



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 10:32 AM UTC

PDB ID : 5K57 / pdb_00005k57
BMRB ID : 30097
Title : HDD domain from human Ddi2
Authors : Veverka, V.
Deposited on : 2016-05-23

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

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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

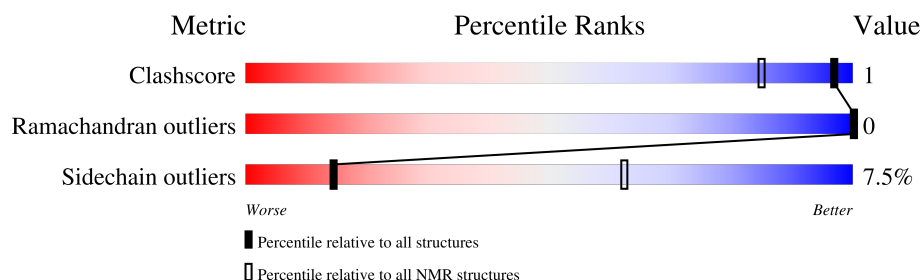
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	98	41% . 56%

2 Ensemble composition and analysis

This entry contains 30 models. Model 13 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:21-A:63 (43)	0.19	13

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 4, 7, 10, 12, 13, 15, 17, 21, 22, 25, 27, 29
2	3, 6, 9, 14, 16, 18, 24, 28, 30
3	2, 5, 8, 11, 20, 26
4	19, 23

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1557 atoms, of which 775 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein DDI1 homolog 2.

Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1557	479	775	144	158	1	

There is a discrepancy between the modelled and reference sequences:

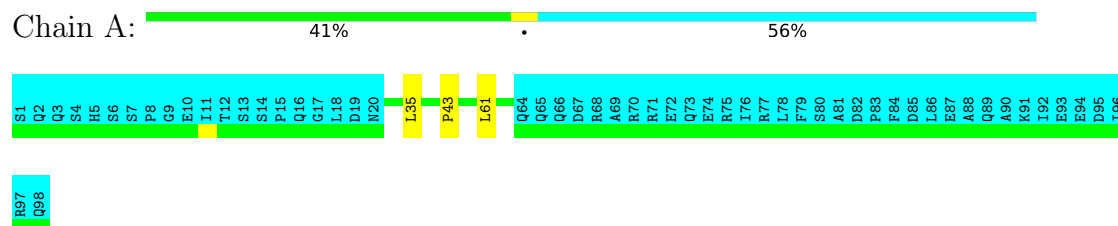
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q5TDH0

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein DDI1 homolog 2

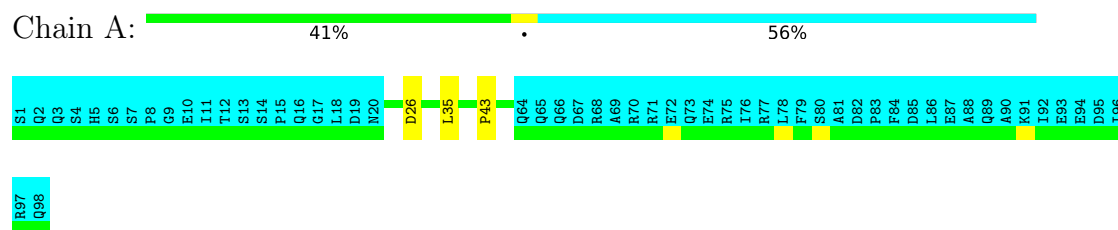


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

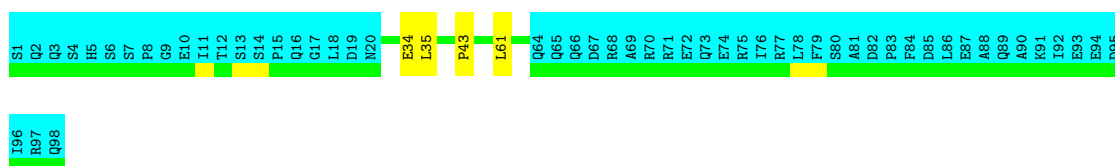
- Molecule 1: Protein DDI1 homolog 2



4.2.2 Score per residue for model 2

- Molecule 1: Protein DDI1 homolog 2

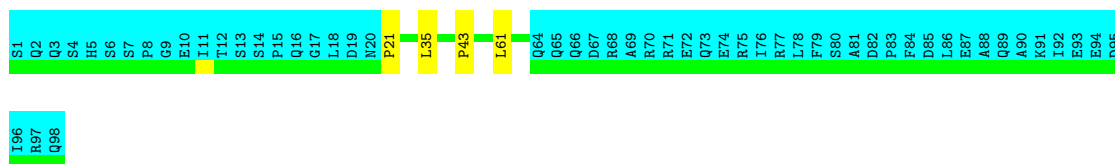




4.2.3 Score per residue for model 3

- Molecule 1: Protein DDI1 homolog 2

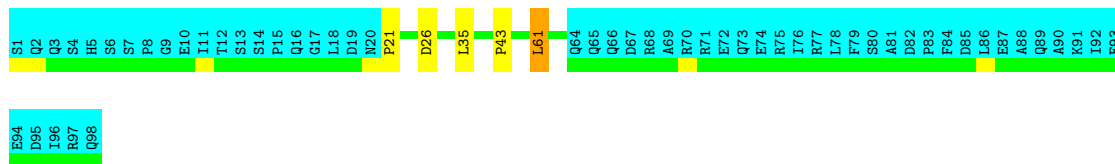
Chain A: 40% 56%



4.2.4 Score per residue for model 4

- Molecule 1: Protein DDI1 homolog 2

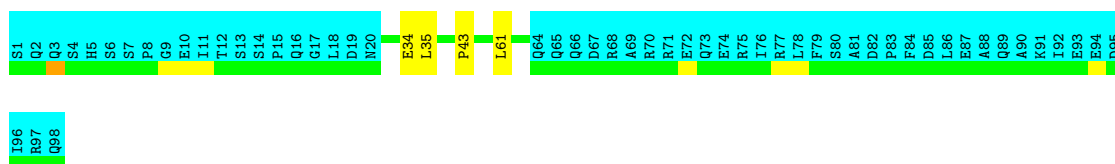
Chain A: 39% 56%



4.2.5 Score per residue for model 5

- Molecule 1: Protein DDI1 homolog 2

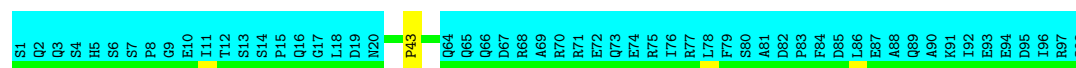
Chain A: 40% 56%



4.2.6 Score per residue for model 6

- Molecule 1: Protein DDI1 homolog 2

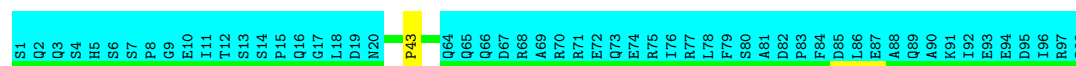
Chain A:  43% 56%



4.2.7 Score per residue for model 7

- Molecule 1: Protein DDI1 homolog 2

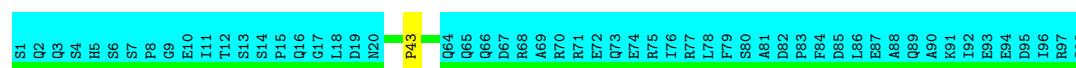
Chain A:  43% 56%



4.2.8 Score per residue for model 8

- Molecule 1: Protein DDI1 homolog 2

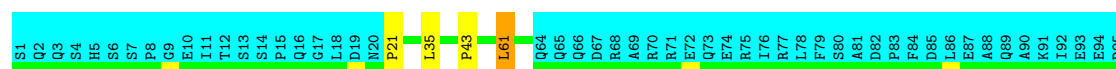
Chain A:  43% 56%



4.2.9 Score per residue for model 9

- Molecule 1: Protein DDI1 homolog 2

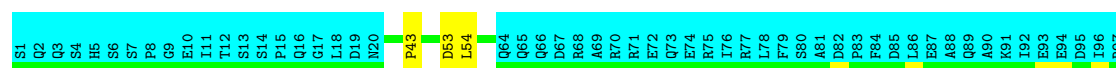
Chain A:  40% 56%



4.2.10 Score per residue for model 10

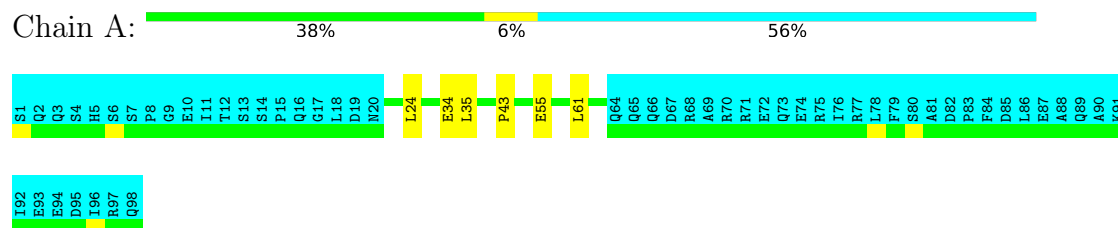
- Molecule 1: Protein DDI1 homolog 2

Chain A:  41% 56%



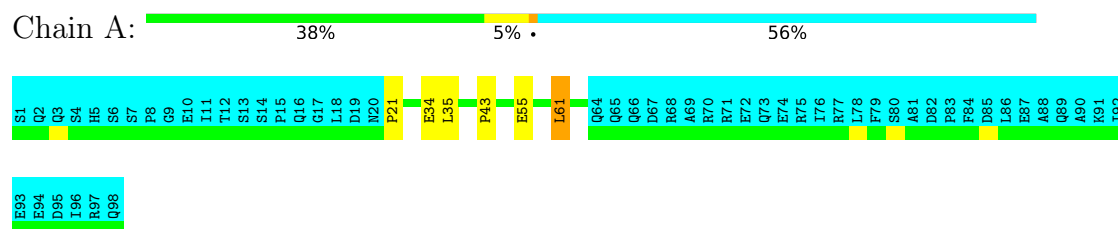
4.2.11 Score per residue for model 11

- Molecule 1: Protein DDI1 homolog 2



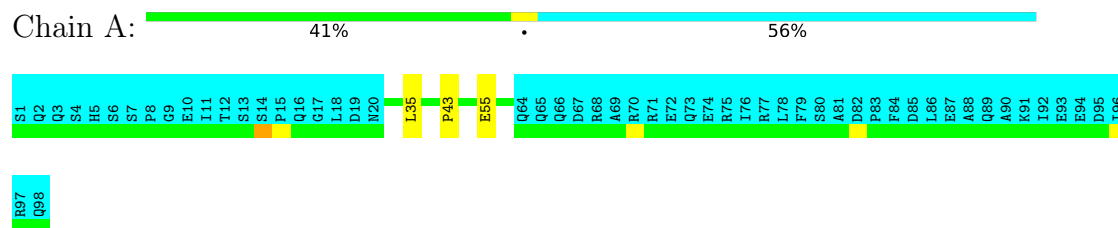
4.2.12 Score per residue for model 12

- Molecule 1: Protein DDI1 homolog 2



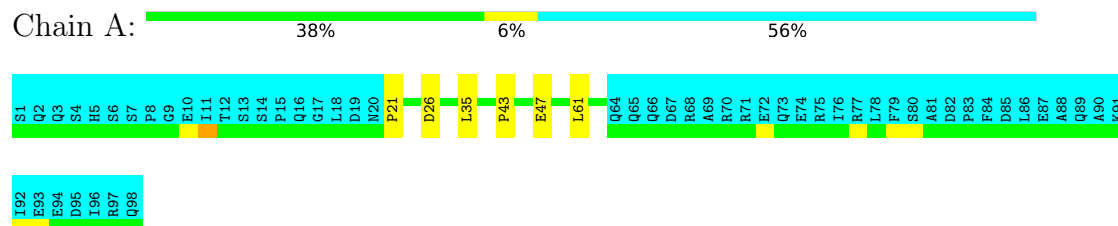
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Protein DDI1 homolog 2



