	0.74
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	3	0.74
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	10	0.74
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	12	0.74
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	13	0.74
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	3	0.74
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	4	0.74
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	15	0.73
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	15	0.73
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	15	0.73
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	15	0.73
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	9	0.73
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	9	0.73
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	9	0.73
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	3	0.73
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	3	0.73
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	15	0.73
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	6	0.72
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	6	0.72
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	18	0.72
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	18	0.72
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	18	0.72
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	18	0.72
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	18	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	18	0.72
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	18	0.72
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	18	0.72
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	18	0.72
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	18	0.72
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	18	0.72
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	18	0.72
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	13	0.71
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	13	0.71
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	13	0.71
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	13	0.7
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	13	0.7
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	1	0.7
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	1	0.7
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	1	0.7
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	1	0.7
(1,201)	1:6:A:ARG:HD2	1:9:A:SER:H	5	0.7
(1,201)	1:6:A:ARG:HD3	1:9:A:SER:H	5	0.7
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD11	13	0.7
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD12	13	0.7
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD13	13	0.7
(1,25)	1:6:A:ARG:HH11	1:18:A:PRO:HA	6	0.7
(1,25)	1:6:A:ARG:HH12	1:18:A:PRO:HA	6	0.7
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	16	0.69
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	16	0.69
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	16	0.69
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB1	7	0.69
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB2	7	0.69
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB3	7	0.69
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB1	7	0.69
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB2	7	0.69
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB3	7	0.69
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	3	0.69
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	3	0.69
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH11	1	0.69
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH12	1	0.69
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	4	0.69
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	17	0.69
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	13	0.69
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	13	0.69
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	11	0.69
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	11	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE2	4	0.68
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE3	4	0.68
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	11	0.68
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	11	0.68
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	11	0.68
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	11	0.68
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	11	0.68
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	11	0.68
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	2	0.68
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	5	0.67
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	12	0.67
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	12	0.67
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	7	0.67
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	9	0.66
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	9	0.66
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	9	0.66
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	14	0.66
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	14	0.66
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	14	0.66
(1,122)	1:10:A:ILE:H	1:10:A:ILE:HB	13	0.66
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	6	0.66
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	20	0.66
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	11	0.66
(1,25)	1:6:A:ARG:HH11	1:18:A:PRO:HA	2	0.66
(1,25)	1:6:A:ARG:HH12	1:18:A:PRO:HA	2	0.66
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	9	0.66
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD11	3	0.65
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD12	3	0.65
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD13	3	0.65
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	11	0.65
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	11	0.65
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	11	0.65
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	16	0.65
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH11	16	0.65
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH12	16	0.65
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG2	10	0.64
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG3	10	0.64
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG2	10	0.64
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG3	10	0.64
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG2	10	0.64
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG3	10	0.64
(1,146)	1:9:A:SER:HB3	1:10:A:ILE:HG12	15	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	12	0.63
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	3	0.63
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	14	0.62
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	14	0.62
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	14	0.62
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB1	19	0.62
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB2	19	0.62
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB3	19	0.62
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	5	0.62
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	5	0.62
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	16	0.62
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	16	0.62
(1,155)	1:12:A:THR:HG21	1:13:A:GLN:HB2	10	0.61
(1,155)	1:12:A:THR:HG21	1:13:A:GLN:HB3	10	0.61
(1,155)	1:12:A:THR:HG22	1:13:A:GLN:HB2	10	0.61
(1,155)	1:12:A:THR:HG22	1:13:A:GLN:HB3	10	0.61
(1,155)	1:12:A:THR:HG23	1:13:A:GLN:HB2	10	0.61
(1,155)	1:12:A:THR:HG23	1:13:A:GLN:HB3	10	0.61
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	10	0.61
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	1	0.61
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	17	0.61
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	14	0.6
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	14	0.6
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	17	0.6
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	17	0.6
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	3	0.6
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	7	0.6
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	7	0.6
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	7	0.6
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	7	0.6
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	19	0.6
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	11	0.59
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB1	4	0.59
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB2	4	0.59
(1,170)	1:6:A:ARG:HD2	1:16:A:ALA:HB3	4	0.59
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB1	4	0.59
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB2	4	0.59
(1,170)	1:6:A:ARG:HD3	1:16:A:ALA:HB3	4	0.59
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	20	0.59
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	9	0.59
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	7	0.59
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	7	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,233)	1:17:A:LYS:HG3	1:17:A:LYS:HD3	9	0.58
(1,233)	1:17:A:LYS:HG3	1:17:A:LYS:HD3	16	0.58
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG2	20	0.58
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG3	20	0.58
(1,182)	1:2:A:VAL:HG11	1:4:A:PHE:H	9	0.58
(1,182)	1:2:A:VAL:HG12	1:4:A:PHE:H	9	0.58
(1,182)	1:2:A:VAL:HG13	1:4:A:PHE:H	9	0.58
(1,182)	1:2:A:VAL:HG21	1:4:A:PHE:H	9	0.58
(1,182)	1:2:A:VAL:HG22	1:4:A:PHE:H	9	0.58
(1,182)	1:2:A:VAL:HG23	1:4:A:PHE:H	9	0.58
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	4	0.58
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	11	0.57
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	11	0.57
(1,138)	1:17:A:LYS:HG3	1:18:A:PRO:HD2	7	0.57
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	19	0.57
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	17	0.56
(1,210)	1:7:A:PRO:HB2	1:9:A:SER:HA	12	0.55
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	14	0.55
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	14	0.55
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	14	0.55
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	14	0.55
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	14	0.55
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	14	0.55
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	14	0.55
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	14	0.55
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	14	0.55
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	14	0.55
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	14	0.55
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	14	0.55
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	15	0.55
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	8	0.55
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	10	0.55
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	17	0.54
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	17	0.54
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	17	0.54
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	17	0.54
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	17	0.54
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	17	0.54
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	2	0.54
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	2	0.54
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	4	0.54
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	10	0.54
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	1	0.54
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	1	0.54
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	5	0.53
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	5	0.53
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	8	0.53
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	8	0.53
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	8	0.53
(1,138)	1:17:A:LYS:HG3	1:18:A:PRO:HD2	14	0.53
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	8	0.53
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	9	0.53
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	6	0.52
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	6	0.52
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	6	0.52
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	6	0.52
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	6	0.52
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	6	0.52
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	6	0.52
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	6	0.52
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	6	0.52
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB1	7	0.52
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB2	7	0.52
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB3	7	0.52
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	2	0.52
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	2	0.52
(1,112)	1:4:A:PHE:H	1:17:A:LYS:HB2	18	0.52
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	13	0.51
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	13	0.51
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	13	0.51
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	13	0.51
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	15	0.51
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	15	0.51
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	15	0.51
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	6	0.51
(1,133)	1:17:A:LYS:HG2	1:18:A:PRO:HD2	18	0.51
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	6	0.51
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	7	0.51