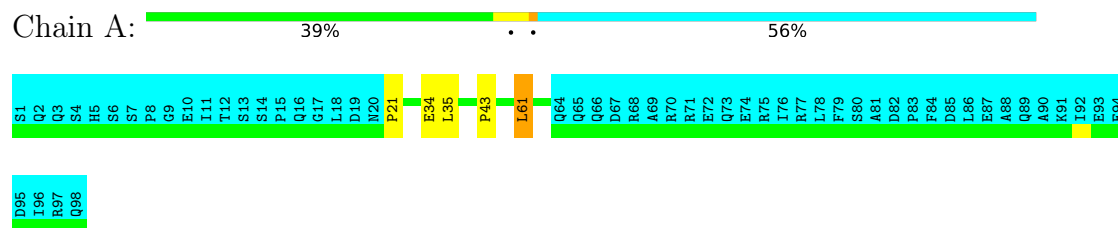
4.2.14 Score per residue for model 14

- Molecule 1: Protein DDI1 homolog 2



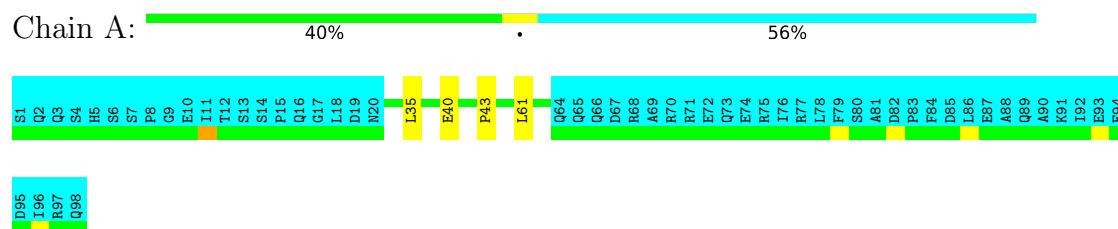
4.2.15 Score per residue for model 15

- Molecule 1: Protein DDI1 homolog 2



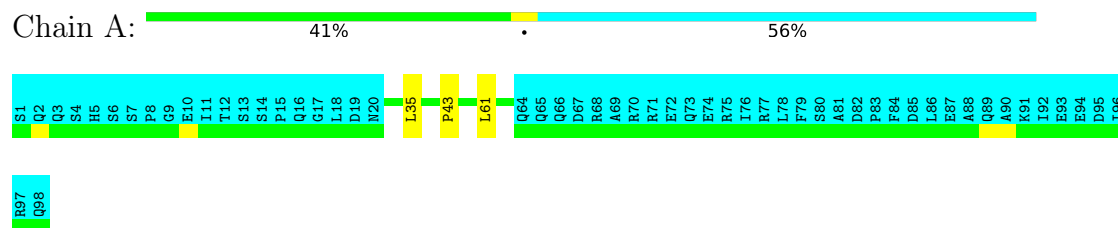
4.2.16 Score per residue for model 16

- Molecule 1: Protein DDI1 homolog 2



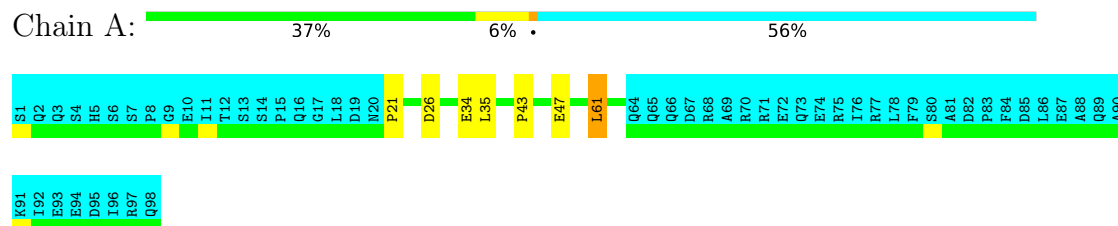
4.2.17 Score per residue for model 17

- Molecule 1: Protein DDI1 homolog 2



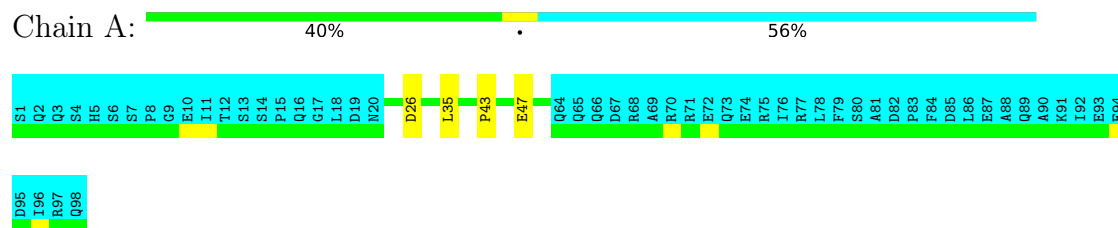
4.2.18 Score per residue for model 18

- Molecule 1: Protein DDI1 homolog 2



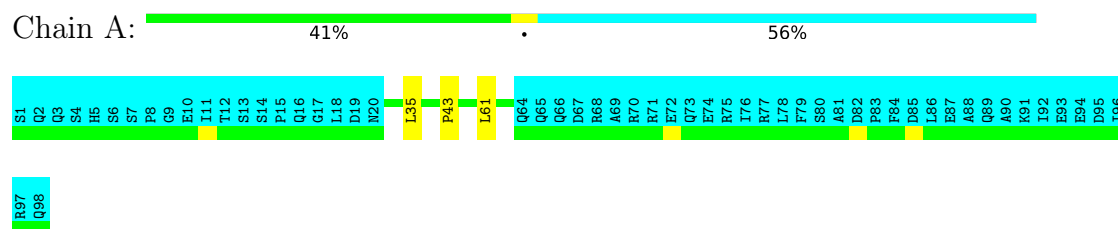
4.2.19 Score per residue for model 19

- Molecule 1: Protein DDI1 homolog 2



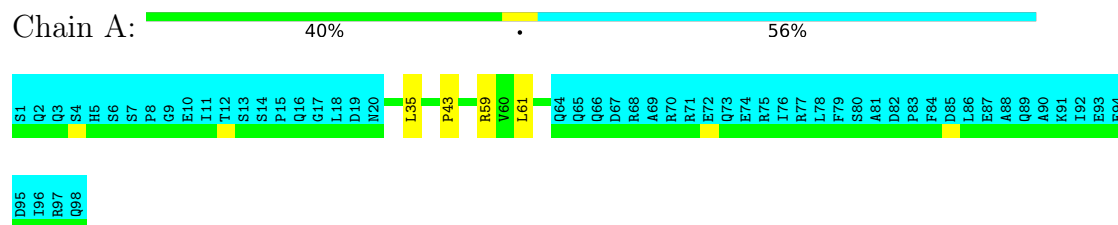
4.2.20 Score per residue for model 20

- Molecule 1: Protein DDI1 homolog 2



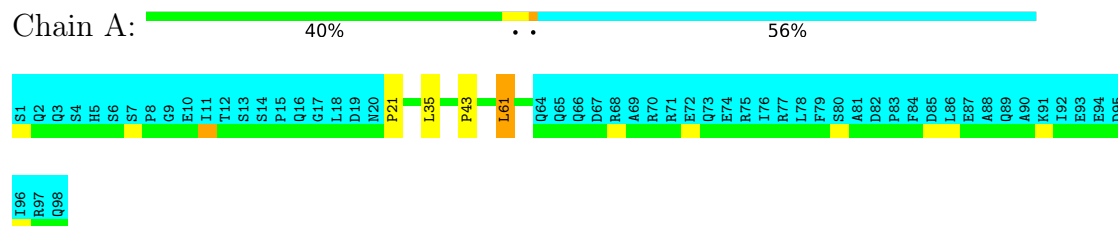
4.2.21 Score per residue for model 21

- Molecule 1: Protein DDI1 homolog 2



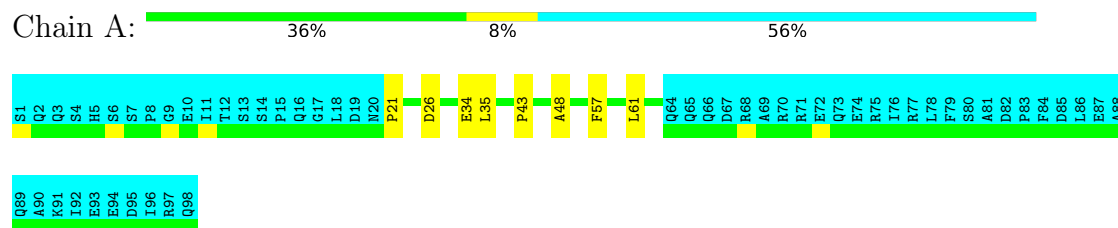
4.2.22 Score per residue for model 22

- Molecule 1: Protein DDI1 homolog 2



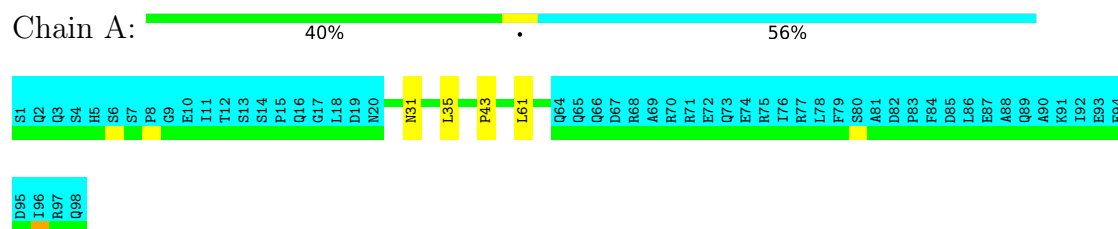
4.2.23 Score per residue for model 23

- Molecule 1: Protein DDI1 homolog 2



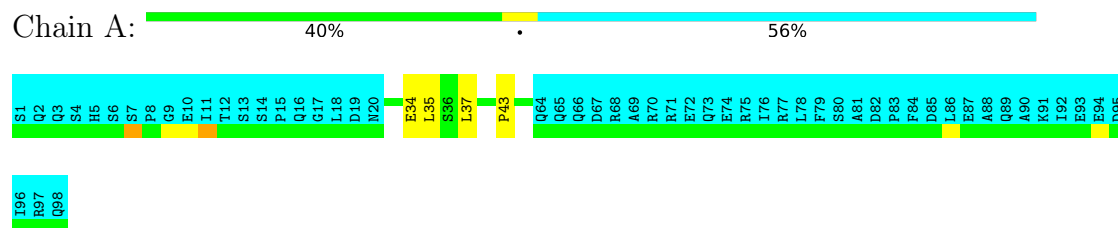
4.2.24 Score per residue for model 24

- Molecule 1: Protein DDI1 homolog 2



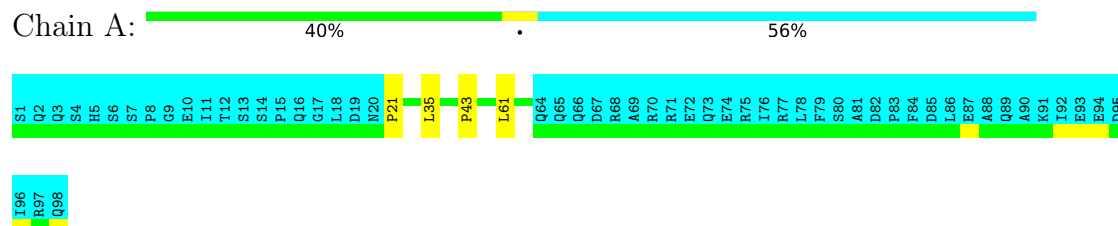
4.2.25 Score per residue for model 25

- Molecule 1: Protein DDI1 homolog 2



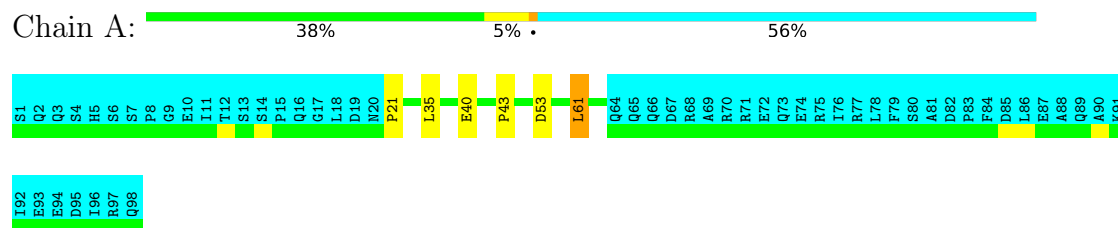
4.2.26 Score per residue for model 26

- Molecule 1: Protein DDI1 homolog 2



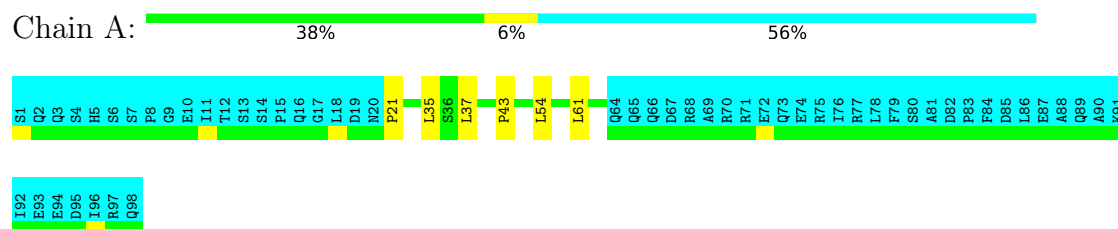
4.2.27 Score per residue for model 27

- Molecule 1: Protein DDI1 homolog 2



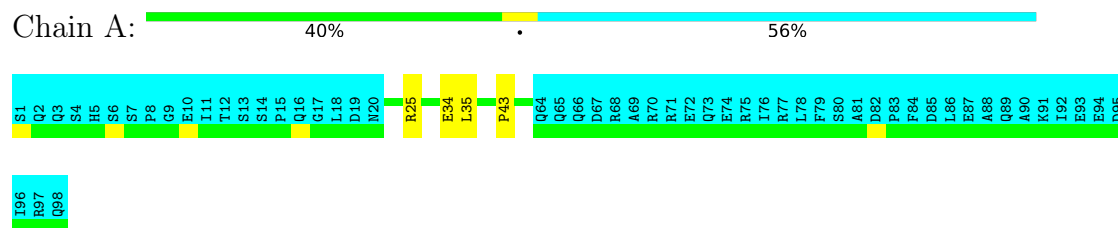
4.2.28 Score per residue for model 28

- Molecule 1: Protein DDI1 homolog 2



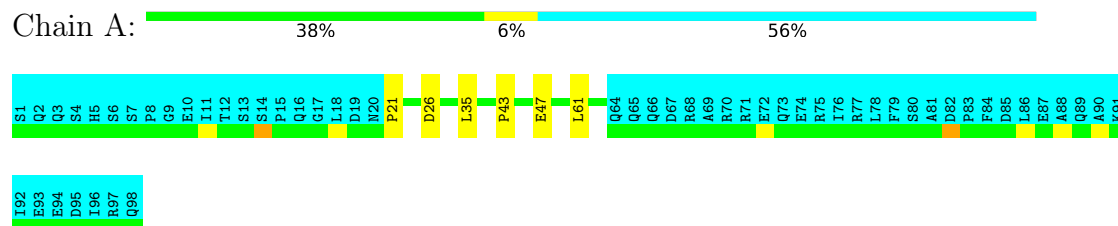
4.2.29 Score per residue for model 29

- Molecule 1: Protein DDI1 homolog 2



4.2.30 Score per residue for model 30

- Molecule 1: Protein DDI1 homolog 2



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 30 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	
YASARA	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	1190
Number of shifts mapped to atoms	1190
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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	0.83±0.04	0±0/343 (0.0± 0.0%)	1.06±0.02	3±0/465 (0.6± 0.0%)
All	All	0.83	0/10290 (0.0%)	1.06	90/13950 (0.6%)

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	43	PRO	N-CA-C	6.87	119.08	110.70	18	30
1	A	43	PRO	CA-C-N	-6.74	112.05	119.19	2	30
1	A	43	PRO	C-N-CA	-6.74	112.05	119.19	2	30

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	337	356	356	0±1
All	All	10110	10680	10680	14

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PRO:HB3	1:A:61:LEU:HD22	0.52	1.82	18	13
1:A:48:ALA:HB1	1:A:57:PHE:HA	0.41	1.92	23	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	43/98 (44%)	43±0 (99±1%)	0±0 (1±1%)	0±0 (0±0%)	100	100
All	All	1290/2940 (44%)	1279 (99%)	11 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	38/87 (44%)	31±11 (81±29%)	2±1 (7±3%)	17	66
All	All	1004/2610 (38%)	929 (93%)	75 (7%)	14	62

All 13 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	35	LEU	26
1	A	61	LEU	15
1	A	34	GLU	9
1	A	26	ASP	7
1	A	47	GLU	4
1	A	55	GLU	3
1	A	53	ASP	2

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Mol	Chain	Res	Type	Models (Total)
1	A	54	LEU	2
1	A	40	GLU	2
1	A	37	LEU	2
1	A	24	LEU	1
1	A	59	ARG	1
1	A	25	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `hdd.star`

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	1190
Number of shifts mapped to atoms	1190
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	97	-0.21 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	94	0.12 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	96	-0.23 ± 0.17	None needed (< 0.5 ppm)
^{15}N	89	-0.36 ± 0.17	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 573 atoms were assigned a chemical shift out of a possible 615. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	207/208 (100%)	83/83 (100%)	85/86 (99%)	39/39 (100%)
Sidechain	357/390 (92%)	244/256 (95%)	108/121 (89%)	5/13 (38%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	9/17 (53%)	6/9 (67%)	3/7 (43%)	0/1 (0%)
Overall	573/615 (93%)	333/348 (96%)	196/214 (92%)	44/53 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1189 atoms were assigned a chemical shift out of a possible 1363. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	470/479 (98%)	188/192 (98%)	193/196 (98%)	89/91 (98%)
Sidechain	699/840 (83%)	478/539 (89%)	207/259 (80%)	14/42 (33%)
Aromatic	20/44 (45%)	15/23 (65%)	5/19 (26%)	0/2 (0%)
Overall	1189/1363 (87%)	681/754 (90%)	405/474 (85%)	103/135 (76%)

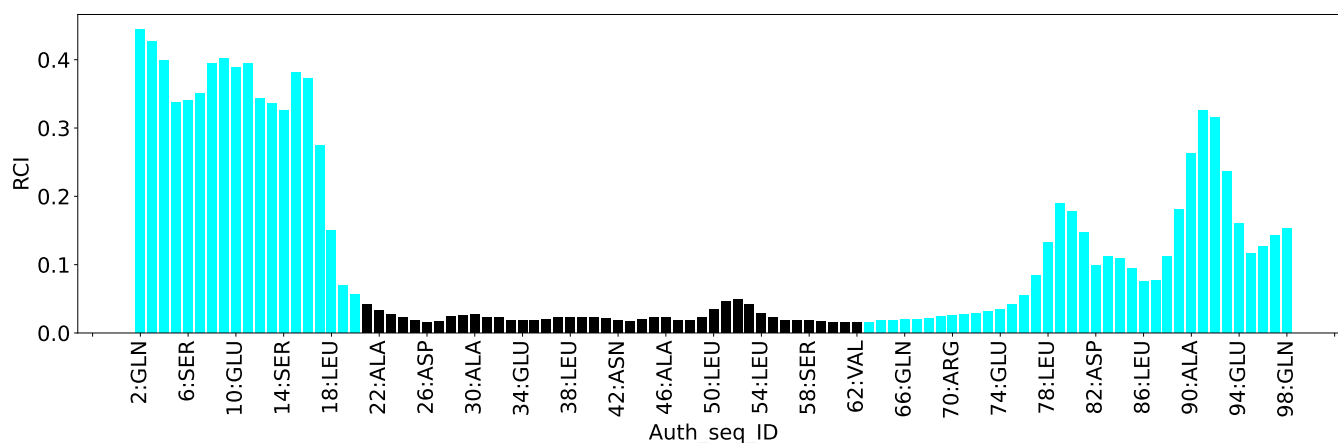
7.1.4 Statistically unusual chemical shifts [i](#)

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	1917
Intra-residue ($ i-j =0$)	495
Sequential ($ i-j =1$)	536
Medium range ($ i-j >1$ and $ i-j <5$)	593
Long range ($ i-j \geq 5$)	293
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	108
Number of unmapped restraints	0
Number of restraints per residue	20.7
Number of long range restraints per residue ¹	3.0

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)	8.2	0.2
0.2-0.5 (Medium)	3.6	0.5
>0.5 (Large)	11.6	1.79

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	3.3	5.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