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	2	0.5
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	2	0.5
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE2	9	0.5
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE3	9	0.5
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	6	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	8	0.5
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	8	0.5
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	12	0.5
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	14	0.49
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	14	0.49
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	14	0.49
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG2	12	0.49
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG3	12	0.49
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	18	0.49
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	18	0.49
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	18	0.49
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB1	4	0.49
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB2	4	0.49
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB3	4	0.49
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB1	5	0.49
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB2	5	0.49
(1,166)	1:6:A:ARG:H	1:16:A:ALA:HB3	5	0.49
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	7	0.49
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	7	0.49
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	7	0.49
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG2	19	0.49
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG3	19	0.49
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG2	19	0.49
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG3	19	0.49
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG2	19	0.49
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG3	19	0.49
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	5	0.49
(1,6)	1:4:A:PHE:HE1	1:5:A:GLY:H	8	0.49
(1,6)	1:4:A:PHE:HE2	1:5:A:GLY:H	8	0.49
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	5	0.48
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	5	0.48
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	5	0.48
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	5	0.48
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	6	0.48
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	6	0.48
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	6	0.48
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	6	0.48
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	5	0.48
(1,82)	1:6:A:ARG:HH11	1:18:A:PRO:HB2	18	0.48
(1,82)	1:6:A:ARG:HH12	1:18:A:PRO:HB2	18	0.48
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	3	0.48
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	3	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:5:A:GLY:H	1:6:A:ARG:H	8	0.48
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	13	0.47
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	13	0.47
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	12	0.47
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	12	0.47
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	12	0.47
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	5	0.47
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	5	0.47
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	5	0.47
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	15	0.47
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	15	0.47
(1,134)	1:17:A:LYS:H	1:17:A:LYS:HG2	2	0.47
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	11	0.46
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	11	0.46
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	11	0.46
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	16	0.46
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD11	18	0.46
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD12	18	0.46
(1,192)	1:9:A:SER:HB2	1:10:A:ILE:HD13	18	0.46
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	7	0.46
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	7	0.46
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	7	0.46
(1,128)	1:7:A:PRO:HG2	1:9:A:SER:H	20	0.46
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	14	0.46
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	5	0.46
(1,105)	1:17:A:LYS:HB3	1:18:A:PRO:HD2	19	0.45
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	20	0.45
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	20	0.45
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	20	0.45
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	20	0.45
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	8	0.44
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	8	0.44
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	8	0.44
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	8	0.44
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	8	0.44
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	8	0.44
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	8	0.44
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	8	0.44
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	8	0.44
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	8	0.44
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	8	0.44
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	6	0.43
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	6	0.43
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	6	0.43
(1,198)	1:4:A:PHE:HD1	1:5:A:GLY:HA3	8	0.43
(1,198)	1:4:A:PHE:HD2	1:5:A:GLY:HA3	8	0.43
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	5	0.43
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	5	0.43
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	5	0.43
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	5	0.43
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	5	0.43
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	5	0.43
(1,138)	1:17:A:LYS:HG3	1:18:A:PRO:HD2	13	0.43
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH11	4	0.43
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH12	4	0.43
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE2	16	0.42
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE3	16	0.42
(1,107)	1:1:A:GLY:HA2	1:2:A:VAL:HB	18	0.42
(1,102)	1:19:A:MET:H	1:19:A:MET:HE1	15	0.42
(1,102)	1:19:A:MET:H	1:19:A:MET:HE2	15	0.42
(1,102)	1:19:A:MET:H	1:19:A:MET:HE3	15	0.42
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	2	0.42
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	2	0.42
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	13	0.42
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	16	0.42
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	19	0.42
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	18	0.42
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	9	0.42
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	9	0.42
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	9	0.42
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	18	0.41
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	17	0.41
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	17	0.41
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	15	0.41
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	15	0.41
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	15	0.41
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	15	0.41
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	15	0.41
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	15	0.41
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	15	0.41
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	15	0.41
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	15	0.41
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	2	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	2	0.41
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	15	0.4
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	15	0.4
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	9	0.4
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	9	0.4
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	9	0.4
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	3	0.4
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	3	0.4
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	3	0.4
(1,107)	1:1:A:GLY:HA2	1:2:A:VAL:HB	9	0.4
(1,65)	1:4:A:PHE:HD1	1:15:A:GLN:HG2	19	0.4
(1,65)	1:4:A:PHE:HD1	1:15:A:GLN:HG3	19	0.4
(1,65)	1:4:A:PHE:HD2	1:15:A:GLN:HG2	19	0.4
(1,65)	1:4:A:PHE:HD2	1:15:A:GLN:HG3	19	0.4
(1,32)	1:3:A:GLY:HA2	1:4:A:PHE:HD1	14	0.4
(1,32)	1:3:A:GLY:HA2	1:4:A:PHE:HD2	14	0.4
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	4	0.39
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	4	0.39
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	4	0.39
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	13	0.39
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	13	0.39
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	13	0.39
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	16	0.39
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	16	0.39
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	16	0.39
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	15	0.39
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	15	0.39
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	18	0.39
(1,68)	1:12:A:THR:HA	1:13:A:GLN:HG2	1	0.39
(1,68)	1:12:A:THR:HA	1:13:A:GLN:HG3	1	0.39
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	13	0.38
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	13	0.38
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	13	0.38
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	16	0.38
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	16	0.38
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	16	0.38
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	16	0.38
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	16	0.38
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	16	0.38
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	16	0.38
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	16	0.38
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	16	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	16	0.38
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	16	0.38
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	16	0.38
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	14	0.38
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	14	0.38
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	14	0.38
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	14	0.38
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	16	0.38
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	16	0.38
(1,146)	1:9:A:SER:HB3	1:10:A:ILE:HG12	16	0.38
(1,139)	1:4:A:PHE:H	1:17:A:LYS:HG3	10	0.38
(1,97)	1:14:A:GLU:HB2	1:15:A:GLN:H	9	0.38
(1,97)	1:14:A:GLU:HB3	1:15:A:GLN:H	9	0.38
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	12	0.38
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG2	19	0.37
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG3	19	0.37
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE2	9	0.37
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE3	9	0.37
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE2	9	0.37
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE3	9	0.37
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	14	0.37
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	1	0.37
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	1	0.37
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	1	0.37
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	1	0.37
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	1	0.37
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	1	0.37
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	1	0.37
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	1	0.37
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	1	0.37
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	1	0.37
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	1	0.37
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	1	0.37
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	1	0.37
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	1	0.37
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	1	0.37
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	9	0.37
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	9	0.37
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	9	0.37
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	9	0.37
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	9	0.37
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	6	0.37
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	6	0.37
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	6	0.37
(1,138)	1:17:A:LYS:HG3	1:18:A:PRO:HD2	11	0.37
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	3	0.37
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	8	0.37
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	8	0.37
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	2	0.37
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	9	0.37
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	13	0.37
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	13	0.37
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	13	0.37
(1,243)	1:2:A:VAL:HG11	1:6:A:ARG:H	9	0.36
(1,243)	1:2:A:VAL:HG12	1:6:A:ARG:H	9	0.36
(1,243)	1:2:A:VAL:HG13	1:6:A:ARG:H	9	0.36
(1,243)	1:2:A:VAL:HG21	1:6:A:ARG:H	9	0.36