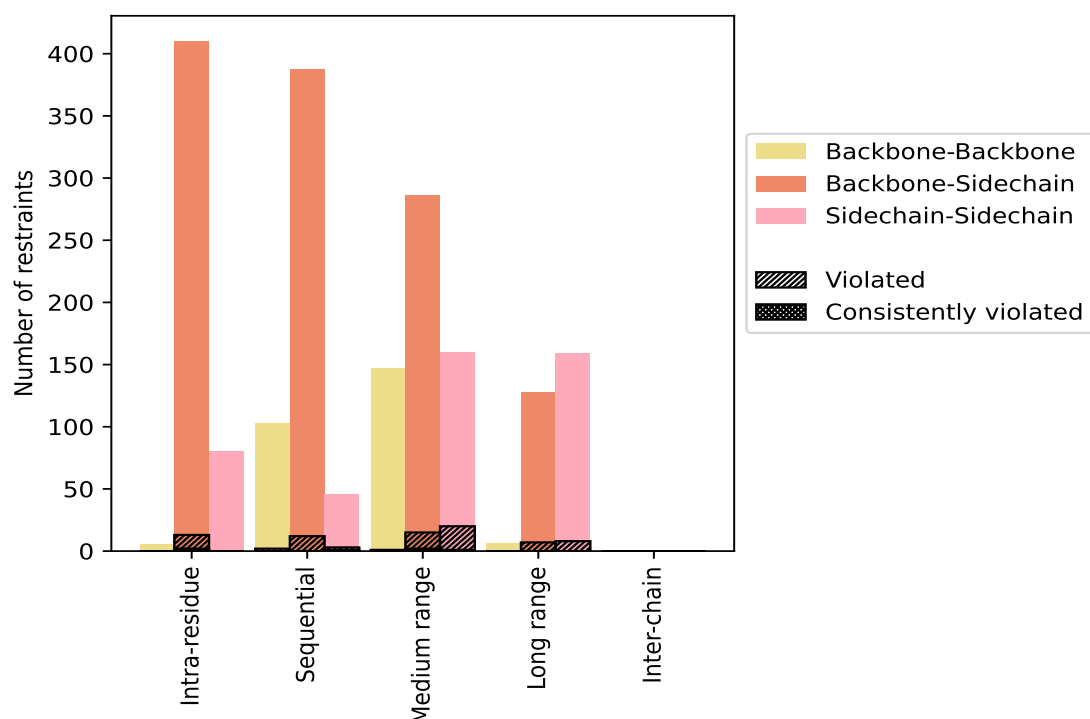
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	495	25.8	13	2.6	0.7	2	0.4	0.1
Backbone-Backbone	5	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	410	21.4	13	3.2	0.7	2	0.5	0.1
Sidechain-Sidechain	80	4.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	536	28.0	17	3.2	0.9	1	0.2	0.1
Backbone-Backbone	103	5.4	2	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	387	20.2	12	3.1	0.6	0	0.0	0.0
Sidechain-Sidechain	46	2.4	3	6.5	0.2	1	2.2	0.1
Medium range ($i-j >1$ & $i-j <5$)	593	30.9	36	6.1	1.9	3	0.5	0.2
Backbone-Backbone	147	7.7	1	0.7	0.1	0	0.0	0.0
Backbone-Sidechain	286	14.9	15	5.2	0.8	2	0.7	0.1
Sidechain-Sidechain	160	8.3	20	12.5	1.0	1	0.6	0.1
Long range ($i-j \geq 5$)	293	15.3	15	5.1	0.8	0	0.0	0.0
Backbone-Backbone	6	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	128	6.7	7	5.5	0.4	0	0.0	0.0
Sidechain-Sidechain	159	8.3	8	5.0	0.4	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	1917	100.0	81	4.2	4.2	6	0.3	0.3
Backbone-Backbone	261	13.6	3	1.1	0.2	0	0.0	0.0
Backbone-Sidechain	1211	63.2	47	3.9	2.5	4	0.3	0.2
Sidechain-Sidechain	445	23.2	31	7.0	1.6	2	0.4	0.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	7	2	9	6	0	24	0.57	1.75	0.46	0.53
2	8	4	16	7	0	35	0.46	1.77	0.44	0.19
3	5	1	6	6	0	18	0.73	1.75	0.46	0.76
4	9	3	10	6	0	28	0.52	1.75	0.44	0.31
5	8	5	9	7	0	29	0.49	1.77	0.45	0.19
6	7	1	6	6	0	20	0.68	1.75	0.45	0.78
7	7	5	12	5	0	29	0.5	1.75	0.45	0.24
8	8	3	11	8	0	30	0.49	1.75	0.44	0.26
9	6	2	11	3	0	22	0.67	1.76	0.52	0.73
10	6	2	8	6	0	22	0.62	1.76	0.45	0.71

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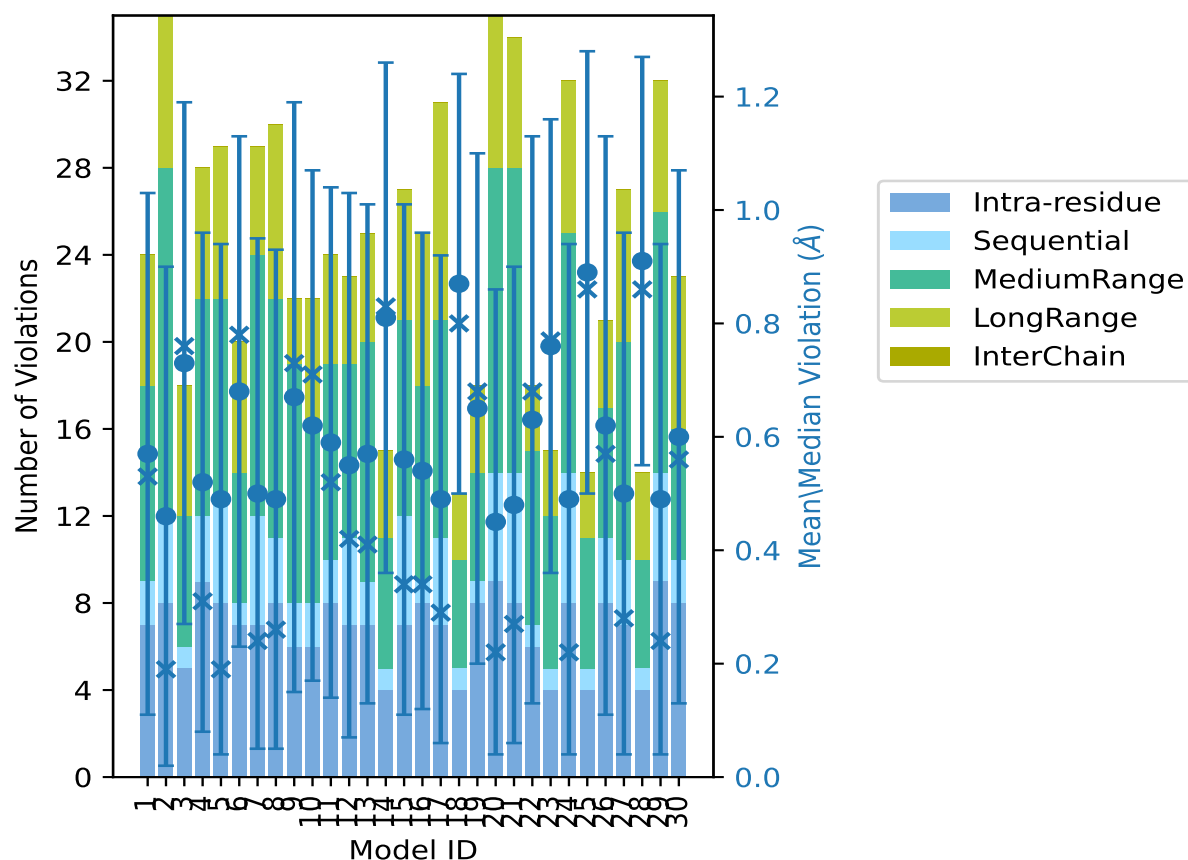
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	8	2	9	5	0	24	0.59	1.76	0.45	0.52
12	7	4	8	4	0	23	0.55	1.75	0.48	0.42
13	7	2	11	5	0	25	0.57	1.74	0.44	0.41
14	4	1	6	4	0	15	0.81	1.75	0.45	0.83
15	7	5	9	6	0	27	0.56	1.76	0.45	0.34
16	8	1	9	7	0	25	0.54	1.73	0.42	0.34
17	7	4	10	10	0	31	0.49	1.75	0.43	0.29
18	4	1	5	3	0	13	0.87	1.76	0.37	0.8
19	8	1	5	4	0	18	0.65	1.74	0.45	0.68
20	9	5	14	7	0	35	0.45	1.79	0.41	0.22
21	8	6	14	6	0	34	0.48	1.74	0.42	0.27
22	6	1	8	3	0	18	0.63	1.75	0.5	0.68
23	4	1	7	3	0	15	0.76	1.72	0.4	0.77
24	8	6	11	7	0	32	0.49	1.67	0.45	0.22
25	4	1	6	3	0	14	0.89	1.75	0.39	0.86
26	8	3	6	4	0	21	0.62	1.75	0.51	0.57
27	7	3	10	7	0	27	0.5	1.74	0.46	0.28
28	4	1	5	4	0	14	0.91	1.74	0.36	0.86
29	9	5	12	6	0	32	0.49	1.78	0.45	0.24
30	8	2	6	7	0	23	0.6	1.76	0.47	0.56

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble [i](#)

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, 1836(IR:482, SQ:519, MR:557, LR:278, 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	%
3	8	14	2	0	27	1	3.3
1	2	4	2	0	9	2	6.7
0	1	3	2	0	6	3	10.0
1	2	3	0	0	6	4	13.3
0	0	0	1	0	1	5	16.7
0	1	0	0	0	1	6	20.0

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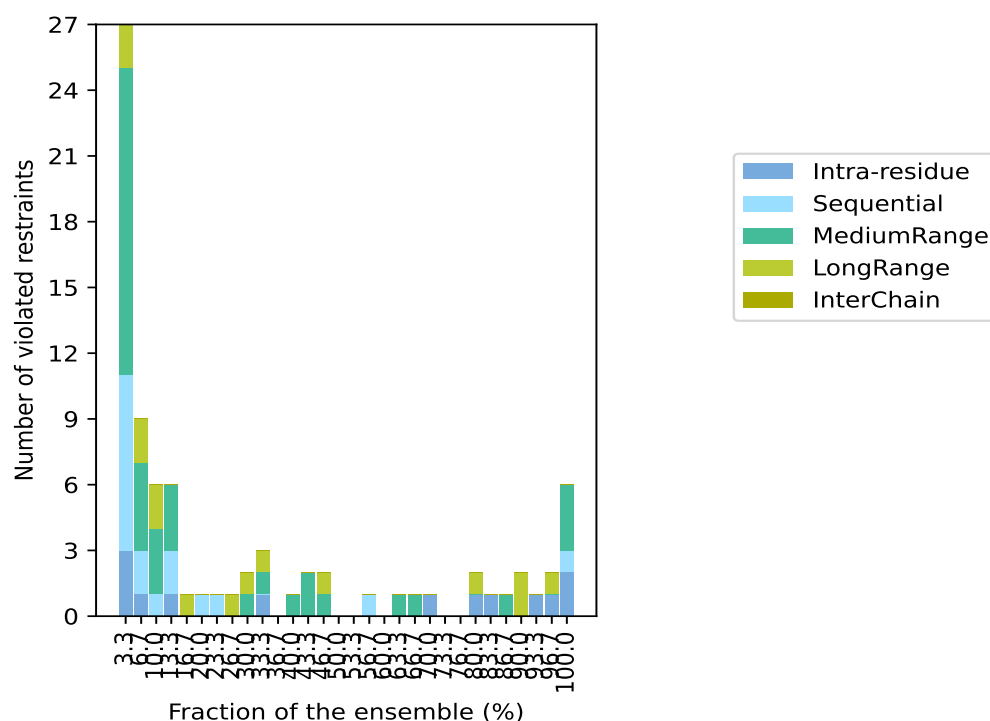
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	1	0	0	0	1	7	23.3
0	0	0	1	0	1	8	26.7
0	0	1	1	0	2	9	30.0
1	0	1	1	0	3	10	33.3
0	0	0	0	0	0	11	36.7
0	0	1	0	0	1	12	40.0
0	0	2	0	0	2	13	43.3
0	0	1	1	0	2	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	1	0	0	0	1	17	56.7
0	0	0	0	0	0	18	60.0
0	0	1	0	0	1	19	63.3
0	0	1	0	0	1	20	66.7
1	0	0	0	0	1	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
1	0	0	1	0	2	24	80.0
1	0	0	0	0	1	25	83.3
0	0	1	0	0	1	26	86.7
0	0	0	2	0	2	27	90.0
1	0	0	0	0	1	28	93.3
1	0	0	1	0	2	29	96.7
2	1	3	0	0	6	30	100.0

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

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

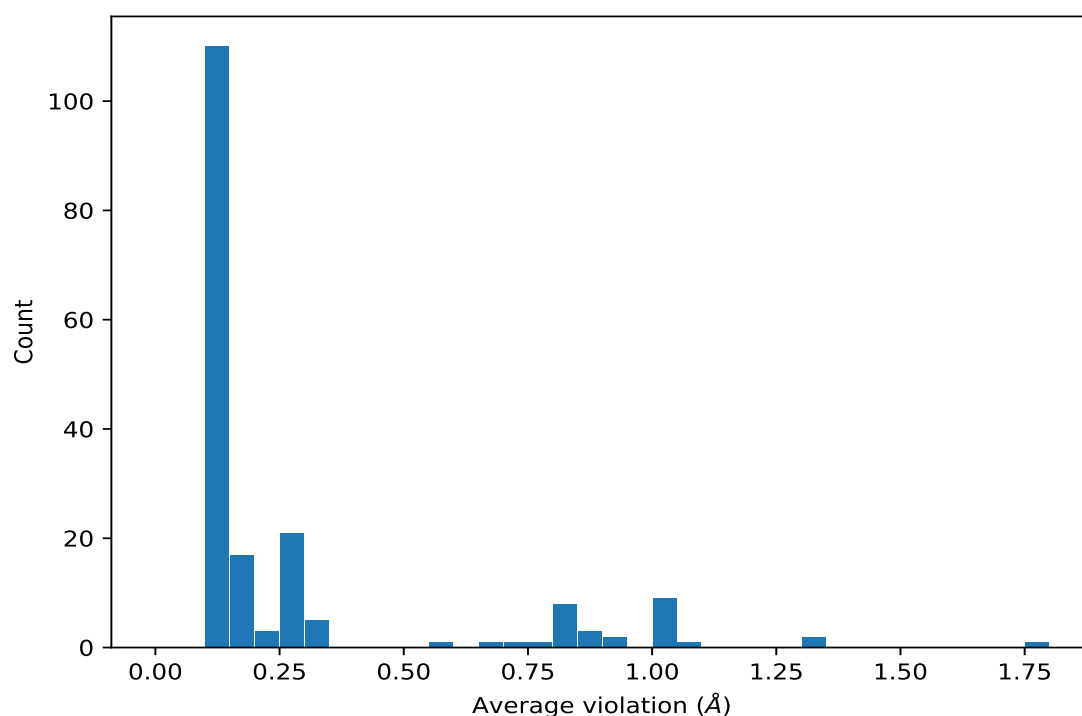
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	30	1.75	0.02	1.75
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	30	1.32	0.08	1.33
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	30	1.32	0.08	1.33
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	30	1.04	0.08	1.04
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	30	1.04	0.08	1.04
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	30	1.04	0.08	1.04
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	30	0.81	0.03	0.82
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	30	0.78	0.04	0.78
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	30	0.72	0.13	0.74
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	29	1.02	0.12	1.02
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	29	1.02	0.12	1.02
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	29	1.02	0.12	1.02
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	29	1.02	0.12	1.02
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	29	1.02	0.12	1.02
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	29	1.02	0.12	1.02
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	29	0.92	0.04	0.92

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	28	0.6	0.04	0.6
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	27	1.06	0.14	1.08
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	27	0.85	0.19	0.86
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	26	0.29	0.08	0.32
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	26	0.29	0.08	0.32
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	26	0.29	0.08	0.32
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	25	0.16	0.03	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	25	0.16	0.03	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	25	0.16	0.03	0.16
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	24	0.34	0.11	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	24	0.34	0.11	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	24	0.34	0.11	0.36
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	24	0.16	0.05	0.16
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	24	0.16	0.05	0.16
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	21	0.14	0.03	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	21	0.14	0.03	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	21	0.14	0.03	0.14
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	20	0.18	0.06	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	20	0.18	0.06	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	20	0.18	0.06	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	20	0.18	0.06	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	20	0.18	0.06	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	20	0.18	0.06	0.15
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	19	0.68	0.32	0.63
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	17	0.14	0.04	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	17	0.14	0.04	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	17	0.14	0.04	0.12
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	14	0.14	0.03	0.13
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	14	0.14	0.03	0.13
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	14	0.14	0.03	0.13
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	14	0.14	0.03	0.13
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	14	0.14	0.03	0.13
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	14	0.14	0.03	0.13
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	14	0.13	0.02	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	14	0.13	0.02	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	14	0.13	0.02	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	14	0.13	0.02	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	14	0.13	0.02	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	14	0.13	0.02	0.12
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	13	0.89	0.25	0.91
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	13	0.89	0.25	0.91
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	13	0.89	0.25	0.91