(1,243)	1:2:A:VAL:HG22	1:6:A:ARG:H	9	0.36
(1,243)	1:2:A:VAL:HG23	1:6:A:ARG:H	9	0.36
(1,210)	1:7:A:PRO:HB2	1:9:A:SER:HA	13	0.36
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	8	0.36
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	8	0.36
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	8	0.36
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	8	0.36
(1,139)	1:4:A:PHE:H	1:17:A:LYS:HG3	20	0.36
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	18	0.35
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	18	0.35
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	15	0.35
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	15	0.35
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	15	0.35
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE2	5	0.35
(1,204)	1:5:A:GLY:HA3	1:17:A:LYS:HE3	5	0.35
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	20	0.35
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	20	0.35
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	20	0.35
(1,181)	1:2:A:VAL:HG11	1:3:A:GLY:H	9	0.35
(1,181)	1:2:A:VAL:HG12	1:3:A:GLY:H	9	0.35
(1,181)	1:2:A:VAL:HG13	1:3:A:GLY:H	9	0.35
(1,181)	1:2:A:VAL:HG21	1:3:A:GLY:H	9	0.35
(1,181)	1:2:A:VAL:HG22	1:3:A:GLY:H	9	0.35
(1,181)	1:2:A:VAL:HG23	1:3:A:GLY:H	9	0.35
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	9	0.35
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	17	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	20	0.35
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	12	0.34
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	12	0.34
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	12	0.34
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	18	0.34
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	18	0.34
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	18	0.34
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB1	3	0.34
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB2	3	0.34
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB3	3	0.34
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB1	3	0.34
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB2	3	0.34
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB3	3	0.34
(1,151)	1:5:A:GLY:H	1:6:A:ARG:HG2	7	0.34
(1,151)	1:5:A:GLY:H	1:6:A:ARG:HG3	7	0.34
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	4	0.34
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	4	0.34
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	19	0.34
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	19	0.34
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	9	0.34
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	9	0.34
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	16	0.34
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	16	0.34
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	16	0.34
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	13	0.34
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	11	0.33
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	11	0.33
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	11	0.33
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	5	0.33
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	5	0.33
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	5	0.33
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	11	0.33
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	11	0.33
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	11	0.33
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	11	0.33
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	11	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	11	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	11	0.33
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	15	0.33
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	15	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	15	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	16	0.33
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	16	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	16	0.33
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	16	0.33
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG2	4	0.32
(1,209)	1:4:A:PHE:HE1	1:15:A:GLN:HG3	4	0.32
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG2	4	0.32
(1,209)	1:4:A:PHE:HE2	1:15:A:GLN:HG3	4	0.32
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE2	15	0.32
(1,205)	1:4:A:PHE:HD1	1:17:A:LYS:HE3	15	0.32
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE2	15	0.32
(1,205)	1:4:A:PHE:HD2	1:17:A:LYS:HE3	15	0.32
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	16	0.32
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	16	0.32
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	16	0.32
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG2	20	0.32
(1,156)	1:12:A:THR:HG21	1:13:A:GLN:HG3	20	0.32
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG2	20	0.32
(1,156)	1:12:A:THR:HG22	1:13:A:GLN:HG3	20	0.32
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG2	20	0.32
(1,156)	1:12:A:THR:HG23	1:13:A:GLN:HG3	20	0.32
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	3	0.32
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	3	0.32
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	3	0.32
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	3	0.32
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	20	0.32
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	20	0.32
(1,139)	1:4:A:PHE:H	1:17:A:LYS:HG3	16	0.32
(1,107)	1:1:A:GLY:HA2	1:2:A:VAL:HB	13	0.32
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	1	0.32
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	1	0.32
(1,32)	1:3:A:GLY:HA2	1:4:A:PHE:HD1	18	0.32
(1,32)	1:3:A:GLY:HA2	1:4:A:PHE:HD2	18	0.32
(1,181)	1:2:A:VAL:HG11	1:3:A:GLY:H	18	0.31
(1,181)	1:2:A:VAL:HG12	1:3:A:GLY:H	18	0.31
(1,181)	1:2:A:VAL:HG13	1:3:A:GLY:H	18	0.31
(1,181)	1:2:A:VAL:HG21	1:3:A:GLY:H	18	0.31
(1,181)	1:2:A:VAL:HG22	1:3:A:GLY:H	18	0.31
(1,181)	1:2:A:VAL:HG23	1:3:A:GLY:H	18	0.31
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	7	0.31
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	7	0.31
(1,103)	1:2:A:VAL:H	1:2:A:VAL:HB	13	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,80)	1:6:A:ARG:HD2	1:18:A:PRO:HB2	11	0.31
(1,80)	1:6:A:ARG:HD3	1:18:A:PRO:HB2	11	0.31
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	10	0.31
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	10	0.31
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	8	0.3
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	8	0.3
(1,125)	1:6:A:ARG:H	1:6:A:ARG:HB3	18	0.3
(1,92)	1:4:A:PHE:HD1	1:15:A:GLN:HB3	9	0.3
(1,92)	1:4:A:PHE:HD2	1:15:A:GLN:HB3	9	0.3
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	20	0.3
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	11	0.3
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	11	0.3
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	11	0.3
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	18	0.29
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	18	0.29
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	18	0.29
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	18	0.29
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH11	19	0.29
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH12	19	0.29
(1,103)	1:2:A:VAL:H	1:2:A:VAL:HB	9	0.29
(1,103)	1:2:A:VAL:H	1:2:A:VAL:HB	18	0.29
(1,101)	1:18:A:PRO:HG2	1:19:A:MET:H	18	0.29
(1,97)	1:14:A:GLU:HB2	1:15:A:GLN:H	7	0.29
(1,97)	1:14:A:GLU:HB3	1:15:A:GLN:H	7	0.29
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	15	0.29
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	15	0.29
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	5	0.28
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	5	0.28
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	5	0.28
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	4	0.28
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	4	0.28
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	4	0.28
(1,160)	1:10:A:ILE:HA	1:10:A:ILE:HG13	10	0.28
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	15	0.28
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	16	0.28
(1,31)	1:6:A:ARG:H	1:18:A:PRO:HD3	10	0.28
(1,25)	1:6:A:ARG:HH11	1:18:A:PRO:HA	1	0.28
(1,25)	1:6:A:ARG:HH12	1:18:A:PRO:HA	1	0.28
(1,6)	1:4:A:PHE:HE1	1:5:A:GLY:H	6	0.28
(1,6)	1:4:A:PHE:HE2	1:5:A:GLY:H	6	0.28
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	1	0.27
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB1	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB2	20	0.27
(1,164)	1:6:A:ARG:HG2	1:16:A:ALA:HB3	20	0.27
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB1	20	0.27
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB2	20	0.27
(1,164)	1:6:A:ARG:HG3	1:16:A:ALA:HB3	20	0.27
(1,97)	1:14:A:GLU:HB2	1:15:A:GLN:H	1	0.27
(1,97)	1:14:A:GLU:HB3	1:15:A:GLN:H	1	0.27
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	18	0.27
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	2	0.26
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	2	0.26
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	2	0.26
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	2	0.26
(1,144)	1:6:A:ARG:HG2	1:18:A:PRO:HD3	9	0.26
(1,144)	1:6:A:ARG:HG3	1:18:A:PRO:HD3	9	0.26
(1,87)	1:6:A:ARG:H	1:15:A:GLN:HB2	11	0.26
(1,37)	1:1:A:GLY:HA2	1:2:A:VAL:H	7	0.26
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	14	0.26
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	12	0.25
(1,189)	1:10:A:ILE:HA	1:10:A:ILE:HD11	13	0.25
(1,189)	1:10:A:ILE:HA	1:10:A:ILE:HD12	13	0.25
(1,189)	1:10:A:ILE:HA	1:10:A:ILE:HD13	13	0.25
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	13	0.25
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	13	0.25
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	13	0.25
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	13	0.25
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	13	0.25
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	13	0.25
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	13	0.25
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	13	0.25
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	13	0.25
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	13	0.25
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	13	0.25
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	13	0.25
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	8	0.25
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	8	0.25
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	8	0.25
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	2	0.25
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	2	0.25
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	2	0.25
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	19	0.25
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	19	0.25
(1,102)	1:19:A:MET:H	1:19:A:MET:HE1	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,102)	1:19:A:MET:H	1:19:A:MET:HE2	13	0.25
(1,102)	1:19:A:MET:H	1:19:A:MET:HE3	13	0.25
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	12	0.25
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH11	10	0.24
(1,196)	1:6:A:ARG:H	1:6:A:ARG:HH12	10	0.24
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG11	7	0.24
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG12	7	0.24
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG13	7	0.24
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG21	7	0.24
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG22	7	0.24
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG23	7	0.24
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG11	7	0.24
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG12	7	0.24
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG13	7	0.24
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG21	7	0.24
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG22	7	0.24
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG23	7	0.24
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	20	0.24
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	20	0.24
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	20	0.24
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	15	0.24
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	15	0.24
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	4	0.24
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	4	0.24
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	4	0.24
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	4	0.24
(1,132)	1:7:A:PRO:HG2	1:9:A:SER:HA	2	0.24
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	16	0.24
(1,6)	1:4:A:PHE:HE1	1:5:A:GLY:H	9	0.24
(1,6)	1:4:A:PHE:HE2	1:5:A:GLY:H	9	0.24
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	10	0.24
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	10	0.24
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	10	0.24
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG2	5	0.23
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG3	5	0.23
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	7	0.23
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	20	0.23
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	20	0.23
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	20	0.23
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	20	0.23
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	20	0.23
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	20	0.23
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	20	0.23
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	20	0.23
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	20	0.23