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	13	0.19	0.05	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	13	0.19	0.05	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	13	0.19	0.05	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	13	0.19	0.05	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	13	0.19	0.05	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	13	0.19	0.05	0.19
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	12	0.32	0.05	0.33
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	12	0.32	0.05	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	10	0.3	0.05	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	10	0.3	0.05	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	10	0.3	0.05	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	10	0.3	0.05	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	10	0.3	0.05	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	10	0.3	0.05	0.31
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	10	0.15	0.04	0.14
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	10	0.15	0.04	0.14
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	10	0.14	0.04	0.12
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	10	0.14	0.04	0.12
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	10	0.14	0.04	0.12
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	9	0.25	0.04	0.25
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	9	0.25	0.04	0.25
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	9	0.25	0.04	0.25
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	9	0.25	0.04	0.25
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	9	0.25	0.04	0.25
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	9	0.25	0.04	0.25
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	9	0.13	0.01	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	9	0.13	0.01	0.12
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	8	0.15	0.02	0.14
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	8	0.15	0.02	0.14
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	8	0.15	0.02	0.14
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	8	0.15	0.02	0.14
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	8	0.15	0.02	0.14
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	8	0.15	0.02	0.14
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	7	0.13	0.02	0.12
(1,845)	1:38:A:LEU:HD11	1:39:A:LYS:H	6	0.11	0.01	0.12
(1,845)	1:38:A:LEU:HD12	1:39:A:LYS:H	6	0.11	0.01	0.12
(1,845)	1:38:A:LEU:HD13	1:39:A:LYS:H	6	0.11	0.01	0.12
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD21	5	0.12	0.02	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD22	5	0.12	0.02	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD23	5	0.12	0.02	0.11
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB2	4	0.15	0.02	0.15
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB3	4	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,837)	1:68:A:ARG:HB2	1:69:A:ALA:H	4	0.14	0.03	0.15
(1,837)	1:68:A:ARG:HB3	1:69:A:ALA:H	4	0.14	0.03	0.15
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD11	4	0.13	0.03	0.13
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD12	4	0.13	0.03	0.13
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD13	4	0.13	0.03	0.13
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD21	4	0.12	0.02	0.12
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD22	4	0.12	0.02	0.12
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD23	4	0.12	0.02	0.12
(1,572)	1:11:A:ILE:HA	1:12:A:THR:H	4	0.12	0.02	0.12
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE1	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE2	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE3	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE1	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE2	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE3	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE1	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE2	4	0.11	0.01	0.11
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE3	4	0.11	0.01	0.11
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD11	3	0.8	0.18	0.74
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD12	3	0.8	0.18	0.74
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD13	3	0.8	0.18	0.74
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD11	3	0.8	0.18	0.74
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD12	3	0.8	0.18	0.74
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD13	3	0.8	0.18	0.74
(1,1762)	1:60:A:VAL:HG11	1:65:A:GLN:H	3	0.15	0.03	0.13
(1,1762)	1:60:A:VAL:HG12	1:65:A:GLN:H	3	0.15	0.03	0.13
(1,1762)	1:60:A:VAL:HG13	1:65:A:GLN:H	3	0.15	0.03	0.13
(1,1762)	1:60:A:VAL:HG21	1:65:A:GLN:H	3	0.15	0.03	0.13
(1,1762)	1:60:A:VAL:HG22	1:65:A:GLN:H	3	0.15	0.03	0.13
(1,1762)	1:60:A:VAL:HG23	1:65:A:GLN:H	3	0.15	0.03	0.13
(1,501)	1:90:A:ALA:HB1	1:91:A:LYS:H	3	0.14	0.04	0.11
(1,501)	1:90:A:ALA:HB2	1:91:A:LYS:H	3	0.14	0.04	0.11
(1,501)	1:90:A:ALA:HB3	1:91:A:LYS:H	3	0.14	0.04	0.11
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB1	3	0.13	0.05	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB2	3	0.13	0.05	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB3	3	0.13	0.05	0.1
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD21	3	0.13	0.02	0.12
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD22	3	0.13	0.02	0.12
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD23	3	0.13	0.02	0.12
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG11	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG12	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG13	3	0.12	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG21	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG22	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG23	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG11	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG12	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG13	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG21	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG22	3	0.12	0.01	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG23	3	0.12	0.01	0.11
(1,1387)	1:63:A:GLU:HA	1:66:A:GLN:HE21	2	0.94	0.4	0.94
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD21	2	0.28	0.16	0.28
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD22	2	0.28	0.16	0.28
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD23	2	0.28	0.16	0.28
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD21	2	0.28	0.16	0.28
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD22	2	0.28	0.16	0.28
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD23	2	0.28	0.16	0.28
(1,1022)	1:54:A:LEU:HD21	1:56:A:LYS:H	2	0.22	0.01	0.22
(1,1022)	1:54:A:LEU:HD22	1:56:A:LYS:H	2	0.22	0.01	0.22
(1,1022)	1:54:A:LEU:HD23	1:56:A:LYS:H	2	0.22	0.01	0.22
(1,1790)	1:62:A:VAL:HG11	1:66:A:GLN:HA	2	0.15	0.0	0.15
(1,1790)	1:62:A:VAL:HG12	1:66:A:GLN:HA	2	0.15	0.0	0.15
(1,1790)	1:62:A:VAL:HG13	1:66:A:GLN:HA	2	0.15	0.0	0.15
(1,1790)	1:62:A:VAL:HG21	1:66:A:GLN:HA	2	0.15	0.0	0.15
(1,1790)	1:62:A:VAL:HG22	1:66:A:GLN:HA	2	0.15	0.0	0.15
(1,1790)	1:62:A:VAL:HG23	1:66:A:GLN:HA	2	0.15	0.0	0.15
(1,1891)	1:87:A:GLU:HB2	1:88:A:ALA:H	2	0.12	0.01	0.12
(1,1891)	1:87:A:GLU:HB3	1:88:A:ALA:H	2	0.12	0.01	0.12
(1,1108)	1:62:A:VAL:HG21	1:63:A:GLU:H	2	0.11	0.0	0.11
(1,1108)	1:62:A:VAL:HG22	1:63:A:GLU:H	2	0.11	0.0	0.11
(1,1108)	1:62:A:VAL:HG23	1:63:A:GLU:H	2	0.11	0.0	0.11
(1,228)	1:37:A:LEU:HD21	1:40:A:GLU:HB2	2	0.11	0.0	0.11
(1,228)	1:37:A:LEU:HD21	1:40:A:GLU:HB3	2	0.11	0.0	0.11
(1,228)	1:37:A:LEU:HD22	1:40:A:GLU:HB2	2	0.11	0.0	0.11
(1,228)	1:37:A:LEU:HD22	1:40:A:GLU:HB3	2	0.11	0.0	0.11
(1,228)	1:37:A:LEU:HD23	1:40:A:GLU:HB2	2	0.11	0.0	0.11
(1,228)	1:37:A:LEU:HD23	1:40:A:GLU:HB3	2	0.11	0.0	0.11
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD11	2	0.11	0.0	0.11
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD12	2	0.11	0.0	0.11
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD13	2	0.11	0.0	0.11
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD11	2	0.11	0.0	0.11
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD12	2	0.11	0.0	0.11
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD13	2	0.11	0.0	0.11