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	20	0.23
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	20	0.23
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	5	0.23
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	5	0.23
(1,102)	1:19:A:MET:H	1:19:A:MET:HE1	11	0.23
(1,102)	1:19:A:MET:H	1:19:A:MET:HE2	11	0.23
(1,102)	1:19:A:MET:H	1:19:A:MET:HE3	11	0.23
(1,94)	1:14:A:GLU:HB2	1:15:A:GLN:HE21	3	0.23
(1,94)	1:14:A:GLU:HB3	1:15:A:GLN:HE21	3	0.23
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	17	0.23
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	17	0.23
(1,46)	1:18:A:PRO:HD2	1:19:A:MET:H	3	0.23
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	3	0.23
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	11	0.22
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	11	0.22
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	11	0.22
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	11	0.22
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	11	0.22
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	11	0.22
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	11	0.22
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	11	0.22
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	11	0.22
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	11	0.22
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	11	0.22
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	11	0.22
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	11	0.22
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	11	0.22
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	13	0.22
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	13	0.22
(1,133)	1:17:A:LYS:HG2	1:18:A:PRO:HD2	7	0.22
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH11	13	0.22
(1,126)	1:6:A:ARG:HB3	1:6:A:ARG:HH12	13	0.22
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	7	0.22
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	13	0.22
(1,6)	1:4:A:PHE:HE1	1:5:A:GLY:H	20	0.22
(1,6)	1:4:A:PHE:HE2	1:5:A:GLY:H	20	0.22
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	13	0.21
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	13	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	13	0.21
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	18	0.21
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	18	0.21
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	18	0.21
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB1	1	0.21
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB2	1	0.21
(1,165)	1:6:A:ARG:HB3	1:16:A:ALA:HB3	1	0.21
(1,133)	1:17:A:LYS:HG2	1:18:A:PRO:HD2	9	0.21
(1,80)	1:6:A:ARG:HD2	1:18:A:PRO:HB2	12	0.21
(1,80)	1:6:A:ARG:HD3	1:18:A:PRO:HB2	12	0.21
(1,46)	1:18:A:PRO:HD2	1:19:A:MET:H	2	0.21
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	10	0.21
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	11	0.21
(1,31)	1:6:A:ARG:H	1:18:A:PRO:HD3	6	0.21
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	12	0.21
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	5	0.2
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB1	4	0.2
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB2	4	0.2
(1,167)	1:5:A:GLY:H	1:16:A:ALA:HB3	4	0.2
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH11	1	0.2
(1,149)	1:6:A:ARG:HG2	1:6:A:ARG:HH12	1	0.2
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH11	1	0.2
(1,149)	1:6:A:ARG:HG3	1:6:A:ARG:HH12	1	0.2
(1,133)	1:17:A:LYS:HG2	1:18:A:PRO:HD2	11	0.2
(1,133)	1:17:A:LYS:HG2	1:18:A:PRO:HD2	14	0.2
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH11	18	0.2
(1,120)	1:6:A:ARG:HB2	1:6:A:ARG:HH12	18	0.2
(1,85)	1:15:A:GLN:HB2	1:15:A:GLN:HE21	14	0.2
(1,85)	1:15:A:GLN:HB2	1:15:A:GLN:HE22	14	0.2
(1,23)	1:2:A:VAL:HA	1:3:A:GLY:H	13	0.2
(1,210)	1:7:A:PRO:HB2	1:9:A:SER:HA	8	0.19
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	13	0.19
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	20	0.19
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	20	0.19
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	20	0.19
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	8	0.19
(1,131)	1:6:A:ARG:HB3	1:18:A:PRO:HA	15	0.19
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	1	0.19
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	1	0.19
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	1	0.19
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB1	9	0.18
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB2	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:1:A:GLY:HA2	1:16:A:ALA:HB3	9	0.18
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	19	0.18
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	19	0.18
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	10	0.18
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	10	0.18
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	10	0.18
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG2	10	0.18
(1,211)	1:12:A:THR:HB	1:13:A:GLN:HG3	10	0.18
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD11	1	0.18
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD12	1	0.18
(1,190)	1:9:A:SER:HB3	1:10:A:ILE:HD13	1	0.18
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	14	0.18
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	14	0.18
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	14	0.18
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	16	0.18
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	16	0.18
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	16	0.18
(1,160)	1:10:A:ILE:HA	1:10:A:ILE:HG13	13	0.18
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	3	0.18
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	3	0.18
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	3	0.18
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	3	0.18
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	2	0.18
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	12	0.18
(1,233)	1:17:A:LYS:HG3	1:17:A:LYS:HD3	1	0.17
(1,197)	1:5:A:GLY:HA3	1:17:A:LYS:H	4	0.17
(1,153)	1:6:A:ARG:HG2	1:18:A:PRO:HA	13	0.17
(1,153)	1:6:A:ARG:HG3	1:18:A:PRO:HA	13	0.17
(1,152)	1:6:A:ARG:HG2	1:19:A:MET:H	13	0.17
(1,152)	1:6:A:ARG:HG3	1:19:A:MET:H	13	0.17
(1,93)	1:6:A:ARG:H	1:15:A:GLN:HB3	3	0.17
(1,49)	1:6:A:ARG:HH11	1:7:A:PRO:HD3	1	0.17
(1,49)	1:6:A:ARG:HH12	1:7:A:PRO:HD3	1	0.17
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	17	0.17
(1,233)	1:17:A:LYS:HG3	1:17:A:LYS:HD3	6	0.16
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG11	16	0.16
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG12	16	0.16
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG13	16	0.16
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG21	16	0.16
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG22	16	0.16