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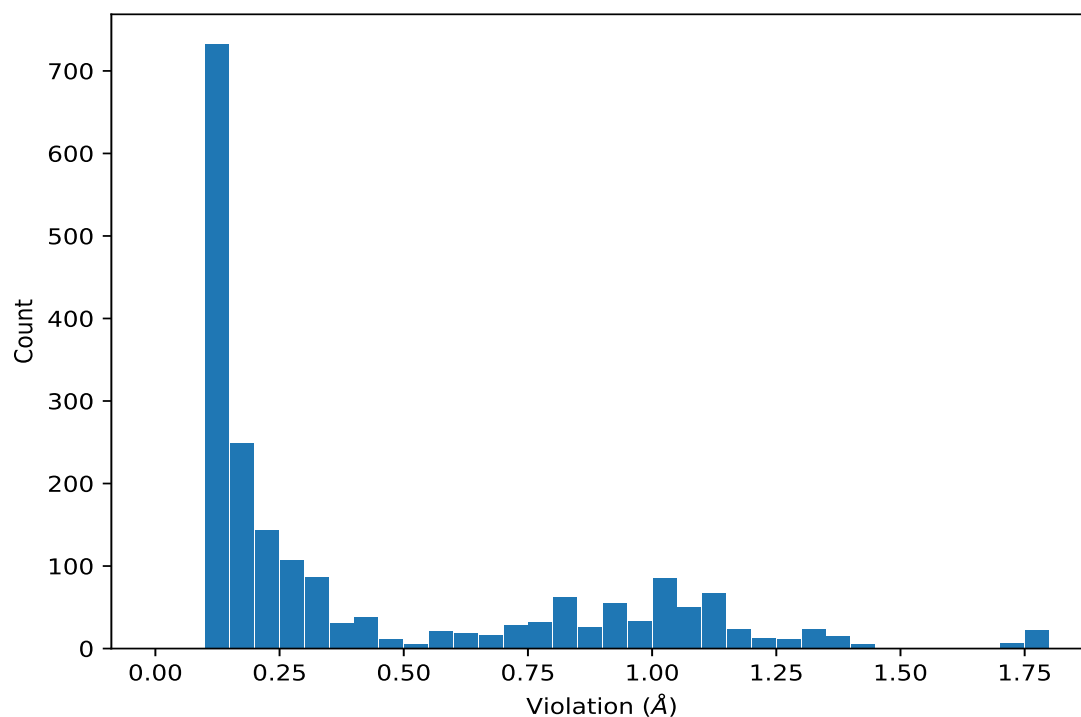
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1850)	1:78:A:LEU:H	1:78:A:LEU:HB2	2	0.11	0.0	0.11
(1,1850)	1:78:A:LEU:H	1:78:A:LEU:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	20	1.79
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	29	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	2	1.77
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	5	1.77
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	9	1.76
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	10	1.76
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	11	1.76
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	15	1.76
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	18	1.76
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	30	1.76
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	1	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	3	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	4	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	6	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	7	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	8	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	12	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	14	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	17	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	22	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	25	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	26	1.75
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	13	1.74
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	19	1.74
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	21	1.74
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	27	1.74
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	28	1.74
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	16	1.73
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	23	1.72
(1,1352)	1:27:A:MET:HA	1:31:A:ASN:HD21	24	1.67
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	9	1.59
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	26	1.48
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	24	1.45
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	24	1.45
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	20	1.44
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	20	1.44
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	25	1.43
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	25	1.43
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	11	1.4
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	11	1.4
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	28	1.4
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	28	1.4
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	17	1.38
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	17	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	18	1.38
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	18	1.38
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	30	1.38
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	30	1.38
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	2	1.36
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	2	1.36
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	13	1.36
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	13	1.36
(1,1387)	1:63:A:GLU:HA	1:66:A:GLN:HE21	9	1.35
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	9	1.34
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	9	1.34
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	14	1.34
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	14	1.34
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	26	1.34
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	26	1.34
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	5	1.33
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	5	1.33
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	15	1.33
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	15	1.33
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	4	1.32
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	4	1.32
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	6	1.32
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	6	1.32
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	12	1.32
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	12	1.32
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	27	1.32
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	27	1.32
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	29	1.32
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	29	1.32
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	22	1.31
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	22	1.31
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	8	1.3
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	8	1.3
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	3	1.29
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	3	1.29
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	7	1.29
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	7	1.29
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	10	1.29
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	10	1.29
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	14	1.28
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	1	1.28
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	1	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	21	1.28
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	21	1.28
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	7	1.24
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	15	1.23
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	24	1.23
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	24	1.23
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	24	1.23
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	3	1.22
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	2	1.21
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	2	1.21
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	2	1.21
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	2	1.21
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	2	1.21
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	2	1.21
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	6	1.21
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	25	1.19
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	27	1.19
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	27	1.19
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	27	1.19
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	8	1.18
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	8	1.18
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	8	1.18
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	8	1.18
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	8	1.18
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	8	1.18
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	22	1.18
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	22	1.18
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	22	1.18
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	22	1.18
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	22	1.18
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	22	1.18
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	16	1.18
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	16	1.18
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	12	1.17
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	12	1.17
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	12	1.17
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	12	1.17
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	12	1.17
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	12	1.17
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	29	1.15
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	29	1.15
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	29	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	29	1.15
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	29	1.15
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	29	1.15
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	23	1.15
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	23	1.15
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	23	1.15
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	29	1.15
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	29	1.15
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	29	1.15
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	11	1.14
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	11	1.14
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	11	1.14
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	11	1.14
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	11	1.14
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	11	1.14
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	30	1.14
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	30	1.14
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	30	1.14
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	30	1.14
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	30	1.14
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	30	1.14
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	30	1.14
(1,1384)	1:62:A:VAL:HG11	1:66:A:GLN:HE21	9	1.14
(1,1384)	1:62:A:VAL:HG12	1:66:A:GLN:HE21	9	1.14
(1,1384)	1:62:A:VAL:HG13	1:66:A:GLN:HE21	9	1.14
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	17	1.13
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	19	1.13
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	19	1.13
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	25	1.13
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	25	1.13
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	25	1.13
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	10	1.12
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	13	1.12
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	13	1.12
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	13	1.12
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	28	1.11
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	28	1.11
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	28	1.11
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	28	1.11
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	28	1.11
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	28	1.11
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	29	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	3	1.11
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	3	1.11
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	3	1.11
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	22	1.11
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	22	1.11
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	22	1.11
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	16	1.11
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	16	1.11
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	16	1.11
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	5	1.1
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	5	1.1
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	5	1.1
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	5	1.1
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	5	1.1
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	5	1.1
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	28	1.1
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	12	1.1
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	12	1.1
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	12	1.1
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	27	1.1
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	27	1.1
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	27	1.1
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	13	1.09
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	21	1.09
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	15	1.09
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	15	1.09
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	15	1.09
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	24	1.08
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	14	1.08
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	8	1.08
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	8	1.08
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	8	1.08
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	13	1.07
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	13	1.07
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	13	1.07
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	13	1.07
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	13	1.07
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	13	1.07
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	2	1.07
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	27	1.07
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	12	1.07
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	26	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	26	1.07
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	26	1.07
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	4	1.07
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	4	1.07
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	4	1.07
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	7	1.07
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	7	1.07
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	7	1.07
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	11	1.07
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	11	1.07
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	11	1.07
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	19	1.07
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	19	1.07
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	19	1.07
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	21	1.07
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	21	1.07
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	21	1.07
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	16	1.05
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	16	1.05
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	16	1.05
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	16	1.05
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	16	1.05
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	16	1.05
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	1	1.05
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	18	1.05
(1,1355)	1:27:A:MET:HB2	1:31:A:ASN:HD21	23	1.05
(1,1355)	1:27:A:MET:HB3	1:31:A:ASN:HD21	23	1.05
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	18	1.05
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	18	1.05
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	18	1.05
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	7	1.04
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	7	1.04
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	7	1.04
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	7	1.04
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	7	1.04
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	7	1.04
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	15	1.04
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	15	1.04
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	15	1.04
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	15	1.04
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	15	1.04
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	15	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	26	1.04
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	26	1.04
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	26	1.04
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	26	1.04
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	26	1.04
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	26	1.04
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	4	1.04
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	5	1.04
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	1	1.04
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	1	1.04
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	1	1.04
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	6	1.04
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	6	1.04
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	6	1.04
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	17	1.04
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	17	1.04
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	17	1.04
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD11	21	1.04
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD12	21	1.04
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD13	21	1.04
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD11	21	1.04
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD12	21	1.04
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD13	21	1.04
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	7	1.03
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	27	1.03
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	28	1.03
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	28	1.03
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	28	1.03
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	3	1.02
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	3	1.02
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	3	1.02
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	3	1.02
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	3	1.02
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	3	1.02
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	14	1.02
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	14	1.02
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	14	1.02
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	14	1.02
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	14	1.02
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	14	1.02
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	19	1.02
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	6	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	24	1.02
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	3	1.02
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	3	1.02
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	3	1.02
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	5	1.02
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	5	1.02
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	5	1.02
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	10	1.02
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	10	1.02
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	10	1.02
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	1	1.01
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	1	1.01
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	1	1.01
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	1	1.01
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	1	1.01
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	1	1.01
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	14	1.01
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	14	1.01
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	14	1.01
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	22	1.01
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	22	1.01
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	22	1.01
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	25	1.0
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	20	1.0
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	20	1.0
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	20	1.0
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	20	1.0
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	26	1.0
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	26	1.0
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	26	1.0
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	24	1.0
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	23	0.99
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	23	0.99
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	23	0.99
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	23	0.99
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	23	0.99
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	23	0.99
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	24	0.99
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	24	0.99
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	24	0.99
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	24	0.99
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	24	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	24	0.99
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	16	0.99
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	30	0.99
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	4	0.98
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	4	0.98
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	4	0.98
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	4	0.98
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	4	0.98
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	4	0.98
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	25	0.97
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	25	0.97
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	25	0.97
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	25	0.97
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	25	0.97
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	25	0.97
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	21	0.97
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	23	0.97
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	2	0.97
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	2	0.97
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	2	0.97
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	3	0.96
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	28	0.96
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	9	0.95
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	9	0.95
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	9	0.95
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	9	0.95
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	9	0.95
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	9	0.95
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	17	0.95
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	17	0.95
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	17	0.95
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	17	0.95
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	17	0.95
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	17	0.95
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	5	0.95
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	14	0.95
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	16	0.95
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	19	0.95
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	9	0.95
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	9	0.95
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	9	0.95
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	30	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	30	0.95
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	30	0.95
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	2	0.94
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	4	0.94
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	17	0.94
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	19	0.93
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	19	0.93
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	19	0.93
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	19	0.93
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	19	0.93
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	19	0.93
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	30	0.93
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	6	0.93
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	29	0.93
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	6	0.92
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	6	0.92
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	6	0.92
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	6	0.92
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	6	0.92
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	6	0.92
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	1	0.92
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	3	0.92
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	2	0.92
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	2	0.92
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	2	0.92
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	8	0.91
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	15	0.91
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	18	0.91
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	26	0.91
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	8	0.91
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	8	0.91
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	8	0.91
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	28	0.9
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	10	0.9
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	25	0.9
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	20	0.89
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	20	0.89
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	20	0.89
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	20	0.89
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	20	0.89
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	20	0.89
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	23	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	8	0.89
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	20	0.89
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	10	0.89
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	11	0.89
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	19	0.88
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	9	0.88
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	12	0.88
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	13	0.88
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	22	0.88
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	15	0.88
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	4	0.87
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	29	0.87
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	30	0.87
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	21	0.87
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	15	0.86
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	21	0.86
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	6	0.86
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	18	0.86
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	30	0.86
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	11	0.85
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	4	0.85
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	7	0.85
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	15	0.85
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	11	0.84
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	1	0.84
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	2	0.84
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	11	0.84
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	12	0.84
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	4	0.84
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	12	0.84
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	21	0.84
(1,1392)	1:65:A:GLN:HA	1:65:A:GLN:HE21	7	0.83
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	12	0.83
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	15	0.83
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	2	0.83
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	14	0.83
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	17	0.83
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	24	0.83
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	25	0.83
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	21	0.82
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	21	0.82
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	21	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	21	0.82
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	21	0.82
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	21	0.82
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	20	0.82
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	5	0.82
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	5	0.82
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	5	0.82
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	28	0.82
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	28	0.82
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	28	0.82
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	9	0.82
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	1	0.82
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	6	0.82
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	10	0.82
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	20	0.82
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	22	0.82
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	11	0.81
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	17	0.81
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	26	0.81
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	5	0.81
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	6	0.81
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	9	0.81
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	29	0.81
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	18	0.8
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	18	0.8
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	18	0.8
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	18	0.8
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	18	0.8
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	18	0.8
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	13	0.8
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	1	0.8
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	5	0.8
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	7	0.8
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	10	0.8
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	19	0.8
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	8	0.8
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	11	0.8
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	26	0.8
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	28	0.8
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	29	0.79
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	26	0.79
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	29	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	16	0.79
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	27	0.79
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	10	0.78
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	17	0.78
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	9	0.78
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	13	0.78
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	1	0.78
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	3	0.78
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	23	0.77
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	23	0.77
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	23	0.77
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	2	0.77
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	5	0.77
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	22	0.77
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	13	0.77
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	23	0.77
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	6	0.76
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	2	0.76
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	10	0.76
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	20	0.76
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	18	0.76
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	27	0.76
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	30	0.76
(1,894)	1:42:A:ASN:H	1:42:A:ASN:HD21	19	0.76
(1,1354)	1:30:A:ALA:HB1	1:31:A:ASN:HD21	24	0.75
(1,1354)	1:30:A:ALA:HB2	1:31:A:ASN:HD21	24	0.75
(1,1354)	1:30:A:ALA:HB3	1:31:A:ASN:HD21	24	0.75
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	15	0.75
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	18	0.75
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	4	0.74
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	22	0.74
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	8	0.74
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD11	10	0.74
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD12	10	0.74
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD13	10	0.74
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD11	10	0.74
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD12	10	0.74
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD13	10	0.74
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	8	0.73
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	23	0.73
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	25	0.73
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	3	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	23	0.73
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	25	0.73
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	28	0.73
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	5	0.72
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	1	0.72
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	1	0.72
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	1	0.72
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	16	0.72
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	20	0.72
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	11	0.71
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	18	0.71
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	24	0.71
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	16	0.71
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	3	0.71
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	24	0.71
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	21	0.7
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	28	0.7
(1,1350)	1:31:A:ASN:H	1:31:A:ASN:HD21	14	0.7
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	27	0.69
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	13	0.69
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	29	0.69
(1,1682)	1:45:A:LEU:HD11	1:65:A:GLN:HE21	10	0.68
(1,1682)	1:45:A:LEU:HD12	1:65:A:GLN:HE21	10	0.68
(1,1682)	1:45:A:LEU:HD13	1:65:A:GLN:HE21	10	0.68
(1,1682)	1:45:A:LEU:HD21	1:65:A:GLN:HE21	10	0.68
(1,1682)	1:45:A:LEU:HD22	1:65:A:GLN:HE21	10	0.68
(1,1682)	1:45:A:LEU:HD23	1:65:A:GLN:HE21	10	0.68
(1,1402)	1:42:A:ASN:HD22	1:64:A:GLN:HE22	9	0.68
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	17	0.65
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	10	0.65
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	27	0.65
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	1	0.64
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	14	0.64
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	22	0.63
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	30	0.63
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	4	0.63
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	12	0.62
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	23	0.62
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	28	0.62
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	7	0.62
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	8	0.62
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	2	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	3	0.61
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	8	0.61
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD11	28	0.61
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD12	28	0.61
(1,387)	1:25:A:ARG:HH11	1:54:A:LEU:HD13	28	0.61
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD11	28	0.61
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD12	28	0.61
(1,387)	1:25:A:ARG:HH12	1:54:A:LEU:HD13	28	0.61
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	11	0.6
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	18	0.6
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	29	0.6
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	21	0.59
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	19	0.59
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	20	0.58
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	4	0.58
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	5	0.58
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	6	0.58
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	14	0.58
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	15	0.58
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	16	0.58
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	7	0.58
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	7	0.58
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	7	0.58
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	17	0.57
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	20	0.57
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	25	0.57
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	26	0.57
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	30	0.56
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	19	0.55
(1,1387)	1:63:A:GLU:HA	1:66:A:GLN:HE21	13	0.54
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	7	0.54
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	25	0.54
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	13	0.53
(1,1386)	1:66:A:GLN:HA	1:66:A:GLN:HE21	24	0.5
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	29	0.49
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	29	0.49
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	29	0.49
(1,1401)	1:42:A:ASN:HD22	1:64:A:GLN:HE21	16	0.48
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	2	0.48
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	2	0.48
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	2	0.48
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	17	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	15	0.45
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	15	0.45
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	15	0.45
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	24	0.44
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	24	0.44
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	24	0.44
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	12	0.43
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	12	0.43
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	12	0.43
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	21	0.43
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	21	0.43
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	21	0.43
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD21	11	0.43
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD22	11	0.43
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD23	11	0.43
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD21	11	0.43
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD22	11	0.43
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD23	11	0.43
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	1	0.42
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	1	0.42
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	1	0.42
(1,489)	1:67:A:ASP:HB3	1:70:A:ARG:HB2	21	0.42
(1,489)	1:67:A:ASP:HB3	1:70:A:ARG:HB3	21	0.42
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	12	0.42
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	12	0.42
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	12	0.42
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	13	0.41
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	13	0.41
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	13	0.41
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	18	0.41
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	18	0.41
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	18	0.41
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	20	0.4
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	20	0.4
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	20	0.4
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	20	0.4
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	20	0.4
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	20	0.4
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	17	0.4
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	17	0.4
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	17	0.4
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	9	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	9	0.39
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	9	0.39
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	11	0.39
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	11	0.39
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	11	0.39
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	23	0.39
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	23	0.39
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	23	0.39
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	21	0.38
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	21	0.38
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	14	0.37
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	5	0.37
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	5	0.37
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	5	0.37
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	8	0.37
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	8	0.37
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	8	0.37
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	7	0.36
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	7	0.36
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	8	0.36
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	8	0.36
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	25	0.36
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	25	0.36
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	16	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	26	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	26	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	26	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	27	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	27	0.36
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	27	0.36
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	17	0.35
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	17	0.35
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	19	0.35
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	4	0.35
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	4	0.35
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	4	0.35
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	20	0.35
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	20	0.35
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	20	0.35
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	13	0.34
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	13	0.34
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	16	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	16	0.34
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	16	0.34
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	17	0.34
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	17	0.34
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	17	0.34
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	15	0.34
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	15	0.34
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	15	0.34
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	22	0.34
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	22	0.34
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	22	0.34
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	11	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	11	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	11	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	11	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	11	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	11	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	13	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	13	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	13	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	13	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	13	0.33
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	13	0.33
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	7	0.33
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	7	0.33
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	7	0.33
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	21	0.33
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	21	0.33
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	21	0.33
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	4	0.32
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	4	0.32
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	15	0.32
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	15	0.32
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	16	0.32
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	16	0.32
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	8	0.32
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	8	0.32
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	8	0.32
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	8	0.32
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	8	0.32
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	8	0.32
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	24	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1383)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	13	0.32
(1,1383)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	13	0.32
(1,1383)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	13	0.32
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	6	0.32
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	6	0.32
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	6	0.32
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	16	0.32
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	16	0.32
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	16	0.32
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	24	0.32
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	24	0.32
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	24	0.32
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	27	0.32
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	27	0.32
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	27	0.32
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	27	0.31
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	27	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	16	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	16	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	16	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	16	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	16	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	16	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	19	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	19	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	19	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	19	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	19	0.31
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	19	0.31
(1,1353)	1:28:A:LEU:HA	1:31:A:ASN:HD21	23	0.31
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	25	0.31
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	25	0.31
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	25	0.31
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	15	0.3
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	15	0.3
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	15	0.3
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	15	0.3
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	15	0.3
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	15	0.3
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	15	0.3
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	15	0.3
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	15	0.3
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	15	0.3
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	15	0.3
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	29	0.3
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	29	0.3
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	4	0.3
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	4	0.3
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	4	0.3
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	17	0.29
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	17	0.29
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	17	0.29
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	17	0.29
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	17	0.29
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	17	0.29
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	20	0.29
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	20	0.29
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	20	0.29
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	20	0.29
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	20	0.29
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	20	0.29
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	21	0.29
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	20	0.29
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	20	0.29
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	20	0.29
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	13	0.29
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	13	0.29
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	13	0.29
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	27	0.28
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	27	0.28
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	27	0.28
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	27	0.28
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	27	0.28
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	27	0.28
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	6	0.28
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	6	0.28
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	6	0.28
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	6	0.28
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	6	0.28
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	6	0.28
(1,1385)	1:62:A:VAL:HB	1:66:A:GLN:HE21	18	0.28
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	3	0.28
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	3	0.28
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	16	0.27
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	16	0.27
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	16	0.27
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	16	0.27
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	16	0.27
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	16	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	26	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	26	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	26	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	26	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	26	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	26	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	27	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	27	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	27	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	27	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	27	0.27
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	27	0.27
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	27	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	27	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	27	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	27	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	27	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	27	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	30	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	30	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	30	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	30	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	30	0.26
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	30	0.26
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	16	0.26
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	16	0.26
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	16	0.26
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	16	0.26
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	16	0.26
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	16	0.26
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	2	0.26
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	2	0.26
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	1	0.26
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	1	0.26
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	29	0.26
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	29	0.26
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	29	0.26
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	30	0.25
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	30	0.25
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	30	0.25
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	30	0.25
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	30	0.25
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	30	0.25
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	21	0.25
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	21	0.25
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	30	0.25
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	30	0.25
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	30	0.25
(1,1786)	1:62:A:VAL:HG11	1:65:A:GLN:HB2	7	0.24
(1,1786)	1:62:A:VAL:HG11	1:65:A:GLN:HB3	7	0.24
(1,1786)	1:62:A:VAL:HG12	1:65:A:GLN:HB2	7	0.24
(1,1786)	1:62:A:VAL:HG12	1:65:A:GLN:HB3	7	0.24
(1,1786)	1:62:A:VAL:HG13	1:65:A:GLN:HB2	7	0.24
(1,1786)	1:62:A:VAL:HG13	1:65:A:GLN:HB3	7	0.24
(1,1786)	1:62:A:VAL:HG21	1:65:A:GLN:HB2	7	0.24
(1,1786)	1:62:A:VAL:HG21	1:65:A:GLN:HB3	7	0.24
(1,1786)	1:62:A:VAL:HG22	1:65:A:GLN:HB2	7	0.24
(1,1786)	1:62:A:VAL:HG22	1:65:A:GLN:HB3	7	0.24
(1,1786)	1:62:A:VAL:HG23	1:65:A:GLN:HB2	7	0.24
(1,1786)	1:62:A:VAL:HG23	1:65:A:GLN:HB3	7	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	6	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	6	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	6	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	6	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	6	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	6	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	17	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	17	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	17	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	17	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	17	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	17	0.24
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	10	0.24
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	10	0.24
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	10	0.24
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	10	0.24
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	10	0.24
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	29	0.24
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	29	0.24
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	29	0.24
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	29	0.24
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	29	0.24
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	29	0.24
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	20	0.24
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	20	0.24
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	24	0.24
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	24	0.24
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	24	0.24
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	3	0.23
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	3	0.23
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	3	0.23
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	3	0.23
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	3	0.23
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	3	0.23
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	3	0.23
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	3	0.23
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	3	0.23
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	3	0.23
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	3	0.23
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	3	0.23
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	6	0.23
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	6	0.23
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	6	0.23
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	6	0.23
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	6	0.23
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	6	0.23
(1,1591)	1:35:A:LEU:HD11	1:39:A:LYS:HD2	21	0.23
(1,1591)	1:35:A:LEU:HD11	1:39:A:LYS:HD3	21	0.23
(1,1591)	1:35:A:LEU:HD12	1:39:A:LYS:HD2	21	0.23
(1,1591)	1:35:A:LEU:HD12	1:39:A:LYS:HD3	21	0.23
(1,1591)	1:35:A:LEU:HD13	1:39:A:LYS:HD2	21	0.23
(1,1591)	1:35:A:LEU:HD13	1:39:A:LYS:HD3	21	0.23
(1,1591)	1:35:A:LEU:HD21	1:39:A:LYS:HD2	21	0.23
(1,1591)	1:35:A:LEU:HD21	1:39:A:LYS:HD3	21	0.23
(1,1591)	1:35:A:LEU:HD22	1:39:A:LYS:HD2	21	0.23
(1,1591)	1:35:A:LEU:HD22	1:39:A:LYS:HD3	21	0.23
(1,1591)	1:35:A:LEU:HD23	1:39:A:LYS:HD2	21	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1591)	1:35:A:LEU:HD23	1:39:A:LYS:HD3	21	0.23
(1,1022)	1:54:A:LEU:HD21	1:56:A:LYS:H	17	0.23
(1,1022)	1:54:A:LEU:HD22	1:56:A:LYS:H	17	0.23
(1,1022)	1:54:A:LEU:HD23	1:56:A:LYS:H	17	0.23
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	17	0.23
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	17	0.23
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	29	0.23
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	29	0.23
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	2	0.23
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	2	0.23
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	2	0.23
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	6	0.23
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	6	0.23
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	6	0.23
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	14	0.22
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	14	0.22
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	14	0.22
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	20	0.22
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	20	0.22
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	20	0.22
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	10	0.21
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	10	0.21
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	10	0.21
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	10	0.21
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	10	0.21
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	10	0.21
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	4	0.21
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	4	0.21
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	4	0.21
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	4	0.21
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	4	0.21
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	4	0.21
(1,1022)	1:54:A:LEU:HD21	1:56:A:LYS:H	11	0.21
(1,1022)	1:54:A:LEU:HD22	1:56:A:LYS:H	11	0.21
(1,1022)	1:54:A:LEU:HD23	1:56:A:LYS:H	11	0.21
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	7	0.21
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	7	0.21
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	7	0.21
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	10	0.21
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	10	0.21
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	10	0.21
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	2	0.21
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	2	0.21
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	16	0.2
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	16	0.2
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	16	0.2
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	16	0.2
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	16	0.2
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	16	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	2	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	2	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	2	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	2	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	2	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	2	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	7	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	7	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	7	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	7	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	7	0.2
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	7	0.2
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB1	20	0.2
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB2	20	0.2
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB3	20	0.2
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	15	0.2
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	15	0.2
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	4	0.2
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	4	0.2
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	4	0.2
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	24	0.2
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	24	0.2
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	24	0.2
(1,1774)	1:61:A:LEU:HD11	1:65:A:GLN:HG2	7	0.19
(1,1774)	1:61:A:LEU:HD11	1:65:A:GLN:HG3	7	0.19
(1,1774)	1:61:A:LEU:HD12	1:65:A:GLN:HG2	7	0.19
(1,1774)	1:61:A:LEU:HD12	1:65:A:GLN:HG3	7	0.19
(1,1774)	1:61:A:LEU:HD13	1:65:A:GLN:HG2	7	0.19
(1,1774)	1:61:A:LEU:HD13	1:65:A:GLN:HG3	7	0.19
(1,1774)	1:61:A:LEU:HD21	1:65:A:GLN:HG2	7	0.19
(1,1774)	1:61:A:LEU:HD21	1:65:A:GLN:HG3	7	0.19
(1,1774)	1:61:A:LEU:HD22	1:65:A:GLN:HG2	7	0.19
(1,1774)	1:61:A:LEU:HD22	1:65:A:GLN:HG3	7	0.19
(1,1774)	1:61:A:LEU:HD23	1:65:A:GLN:HG2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:61:A:LEU:HD23	1:65:A:GLN:HG3	7	0.19
(1,1762)	1:60:A:VAL:HG11	1:65:A:GLN:H	12	0.19
(1,1762)	1:60:A:VAL:HG12	1:65:A:GLN:H	12	0.19
(1,1762)	1:60:A:VAL:HG13	1:65:A:GLN:H	12	0.19
(1,1762)	1:60:A:VAL:HG21	1:65:A:GLN:H	12	0.19
(1,1762)	1:60:A:VAL:HG22	1:65:A:GLN:H	12	0.19
(1,1762)	1:60:A:VAL:HG23	1:65:A:GLN:H	12	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	8	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	8	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	8	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	8	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	8	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	8	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	9	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	9	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	9	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	9	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	9	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	9	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	12	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	12	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	12	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	12	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	12	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	12	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	16	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	16	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	16	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	16	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	16	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	16	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	17	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	17	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	17	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	17	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	17	0.19
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	17	0.19
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD11	30	0.19
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD12	30	0.19
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD13	30	0.19
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD21	30	0.19
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD22	30	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1432)	1:18:A:LEU:HA	1:18:A:LEU:HD23	30	0.19
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	7	0.19
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	7	0.19
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	24	0.19
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	24	0.19
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	24	0.19
(1,501)	1:90:A:ALA:HB1	1:91:A:LYS:H	17	0.19
(1,501)	1:90:A:ALA:HB2	1:91:A:LYS:H	17	0.19
(1,501)	1:90:A:ALA:HB3	1:91:A:LYS:H	17	0.19
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	5	0.19
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	5	0.19
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	5	0.19
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	5	0.19
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	5	0.19
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	21	0.19
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	21	0.19
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	21	0.19
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	4	0.19
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	4	0.19
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	4	0.19
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	21	0.19
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	21	0.19
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	21	0.19
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	2	0.19
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	2	0.19
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	2	0.19
(1,1793)	1:62:A:VAL:HG11	1:66:A:GLN:HE21	9	0.18
(1,1793)	1:62:A:VAL:HG12	1:66:A:GLN:HE21	9	0.18
(1,1793)	1:62:A:VAL:HG13	1:66:A:GLN:HE21	9	0.18
(1,1793)	1:62:A:VAL:HG21	1:66:A:GLN:HE21	9	0.18
(1,1793)	1:62:A:VAL:HG22	1:66:A:GLN:HE21	9	0.18
(1,1793)	1:62:A:VAL:HG23	1:66:A:GLN:HE21	9	0.18
(1,1622)	1:41:A:ARG:HB2	1:42:A:ASN:H	29	0.18
(1,1622)	1:41:A:ARG:HB3	1:42:A:ASN:H	29	0.18
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	4	0.18
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	4	0.18
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	9	0.18
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	9	0.18
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	13	0.18
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	13	0.18
(1,837)	1:68:A:ARG:HB2	1:69:A:ALA:H	8	0.18
(1,837)	1:68:A:ARG:HB3	1:69:A:ALA:H	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	20	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	20	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	20	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	21	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	21	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	21	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	29	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	29	0.18
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	29	0.18
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	10	0.18
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	10	0.18
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	10	0.18
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	29	0.18
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	29	0.18
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	29	0.18
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	2	0.18
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	2	0.18
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	2	0.18
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	24	0.18
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	24	0.18
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	24	0.18
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB2	29	0.17
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB3	29	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	2	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	2	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	2	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	2	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	2	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	2	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	20	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	20	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	20	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	20	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	20	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	20	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	29	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	29	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	29	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	29	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	29	0.17
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	29	0.17
(1,1674)	1:45:A:LEU:HD11	1:60:A:VAL:HB	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1674)	1:45:A:LEU:HD12	1:60:A:VAL:HB	14	0.17
(1,1674)	1:45:A:LEU:HD13	1:60:A:VAL:HB	14	0.17
(1,1674)	1:45:A:LEU:HD21	1:60:A:VAL:HB	14	0.17
(1,1674)	1:45:A:LEU:HD22	1:60:A:VAL:HB	14	0.17
(1,1674)	1:45:A:LEU:HD23	1:60:A:VAL:HB	14	0.17
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	15	0.17
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	15	0.17
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	15	0.17
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	15	0.17
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	15	0.17
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	15	0.17
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	1	0.17
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	1	0.17
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	1	0.17
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	1	0.17
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	1	0.17
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	1	0.17
(1,1438)	1:19:A:ASP:H	1:61:A:LEU:HD11	5	0.17
(1,1438)	1:19:A:ASP:H	1:61:A:LEU:HD12	5	0.17
(1,1438)	1:19:A:ASP:H	1:61:A:LEU:HD13	5	0.17
(1,1438)	1:19:A:ASP:H	1:61:A:LEU:HD21	5	0.17
(1,1438)	1:19:A:ASP:H	1:61:A:LEU:HD22	5	0.17
(1,1438)	1:19:A:ASP:H	1:61:A:LEU:HD23	5	0.17
(1,1146)	1:65:A:GLN:HB2	1:66:A:GLN:H	7	0.17
(1,1146)	1:65:A:GLN:HB3	1:66:A:GLN:H	7	0.17
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD11	2	0.17
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD12	2	0.17
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD13	2	0.17
(1,837)	1:68:A:ARG:HB2	1:69:A:ALA:H	24	0.17
(1,837)	1:68:A:ARG:HB3	1:69:A:ALA:H	24	0.17
(1,564)	1:11:A:ILE:H	1:11:A:ILE:HB	20	0.17
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	30	0.17
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	30	0.17
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	30	0.17
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	2	0.17
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	2	0.17
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	2	0.17
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	28	0.17
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	28	0.17
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	28	0.17
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	17	0.17
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	17	0.17
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	20	0.17
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	20	0.17
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	20	0.17
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	20	0.17
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	20	0.17
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	20	0.17
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB2	2	0.16
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB3	2	0.16
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	17	0.16
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	17	0.16
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	17	0.16
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	17	0.16
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	17	0.16
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	17	0.16
(1,1529)	1:27:A:MET:HG2	1:31:A:ASN:HD21	23	0.16
(1,1529)	1:27:A:MET:HG3	1:31:A:ASN:HD21	23	0.16
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	2	0.16
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	2	0.16
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	2	0.16
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	2	0.16
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	2	0.16
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	2	0.16
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	20	0.16
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	20	0.16
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	20	0.16
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	20	0.16
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	20	0.16
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	20	0.16
(1,1241)	1:80:A:SER:H	1:81:A:ALA:HB1	12	0.16
(1,1241)	1:80:A:SER:H	1:81:A:ALA:HB2	12	0.16
(1,1241)	1:80:A:SER:H	1:81:A:ALA:HB3	12	0.16
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD21	2	0.16
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD22	2	0.16
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD23	2	0.16
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	5	0.16
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	5	0.16
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	16	0.16
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	16	0.16
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	20	0.16
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	20	0.16
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	1	0.16
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	4	0.16
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	4	0.16
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	19	0.16
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	19	0.16
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	19	0.16
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	29	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	1	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	1	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	1	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	8	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	8	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	8	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	9	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	9	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	9	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	11	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	11	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	11	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	15	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	15	0.16
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	15	0.16
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	7	0.16
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	7	0.16
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	7	0.16
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	17	0.16
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	17	0.16
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	17	0.16
(1,1790)	1:62:A:VAL:HG11	1:66:A:GLN:HA	2	0.15
(1,1790)	1:62:A:VAL:HG12	1:66:A:GLN:HA	2	0.15
(1,1790)	1:62:A:VAL:HG13	1:66:A:GLN:HA	2	0.15
(1,1790)	1:62:A:VAL:HG21	1:66:A:GLN:HA	2	0.15
(1,1790)	1:62:A:VAL:HG22	1:66:A:GLN:HA	2	0.15
(1,1790)	1:62:A:VAL:HG23	1:66:A:GLN:HA	2	0.15
(1,1790)	1:62:A:VAL:HG11	1:66:A:GLN:HA	13	0.15
(1,1790)	1:62:A:VAL:HG12	1:66:A:GLN:HA	13	0.15
(1,1790)	1:62:A:VAL:HG13	1:66:A:GLN:HA	13	0.15
(1,1790)	1:62:A:VAL:HG21	1:66:A:GLN:HA	13	0.15
(1,1790)	1:62:A:VAL:HG22	1:66:A:GLN:HA	13	0.15
(1,1790)	1:62:A:VAL:HG23	1:66:A:GLN:HA	13	0.15
(1,1787)	1:62:A:VAL:HG11	1:65:A:GLN:HE21	27	0.15
(1,1787)	1:62:A:VAL:HG12	1:65:A:GLN:HE21	27	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1787)	1:62:A:VAL:HG13	1:65:A:GLN:HE21	27	0.15
(1,1787)	1:62:A:VAL:HG21	1:65:A:GLN:HE21	27	0.15
(1,1787)	1:62:A:VAL:HG22	1:65:A:GLN:HE21	27	0.15
(1,1787)	1:62:A:VAL:HG23	1:65:A:GLN:HE21	27	0.15
(1,1761)	1:60:A:VAL:HG11	1:64:A:GLN:HE21	26	0.15
(1,1761)	1:60:A:VAL:HG11	1:64:A:GLN:HE22	26	0.15
(1,1761)	1:60:A:VAL:HG12	1:64:A:GLN:HE21	26	0.15
(1,1761)	1:60:A:VAL:HG12	1:64:A:GLN:HE22	26	0.15
(1,1761)	1:60:A:VAL:HG13	1:64:A:GLN:HE21	26	0.15
(1,1761)	1:60:A:VAL:HG13	1:64:A:GLN:HE22	26	0.15
(1,1761)	1:60:A:VAL:HG21	1:64:A:GLN:HE21	26	0.15
(1,1761)	1:60:A:VAL:HG21	1:64:A:GLN:HE22	26	0.15
(1,1761)	1:60:A:VAL:HG22	1:64:A:GLN:HE21	26	0.15
(1,1761)	1:60:A:VAL:HG22	1:64:A:GLN:HE22	26	0.15
(1,1761)	1:60:A:VAL:HG23	1:64:A:GLN:HE21	26	0.15
(1,1761)	1:60:A:VAL:HG23	1:64:A:GLN:HE22	26	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	9	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	9	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	9	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	9	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	9	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	9	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	14	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	14	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	14	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	14	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	14	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	14	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	20	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	20	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	20	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	20	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	20	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	20	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	21	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	21	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	21	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	21	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	21	0.15
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	21	0.15
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	2	0.15
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	2	0.15
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	2	0.15
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	2	0.15
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	2	0.15
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	11	0.15
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	11	0.15
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	11	0.15
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	11	0.15
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	11	0.15
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	11	0.15
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	8	0.15
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	8	0.15
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	8	0.15
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	8	0.15
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	8	0.15
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	8	0.15
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	13	0.15
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	13	0.15
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	13	0.15
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	13	0.15
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	13	0.15
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	13	0.15
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD21	2	0.15
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD22	2	0.15
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD23	2	0.15
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	24	0.15
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	24	0.15
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	4	0.15
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	4	0.15
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	4	0.15
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD21	20	0.15
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD22	20	0.15
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD23	20	0.15
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	2	0.15
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	2	0.15
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	20	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	7	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	7	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	7	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	13	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	13	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	13	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	27	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	27	0.15
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	27	0.15
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	15	0.15
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	15	0.15
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	15	0.15
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	27	0.15
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	27	0.15
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	27	0.15
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	4	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	4	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	4	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	4	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	4	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	4	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	21	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	21	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	21	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	21	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	21	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	21	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	24	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	24	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	24	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	24	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	24	0.14
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	24	0.14
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	6	0.14
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	6	0.14
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	6	0.14
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	6	0.14
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	6	0.14
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	6	0.14
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	24	0.14
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	24	0.14
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	24	0.14
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	24	0.14
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	24	0.14
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	24	0.14
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	29	0.14
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	29	0.14
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	29	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	29	0.14
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	29	0.14
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	29	0.14
(1,1172)	1:70:A:ARG:H	1:70:A:ARG:HD2	4	0.14
(1,1172)	1:70:A:ARG:H	1:70:A:ARG:HD3	4	0.14
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD11	20	0.14
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD12	20	0.14
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD13	20	0.14
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	19	0.14
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	19	0.14
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	5	0.14
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	5	0.14
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	5	0.14
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD21	27	0.14
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD22	27	0.14
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD23	27	0.14
(1,572)	1:11:A:ILE:HA	1:12:A:THR:H	21	0.14
(1,572)	1:11:A:ILE:HA	1:12:A:THR:H	24	0.14
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	22	0.14
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	22	0.14
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	22	0.14
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	8	0.14
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	8	0.14
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	24	0.14
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	24	0.14
(1,321)	1:42:A:ASN:HD21	1:45:A:LEU:HG	22	0.14
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	2	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	12	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	12	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	12	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	16	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	16	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	16	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	26	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	26	0.14
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	26	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	16	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	16	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	16	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	29	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	29	0.14
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	29	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1891)	1:87:A:GLU:HB2	1:88:A:ALA:H	15	0.13
(1,1891)	1:87:A:GLU:HB3	1:88:A:ALA:H	15	0.13
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB2	5	0.13
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB3	5	0.13
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB2	24	0.13
(1,1858)	1:79:A:PHE:H	1:79:A:PHE:HB3	24	0.13
(1,1762)	1:60:A:VAL:HG11	1:65:A:GLN:H	22	0.13
(1,1762)	1:60:A:VAL:HG12	1:65:A:GLN:H	22	0.13
(1,1762)	1:60:A:VAL:HG13	1:65:A:GLN:H	22	0.13
(1,1762)	1:60:A:VAL:HG21	1:65:A:GLN:H	22	0.13
(1,1762)	1:60:A:VAL:HG22	1:65:A:GLN:H	22	0.13
(1,1762)	1:60:A:VAL:HG23	1:65:A:GLN:H	22	0.13
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG11	8	0.13
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG12	8	0.13
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG13	8	0.13
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG21	8	0.13
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG22	8	0.13
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG23	8	0.13
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG11	8	0.13
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG12	8	0.13
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG13	8	0.13
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG21	8	0.13
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG22	8	0.13
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG23	8	0.13
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	5	0.13
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	5	0.13
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	5	0.13
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	5	0.13
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	5	0.13
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	5	0.13
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	3	0.13
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	3	0.13
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	3	0.13
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	3	0.13
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	3	0.13
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	3	0.13
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	30	0.13
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	30	0.13
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	30	0.13
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	30	0.13
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	30	0.13
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	30	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	1	0.13
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	1	0.13
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	11	0.13
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	11	0.13
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	30	0.13
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	30	0.13
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	9	0.13
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	9	0.13
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	15	0.13
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	15	0.13
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	21	0.13
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	21	0.13
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	12	0.13
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	12	0.13
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	27	0.13
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	27	0.13
(1,322)	1:24:A:LEU:HG	1:57:A:PHE:HZ	24	0.13
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	10	0.13
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	10	0.13
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	10	0.13
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	19	0.13
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	19	0.13
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	19	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	1	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	1	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	1	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	5	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	5	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	5	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	8	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	8	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	8	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	9	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	9	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	9	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	13	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	13	0.13
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	13	0.13
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	4	0.13
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	4	0.13
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	4	0.13
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	5	0.13
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	5	0.13
(1,1860)	1:79:A:PHE:HB2	1:81:A:ALA:H	21	0.12
(1,1860)	1:79:A:PHE:HB3	1:81:A:ALA:H	21	0.12
(1,1855)	1:78:A:LEU:HD11	1:79:A:PHE:H	15	0.12
(1,1855)	1:78:A:LEU:HD12	1:79:A:PHE:H	15	0.12
(1,1855)	1:78:A:LEU:HD13	1:79:A:PHE:H	15	0.12
(1,1855)	1:78:A:LEU:HD21	1:79:A:PHE:H	15	0.12
(1,1855)	1:78:A:LEU:HD22	1:79:A:PHE:H	15	0.12
(1,1855)	1:78:A:LEU:HD23	1:79:A:PHE:H	15	0.12
(1,1762)	1:60:A:VAL:HG11	1:65:A:GLN:H	27	0.12
(1,1762)	1:60:A:VAL:HG12	1:65:A:GLN:H	27	0.12
(1,1762)	1:60:A:VAL:HG13	1:65:A:GLN:H	27	0.12
(1,1762)	1:60:A:VAL:HG21	1:65:A:GLN:H	27	0.12
(1,1762)	1:60:A:VAL:HG22	1:65:A:GLN:H	27	0.12
(1,1762)	1:60:A:VAL:HG23	1:65:A:GLN:H	27	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	1	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	1	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	1	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	1	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	1	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	1	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	13	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	13	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	13	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	13	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	13	0.12
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	13	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	2	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	2	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	2	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	2	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	2	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	2	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	4	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	4	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	4	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	4	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	4	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	4	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	5	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	5	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	5	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	5	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	5	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	8	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	8	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	8	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	8	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	8	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	8	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	29	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	29	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	29	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	29	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	29	0.12
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	29	0.12
(1,1672)	1:45:A:LEU:HD11	1:59:A:ARG:H	15	0.12
(1,1672)	1:45:A:LEU:HD12	1:59:A:ARG:H	15	0.12
(1,1672)	1:45:A:LEU:HD13	1:59:A:ARG:H	15	0.12
(1,1672)	1:45:A:LEU:HD21	1:59:A:ARG:H	15	0.12
(1,1672)	1:45:A:LEU:HD22	1:59:A:ARG:H	15	0.12
(1,1672)	1:45:A:LEU:HD23	1:59:A:ARG:H	15	0.12
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	5	0.12
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	5	0.12
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	5	0.12
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	5	0.12
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	5	0.12
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	5	0.12
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	17	0.12
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	17	0.12
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	17	0.12
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	17	0.12
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	17	0.12
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	17	0.12
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	21	0.12
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	21	0.12
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	21	0.12
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	21	0.12
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	21	0.12
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	21	0.12
(1,1344)	1:20:A:ASN:HD21	1:23:A:LEU:HD11	20	0.12
(1,1344)	1:20:A:ASN:HD21	1:23:A:LEU:HD12	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:20:A:ASN:HD21	1:23:A:LEU:HD13	20	0.12
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD21	24	0.12
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD22	24	0.12
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD23	24	0.12
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD11	29	0.12
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD12	29	0.12
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD13	29	0.12
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD21	21	0.12
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD22	21	0.12
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD23	21	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	6	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	6	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	8	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	8	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	12	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	12	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	22	0.12
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	22	0.12
(1,845)	1:38:A:LEU:HD11	1:39:A:LYS:H	2	0.12
(1,845)	1:38:A:LEU:HD12	1:39:A:LYS:H	2	0.12
(1,845)	1:38:A:LEU:HD13	1:39:A:LYS:H	2	0.12
(1,845)	1:38:A:LEU:HD11	1:39:A:LYS:H	5	0.12
(1,845)	1:38:A:LEU:HD12	1:39:A:LYS:H	5	0.12
(1,845)	1:38:A:LEU:HD13	1:39:A:LYS:H	5	0.12
(1,845)	1:38:A:LEU:HD11	1:39:A:LYS:H	24	0.12
(1,845)	1:38:A:LEU:HD12	1:39:A:LYS:H	24	0.12
(1,845)	1:38:A:LEU:HD13	1:39:A:LYS:H	24	0.12
(1,837)	1:68:A:ARG:HB2	1:69:A:ALA:H	27	0.12
(1,837)	1:68:A:ARG:HB3	1:69:A:ALA:H	27	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	8	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	8	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	8	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	12	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	12	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	12	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	15	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	15	0.12
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	15	0.12
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD21	17	0.12
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD22	17	0.12
(1,542)	1:25:A:ARG:HH11	1:54:A:LEU:HD23	17	0.12
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD21	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD22	17	0.12
(1,542)	1:25:A:ARG:HH12	1:54:A:LEU:HD23	17	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	7	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	7	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	13	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	13	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	17	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	17	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	29	0.12
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	29	0.12
(1,236)	1:38:A:LEU:HD11	1:42:A:ASN:HD21	8	0.12
(1,236)	1:38:A:LEU:HD12	1:42:A:ASN:HD21	8	0.12
(1,236)	1:38:A:LEU:HD13	1:42:A:ASN:HD21	8	0.12
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	4	0.12
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	6	0.12
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	6	0.12
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	6	0.12
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	30	0.12
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	30	0.12
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	30	0.12
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	26	0.12
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	26	0.12
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	26	0.12
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	30	0.12
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	30	0.12
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	30	0.12
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE1	1	0.12
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE2	1	0.12
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE3	1	0.12
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE1	1	0.12
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE2	1	0.12
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE3	1	0.12
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE1	1	0.12
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE2	1	0.12
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE3	1	0.12
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	8	0.12
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	8	0.12
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	8	0.12
(1,1897)	1:91:A:LYS:HB2	1:92:A:ILE:H	5	0.11
(1,1897)	1:91:A:LYS:HB3	1:92:A:ILE:H	5	0.11
(1,1891)	1:87:A:GLU:HB2	1:88:A:ALA:H	7	0.11
(1,1891)	1:87:A:GLU:HB3	1:88:A:ALA:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1873)	1:84:A:PHE:H	1:85:A:ASP:HB2	21	0.11
(1,1873)	1:84:A:PHE:H	1:85:A:ASP:HB3	21	0.11
(1,1850)	1:78:A:LEU:H	1:78:A:LEU:HB2	4	0.11
(1,1850)	1:78:A:LEU:H	1:78:A:LEU:HB3	4	0.11
(1,1828)	1:70:A:ARG:HG2	1:72:A:GLU:H	20	0.11
(1,1828)	1:70:A:ARG:HG3	1:72:A:GLU:H	20	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG11	2	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG12	2	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG13	2	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG21	2	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG22	2	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG23	2	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG11	2	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG12	2	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG13	2	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG21	2	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG22	2	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG23	2	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG11	22	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG12	22	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG13	22	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG21	22	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG22	22	0.11
(1,1747)	1:59:A:ARG:HD2	1:62:A:VAL:HG23	22	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG11	22	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG12	22	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG13	22	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG21	22	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG22	22	0.11
(1,1747)	1:59:A:ARG:HD3	1:62:A:VAL:HG23	22	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	7	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	7	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	7	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	7	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	7	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	7	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	9	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	9	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	9	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	9	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	9	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	11	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	11	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	11	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	11	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	11	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	11	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	26	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	26	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	26	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	26	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	26	0.11
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	26	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	11	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	11	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	11	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	11	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	11	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	11	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	12	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	12	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	12	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	12	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	12	0.11
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	12	0.11
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	24	0.11
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	24	0.11
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	24	0.11
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	24	0.11
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	24	0.11
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	24	0.11
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	27	0.11
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	27	0.11
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	27	0.11
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	27	0.11
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	27	0.11
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	27	0.11
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	30	0.11
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	30	0.11
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	30	0.11
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	30	0.11
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	30	0.11
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	30	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:62:A:VAL:HG21	1:63:A:GLU:H	7	0.11
(1,1108)	1:62:A:VAL:HG22	1:63:A:GLU:H	7	0.11
(1,1108)	1:62:A:VAL:HG23	1:63:A:GLU:H	7	0.11
(1,1108)	1:62:A:VAL:HG21	1:63:A:GLU:H	27	0.11
(1,1108)	1:62:A:VAL:HG22	1:63:A:GLU:H	27	0.11
(1,1108)	1:62:A:VAL:HG23	1:63:A:GLU:H	27	0.11
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD21	5	0.11
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD22	5	0.11
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD23	5	0.11
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD21	29	0.11
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD22	29	0.11
(1,1052)	1:58:A:SER:H	1:61:A:LEU:HD23	29	0.11
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD21	20	0.11
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD22	20	0.11
(1,941)	1:48:A:ALA:H	1:50:A:LEU:HD23	20	0.11
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	3	0.11
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	3	0.11
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	26	0.11
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	26	0.11
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB2	27	0.11
(1,939)	1:48:A:ALA:H	1:56:A:LYS:HB3	27	0.11
(1,845)	1:38:A:LEU:HD11	1:39:A:LYS:H	20	0.11
(1,845)	1:38:A:LEU:HD12	1:39:A:LYS:H	20	0.11
(1,845)	1:38:A:LEU:HD13	1:39:A:LYS:H	20	0.11
(1,845)	1:38:A:LEU:HD11	1:39:A:LYS:H	29	0.11
(1,845)	1:38:A:LEU:HD12	1:39:A:LYS:H	29	0.11
(1,845)	1:38:A:LEU:HD13	1:39:A:LYS:H	29	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	1	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	1	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	1	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	7	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	7	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	7	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	11	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	11	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	11	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	13	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	13	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	13	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	17	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	17	0.11
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD21	7	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD22	7	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD23	7	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD21	8	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD22	8	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD23	8	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD21	17	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD22	17	0.11
(1,658)	1:25:A:ARG:H	1:61:A:LEU:HD23	17	0.11
(1,639)	1:23:A:LEU:H	1:23:A:LEU:HD11	29	0.11
(1,639)	1:23:A:LEU:H	1:23:A:LEU:HD12	29	0.11
(1,639)	1:23:A:LEU:H	1:23:A:LEU:HD13	29	0.11
(1,572)	1:11:A:ILE:HA	1:12:A:THR:H	17	0.11
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG21	19	0.11
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG22	19	0.11
(1,562)	1:11:A:ILE:H	1:11:A:ILE:HG23	19	0.11
(1,561)	1:10:A:GLU:HA	1:11:A:ILE:H	15	0.11
(1,516)	1:20:A:ASN:HD21	1:23:A:LEU:HD21	2	0.11
(1,516)	1:20:A:ASN:HD21	1:23:A:LEU:HD22	2	0.11
(1,516)	1:20:A:ASN:HD21	1:23:A:LEU:HD23	2	0.11
(1,501)	1:90:A:ALA:HB1	1:91:A:LYS:H	10	0.11
(1,501)	1:90:A:ALA:HB2	1:91:A:LYS:H	10	0.11
(1,501)	1:90:A:ALA:HB3	1:91:A:LYS:H	10	0.11
(1,501)	1:90:A:ALA:HB1	1:91:A:LYS:H	30	0.11
(1,501)	1:90:A:ALA:HB2	1:91:A:LYS:H	30	0.11
(1,501)	1:90:A:ALA:HB3	1:91:A:LYS:H	30	0.11
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD11	10	0.11
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD12	10	0.11
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD13	10	0.11
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD11	10	0.11
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD12	10	0.11
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD13	10	0.11
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB2	16	0.11
(1,402)	1:53:A:ASP:HB2	1:56:A:LYS:HB3	16	0.11
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	10	0.11
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	10	0.11
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB2	11	0.11
(1,400)	1:53:A:ASP:HA	1:56:A:LYS:HB3	11	0.11
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	5	0.11
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	21	0.11
(1,232)	1:37:A:LEU:HB3	1:38:A:LEU:HB2	24	0.11
(1,228)	1:37:A:LEU:HD21	1:40:A:GLU:HB2	24	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,228)	1:37:A:LEU:HD21	1:40:A:GLU:HB3	24	0.11
(1,228)	1:37:A:LEU:HD22	1:40:A:GLU:HB2	24	0.11
(1,228)	1:37:A:LEU:HD22	1:40:A:GLU:HB3	24	0.11
(1,228)	1:37:A:LEU:HD23	1:40:A:GLU:HB2	24	0.11
(1,228)	1:37:A:LEU:HD23	1:40:A:GLU:HB3	24	0.11
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	3	0.11
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	3	0.11
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	3	0.11
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD21	22	0.11
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD22	22	0.11
(1,207)	1:35:A:LEU:HA	1:35:A:LEU:HD23	22	0.11
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	11	0.11
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	11	0.11
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	11	0.11
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE1	27	0.11
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE2	27	0.11
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE3	27	0.11
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE1	27	0.11
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE2	27	0.11
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE3	27	0.11
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE1	27	0.11
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE2	27	0.11
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE3	27	0.11
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	1	0.11
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	1	0.11
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	1	0.11
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	17	0.11
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	17	0.11
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	17	0.11
(1,1854)	1:78:A:LEU:HB2	1:79:A:PHE:HD1	12	0.1
(1,1854)	1:78:A:LEU:HB2	1:79:A:PHE:HD2	12	0.1
(1,1854)	1:78:A:LEU:HB3	1:79:A:PHE:HD1	12	0.1
(1,1854)	1:78:A:LEU:HB3	1:79:A:PHE:HD2	12	0.1
(1,1850)	1:78:A:LEU:H	1:78:A:LEU:HB2	21	0.1
(1,1850)	1:78:A:LEU:H	1:78:A:LEU:HB3	21	0.1
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG11	8	0.1
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG12	8	0.1
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG13	8	0.1
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG21	8	0.1
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG22	8	0.1
(1,1735)	1:58:A:SER:HA	1:60:A:VAL:HG23	8	0.1
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG11	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG12	7	0.1
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG13	7	0.1
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG21	7	0.1
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG22	7	0.1
(1,1724)	1:56:A:LYS:H	1:60:A:VAL:HG23	7	0.1
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD11	23	0.1
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD12	23	0.1
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD13	23	0.1
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD21	23	0.1
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD22	23	0.1
(1,1498)	1:25:A:ARG:H	1:29:A:LEU:HD23	23	0.1
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	12	0.1
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	12	0.1
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	12	0.1
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	12	0.1
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	12	0.1
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	12	0.1
(1,1491)	1:24:A:LEU:HD11	1:29:A:LEU:H	16	0.1
(1,1491)	1:24:A:LEU:HD12	1:29:A:LEU:H	16	0.1
(1,1491)	1:24:A:LEU:HD13	1:29:A:LEU:H	16	0.1
(1,1491)	1:24:A:LEU:HD21	1:29:A:LEU:H	16	0.1
(1,1491)	1:24:A:LEU:HD22	1:29:A:LEU:H	16	0.1
(1,1491)	1:24:A:LEU:HD23	1:29:A:LEU:H	16	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB1	1	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB2	1	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB3	1	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB1	10	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB2	10	0.1
(1,1266)	1:85:A:ASP:H	1:88:A:ALA:HB3	10	0.1
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD11	5	0.1
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD12	5	0.1
(1,942)	1:48:A:ALA:H	1:50:A:LEU:HD13	5	0.1
(1,845)	1:38:A:LEU:HD11	1:39:A:LYS:H	21	0.1
(1,845)	1:38:A:LEU:HD12	1:39:A:LYS:H	21	0.1
(1,845)	1:38:A:LEU:HD13	1:39:A:LYS:H	21	0.1
(1,837)	1:68:A:ARG:HB2	1:69:A:ALA:H	26	0.1
(1,837)	1:68:A:ARG:HB3	1:69:A:ALA:H	26	0.1
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	9	0.1
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	9	0.1
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	9	0.1
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD11	26	0.1
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD12	26	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:34:A:GLU:H	1:35:A:LEU:HD13	26	0.1
(1,572)	1:11:A:ILE:HA	1:12:A:THR:H	20	0.1
(1,571)	1:9:A:GLY:HA2	1:12:A:THR:H	22	0.1
(1,571)	1:9:A:GLY:HA3	1:12:A:THR:H	22	0.1
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD11	8	0.1
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD12	8	0.1
(1,464)	1:17:A:GLY:HA2	1:61:A:LEU:HD13	8	0.1
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD11	8	0.1
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD12	8	0.1
(1,464)	1:17:A:GLY:HA3	1:61:A:LEU:HD13	8	0.1
(1,228)	1:37:A:LEU:HD21	1:40:A:GLU:HB2	2	0.1
(1,228)	1:37:A:LEU:HD21	1:40:A:GLU:HB3	2	0.1
(1,228)	1:37:A:LEU:HD22	1:40:A:GLU:HB2	2	0.1
(1,228)	1:37:A:LEU:HD22	1:40:A:GLU:HB3	2	0.1
(1,228)	1:37:A:LEU:HD23	1:40:A:GLU:HB2	2	0.1
(1,228)	1:37:A:LEU:HD23	1:40:A:GLU:HB3	2	0.1
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	12	0.1
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	12	0.1
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	12	0.1
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD11	19	0.1
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD12	19	0.1
(1,160)	1:28:A:LEU:HA	1:28:A:LEU:HD13	19	0.1
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE1	4	0.1
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE2	4	0.1
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE3	4	0.1
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE1	4	0.1
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE2	4	0.1
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE3	4	0.1
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE1	4	0.1
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE2	4	0.1
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE3	4	0.1
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE1	21	0.1
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE2	21	0.1
(1,138)	1:24:A:LEU:HD21	1:27:A:MET:HE3	21	0.1
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE1	21	0.1
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE2	21	0.1
(1,138)	1:24:A:LEU:HD22	1:27:A:MET:HE3	21	0.1
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE1	21	0.1
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE2	21	0.1
(1,138)	1:24:A:LEU:HD23	1:27:A:MET:HE3	21	0.1
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	26	0.1
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	26	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	26	0.1
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD11	29	0.1
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD12	29	0.1
(1,78)	1:21:A:PRO:HG2	1:61:A:LEU:HD13	29	0.1