(1,177)	1:1:A:GLY:HA2	1:2:A:VAL:HG23	16	0.16
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG11	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG12	16	0.16
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG13	16	0.16
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG21	16	0.16
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG22	16	0.16
(1,177)	1:1:A:GLY:HA3	1:2:A:VAL:HG23	16	0.16
(1,151)	1:5:A:GLY:H	1:6:A:ARG:HG2	5	0.16
(1,151)	1:5:A:GLY:H	1:6:A:ARG:HG3	5	0.16
(1,146)	1:9:A:SER:HB3	1:10:A:ILE:HG12	9	0.16
(1,138)	1:17:A:LYS:HG3	1:18:A:PRO:HD2	1	0.16
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	17	0.16
(1,1)	1:9:A:SER:H	1:10:A:ILE:H	3	0.16
(1,223)	1:18:A:PRO:HG2	1:18:A:PRO:HB2	8	0.15
(1,182)	1:2:A:VAL:HG11	1:4:A:PHE:H	18	0.15
(1,182)	1:2:A:VAL:HG12	1:4:A:PHE:H	18	0.15
(1,182)	1:2:A:VAL:HG13	1:4:A:PHE:H	18	0.15
(1,182)	1:2:A:VAL:HG21	1:4:A:PHE:H	18	0.15
(1,182)	1:2:A:VAL:HG22	1:4:A:PHE:H	18	0.15
(1,182)	1:2:A:VAL:HG23	1:4:A:PHE:H	18	0.15
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	10	0.15
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	10	0.15
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	10	0.15
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE2	6	0.15
(1,56)	1:6:A:ARG:H	1:17:A:LYS:HE3	6	0.15
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	4	0.15
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	8	0.15
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	8	0.15
(1,6)	1:4:A:PHE:HE1	1:5:A:GLY:H	12	0.15
(1,6)	1:4:A:PHE:HE2	1:5:A:GLY:H	12	0.15
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	7	0.14
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	7	0.14
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	7	0.14
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	7	0.14
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	7	0.14
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	7	0.14
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	7	0.14
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	7	0.14
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	7	0.14
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	7	0.14
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	7	0.14
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	7	0.14
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB1	1	0.14
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:13:A:GLN:HG2	1:16:A:ALA:HB3	1	0.14
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB1	1	0.14
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB2	1	0.14
(1,171)	1:13:A:GLN:HG3	1:16:A:ALA:HB3	1	0.14
(1,143)	1:10:A:ILE:H	1:10:A:ILE:HG12	17	0.14
(1,52)	1:6:A:ARG:HD2	1:18:A:PRO:HA	17	0.14
(1,52)	1:6:A:ARG:HD3	1:18:A:PRO:HA	17	0.14
(1,46)	1:18:A:PRO:HD2	1:19:A:MET:H	16	0.14
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	20	0.14
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	2	0.14
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	2	0.14
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	2	0.14
(1,3)	1:6:A:ARG:H	1:17:A:LYS:H	8	0.14
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	13	0.13
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	13	0.13
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	13	0.13
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	13	0.13
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	13	0.13
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	13	0.13
(1,94)	1:14:A:GLU:HB2	1:15:A:GLN:HE21	9	0.13
(1,94)	1:14:A:GLU:HB3	1:15:A:GLN:HE21	9	0.13
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	17	0.13
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	17	0.13
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	17	0.13
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	17	0.13
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	20	0.13
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	1	0.13
(1,12)	1:6:A:ARG:H	1:17:A:LYS:HA	5	0.13
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ1	14	0.13
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ2	14	0.13
(1,4)	1:17:A:LYS:H	1:17:A:LYS:HZ3	14	0.13
(1,148)	1:6:A:ARG:HG2	1:7:A:PRO:HD3	10	0.12
(1,148)	1:6:A:ARG:HG3	1:7:A:PRO:HD3	10	0.12
(1,147)	1:6:A:ARG:HG2	1:9:A:SER:H	2	0.12
(1,147)	1:6:A:ARG:HG3	1:9:A:SER:H	2	0.12
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE2	5	0.12
(1,57)	1:4:A:PHE:HE1	1:17:A:LYS:HE3	5	0.12
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE2	5	0.12
(1,57)	1:4:A:PHE:HE2	1:17:A:LYS:HE3	5	0.12
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	6	0.12
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	11	0.12
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH11	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,10)	1:6:A:ARG:HA	1:6:A:ARG:HH12	15	0.12
(1,238)	1:6:A:ARG:HG2	1:18:A:PRO:HB2	14	0.11
(1,238)	1:6:A:ARG:HG3	1:18:A:PRO:HB2	14	0.11
(1,233)	1:17:A:LYS:HG3	1:17:A:LYS:HD3	3	0.11
(1,233)	1:17:A:LYS:HG3	1:17:A:LYS:HD3	10	0.11
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE1	7	0.11
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE2	7	0.11
(1,220)	1:19:A:MET:HA	1:19:A:MET:HE3	7	0.11
(1,187)	1:11:A:LEU:HD11	1:13:A:GLN:HE22	16	0.11
(1,187)	1:11:A:LEU:HD12	1:13:A:GLN:HE22	16	0.11
(1,187)	1:11:A:LEU:HD13	1:13:A:GLN:HE22	16	0.11
(1,187)	1:11:A:LEU:HD21	1:13:A:GLN:HE22	16	0.11
(1,187)	1:11:A:LEU:HD22	1:13:A:GLN:HE22	16	0.11
(1,187)	1:11:A:LEU:HD23	1:13:A:GLN:HE22	16	0.11
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE2	12	0.11
(1,174)	1:2:A:VAL:HG11	1:17:A:LYS:HE3	12	0.11
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE2	12	0.11
(1,174)	1:2:A:VAL:HG12	1:17:A:LYS:HE3	12	0.11
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE2	12	0.11
(1,174)	1:2:A:VAL:HG13	1:17:A:LYS:HE3	12	0.11
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE2	12	0.11
(1,174)	1:2:A:VAL:HG21	1:17:A:LYS:HE3	12	0.11
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE2	12	0.11
(1,174)	1:2:A:VAL:HG22	1:17:A:LYS:HE3	12	0.11
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE2	12	0.11
(1,174)	1:2:A:VAL:HG23	1:17:A:LYS:HE3	12	0.11
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB1	7	0.11
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB2	7	0.11
(1,173)	1:1:A:GLY:HA3	1:16:A:ALA:HB3	7	0.11
(1,146)	1:9:A:SER:HB3	1:10:A:ILE:HG12	14	0.11
(1,47)	1:4:A:PHE:H	1:18:A:PRO:HD2	7	0.11
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	12	0.11
(1,34)	1:3:A:GLY:HA2	1:4:A:PHE:H	8	0.11
(1,6)	1:4:A:PHE:HE1	1:5:A:GLY:H	19	0.11
(1,6)	1:4:A:PHE:HE2	1:5:A:GLY:H	19	0.11
(1,1)	1:9:A:SER:H	1:10:A:ILE:H	19	0.11
(1,198)	1:4:A:PHE:HD1	1:5:A:GLY:HA3	7	0.1
(1,198)	1:4:A:PHE:HD2	1:5:A:GLY:HA3	7	0.1
(1,194)	1:3:A:GLY:H	1:4:A:PHE:H	7	0.1
(1,162)	1:10:A:ILE:H	1:10:A:ILE:HG13	10	0.1
(1,41)	1:9:A:SER:H	1:9:A:SER:HB3	8	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found