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

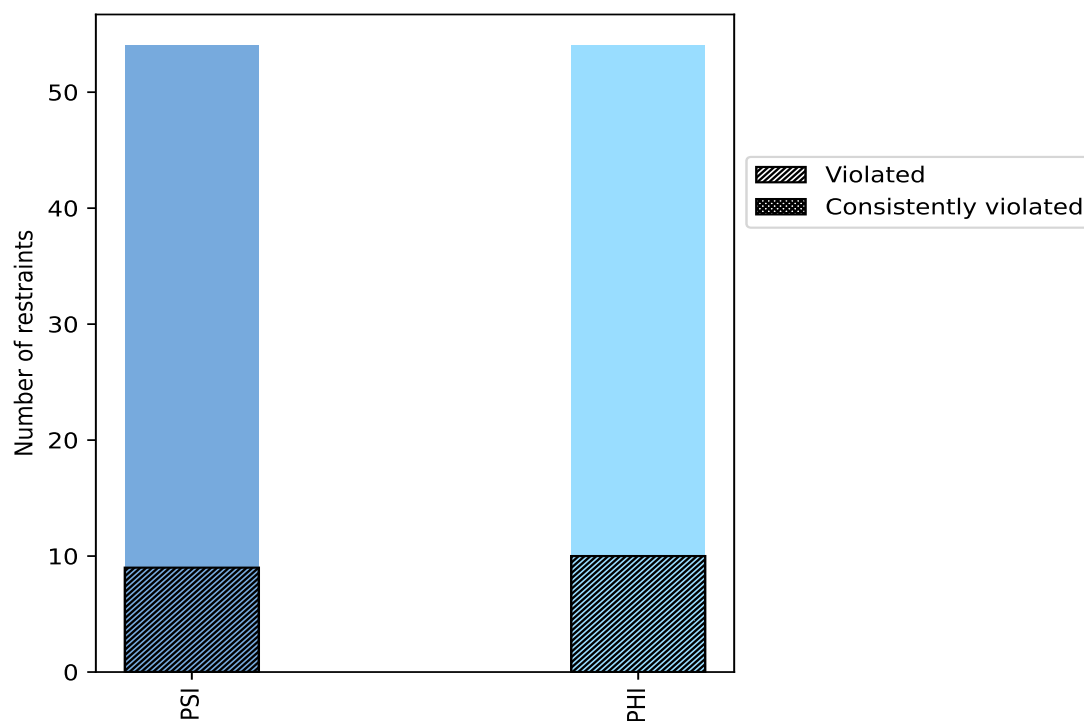
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	54	50.0	9	16.7	8.3	0	0.0	0.0
PHI	54	50.0	10	18.5	9.3	0	0.0	0.0
Total	108	100.0	19	17.6	17.6	0	0.0	0.0

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

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



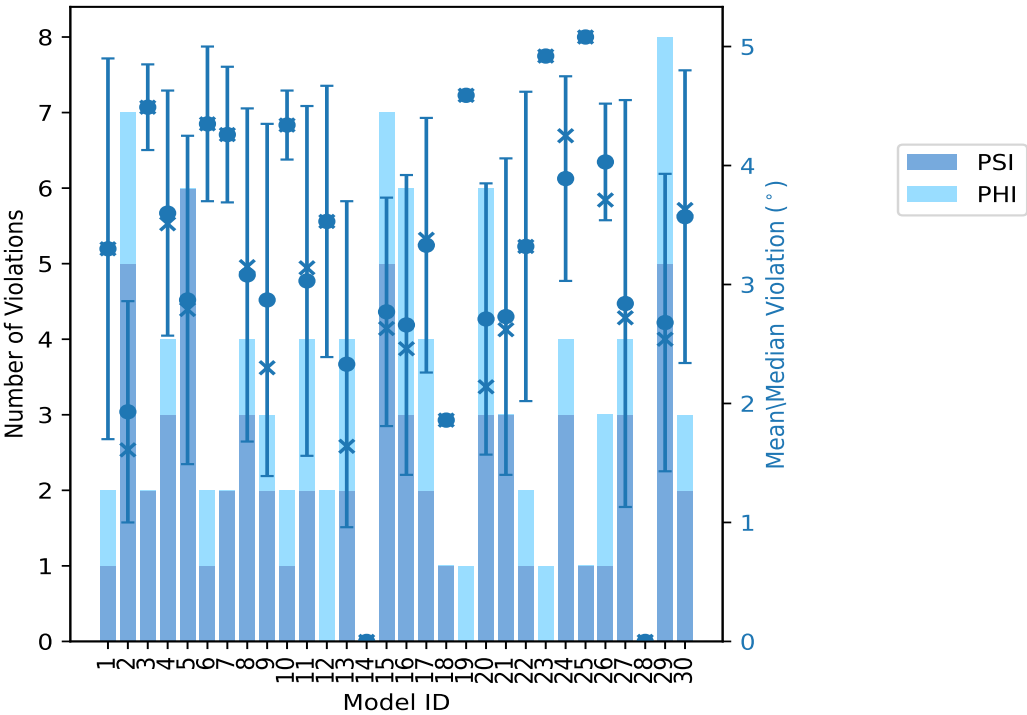
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	1	2	3.3	4.9	1.6	3.3
2	5	2	7	1.93	3.96	0.93	1.61
3	2	0	2	4.49	4.85	0.36	4.49
4	3	1	4	3.6	5.1	1.03	3.51
5	6	0	6	2.87	4.69	1.38	2.79
6	1	1	2	4.35	5.0	0.65	4.35
7	2	0	2	4.26	4.84	0.57	4.26
8	3	1	4	3.08	4.89	1.4	3.15
9	2	1	3	2.87	4.9	1.48	2.3
10	1	1	2	4.34	4.62	0.29	4.34
11	2	2	4	3.03	4.79	1.47	3.14
12	0	2	2	3.53	4.67	1.14	3.53
13	2	2	4	2.33	4.69	1.37	1.64
14	0	0	0	0.0	0.0	0.0	0.0
15	5	2	7	2.77	4.76	0.96	2.63
16	3	3	6	2.66	4.77	1.26	2.46
17	2	2	4	3.33	4.6	1.07	3.38
18	1	0	1	1.86	1.86	0.0	1.86
19	0	1	1	4.59	4.59	0.0	4.59
20	3	3	6	2.71	4.94	1.14	2.14
21	3	0	3	2.73	4.42	1.33	2.62
22	1	1	2	3.32	4.62	1.3	3.32
23	0	1	1	4.92	4.92	0.0	4.92
24	3	1	4	3.89	4.63	0.86	4.25
25	1	0	1	5.08	5.08	0.0	5.08
26	1	2	3	4.03	4.72	0.49	3.71
27	3	1	4	2.84	4.92	1.71	2.72
28	0	0	0	0.0	0.0	0.0	0.0
29	5	3	8	2.68	4.67	1.25	2.54
30	2	1	3	3.57	5.04	1.23	3.63

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
3	4	7	1	3.3
0	1	1	2	6.7
0	1	1	3	10.0
0	2	2	4	13.3
1	0	1	5	16.7
1	0	1	6	20.0
0	0	0	7	23.3
2	0	2	8	26.7
0	2	2	9	30.0
0	0	0	10	33.3
0	0	0	11	36.7

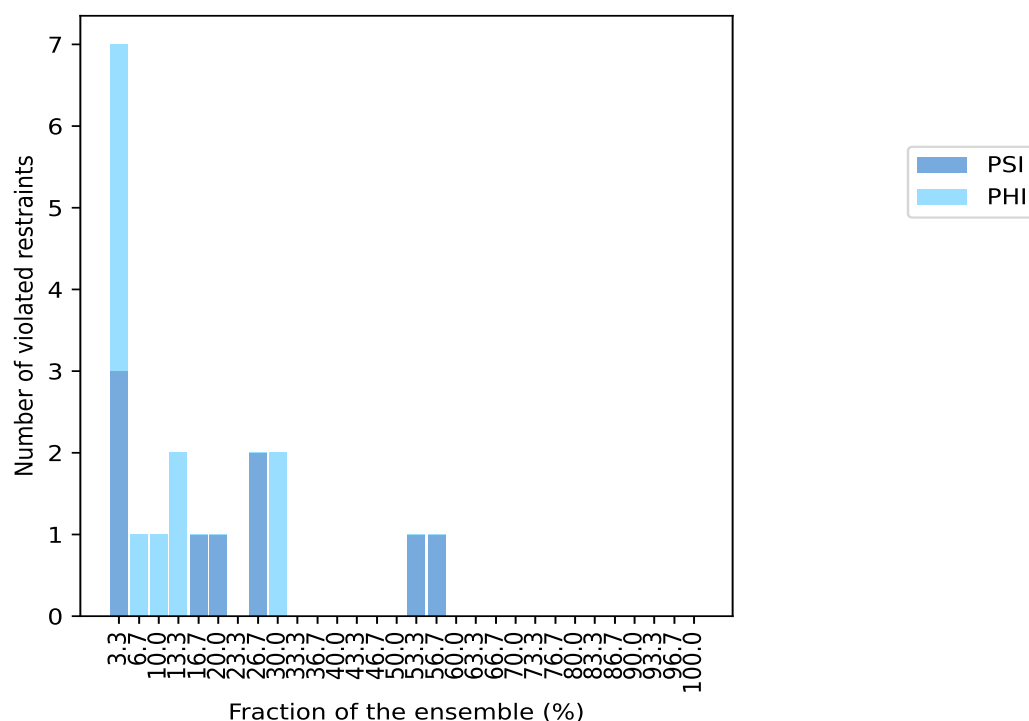
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	40.0
0	0	0	13	43.3
0	0	0	14	46.7
0	0	0	15	50.0
1	0	1	16	53.3
1	0	1	17	56.7
0	0	0	18	60.0
0	0	0	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
0	0	0	23	76.7
0	0	0	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
0	0	0	30	100.0

¹ Number of models with violations

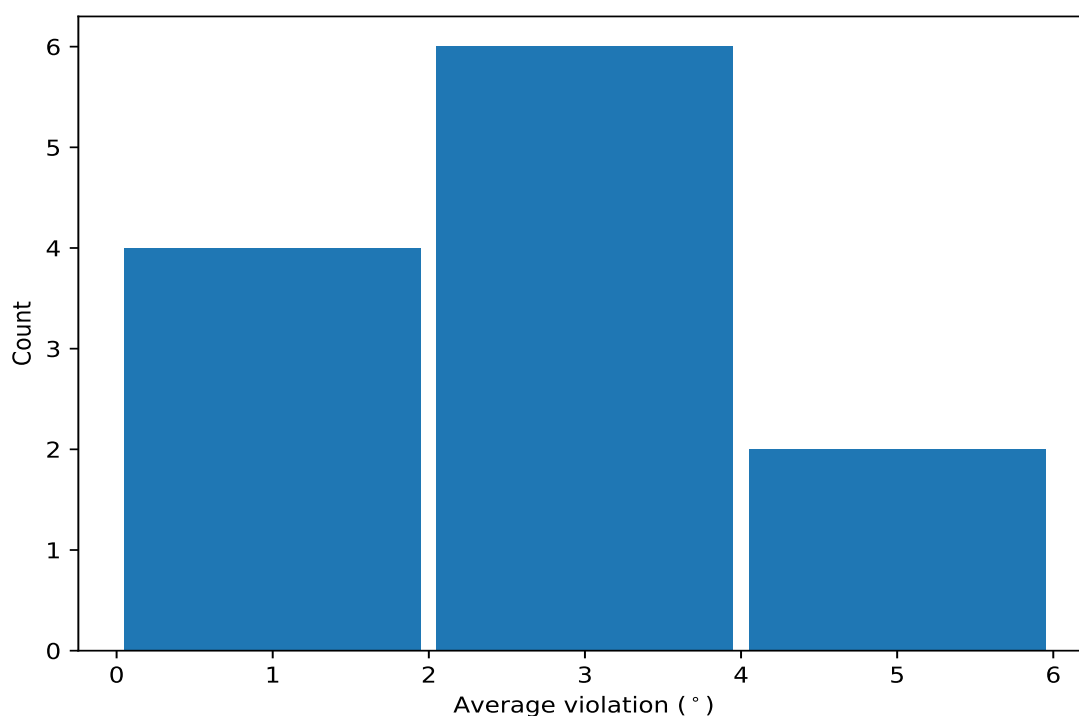
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

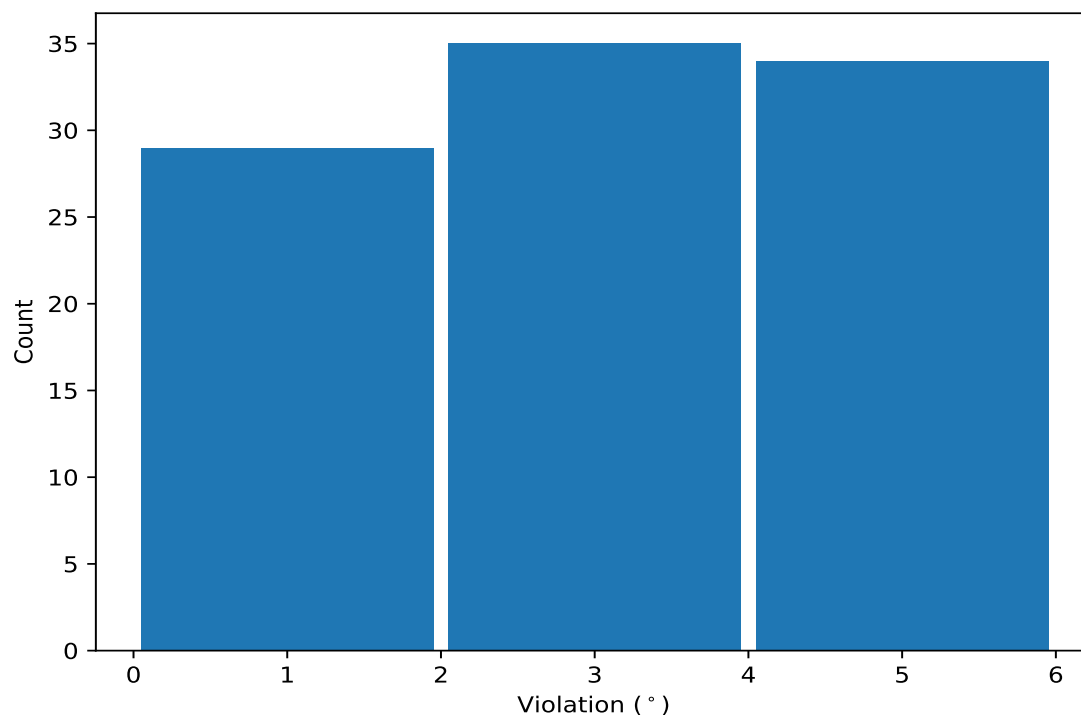
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	17	3.05	0.88	2.79
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	16	3.1	1.54	2.9
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	9	4.52	0.39	4.67
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	9	4.3	0.56	4.13
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	8	3.15	1.37	3.14
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	8	3.15	1.16	3.36
(1,26)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	6	1.53	0.45	1.48
(1,36)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:ARG:N	5	1.78	0.56	1.52
(1,105)	1:85:A:ASP:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	4	2.44	1.3	2.03
(1,27)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	4	1.84	0.49	1.95
(1,89)	1:70:A:ARG:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	3	3.85	1.34	4.69
(1,21)	1:32:A:PRO:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	2	1.72	0.18	1.72

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	4	5.1
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	25	5.08
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	30	5.04
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	6	5.0
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	20	4.94
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	23	4.92
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	27	4.92
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	9	4.9
(1,89)	1:70:A:ARG:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	1	4.9
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	8	4.89
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	3	4.85
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	7	4.84
(1,59)	1:55:A:GLU:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	11	4.79
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	16	4.77

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	15	4.76
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	26	4.72
(1,104)	1:82:A:ASP:N	1:82:A:ASP:CA	1:82:A:ASP:C	1:83:A:PRO:N	5	4.69
(1,89)	1:70:A:ARG:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	13	4.69
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	12	4.67
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	29	4.67
(1,86)	1:69:A:ALA:N	1:69:A:ALA:CA	1:69:A:ALA:C	1:70:A:ARG:N	24	4.63
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	22	4.62
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	10	4.62
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	17	4.6
(1,105)	1:85:A:ASP:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	19	4.59
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	21	4.42
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	24	4.34
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	5	4.21
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	24	4.16
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	27	4.14
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	3	4.14
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	17	4.13
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	11	4.05
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	10	4.05
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	2	3.96
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	29	3.95
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	4	3.88
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	5	3.76
(1,95)	1:73:A:GLN:C	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	8	3.75
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	26	3.71
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	6	3.7
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	7	3.69
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	16	3.67
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	26	3.67
(1,107)	1:86:A:LEU:C	1:87:A:GLU:N	1:87:A:GLU:CA	1:87:A:GLU:C	30	3.63
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	29	3.57
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	20	3.43
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	29	3.22
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	4	3.14
(1,91)	1:71:A:ARG:C	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	15	3.13
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	15	3.05
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	16	2.79
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	15	2.63
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	17	2.63
(1,36)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:ARG:N	21	2.62
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	8	2.55
(1,26)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	24	2.42
(1,27)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	12	2.39
(1,96)	1:74:A:GLU:N	1:74:A:GLU:CA	1:74:A:GLU:C	1:75:A:ARG:N	4	2.3
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	9	2.3
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	2	2.23
(1,36)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:ARG:N	15	2.22
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	11	2.22
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	20	2.2
(1,27)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	16	2.14

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	2	2.1
(1,105)	1:85:A:ASP:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	20	2.09
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	30	2.04
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	22	2.03
(1,105)	1:85:A:ASP:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	17	1.97
(1,89)	1:70:A:ARG:C	1:71:A:ARG:N	1:71:A:ARG:CA	1:71:A:ARG:C	15	1.95
(1,21)	1:32:A:PRO:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	20	1.9
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	18	1.86
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	29	1.86
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	5	1.82
(1,27)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	13	1.76
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	1	1.7
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	20	1.68
(1,26)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	15	1.62
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	2	1.61
(1,26)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	5	1.55
(1,21)	1:32:A:PRO:C	1:33:A:HIS:N	1:33:A:HIS:CA	1:33:A:HIS:C	29	1.53
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	13	1.52
(1,36)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:ARG:N	29	1.52
(1,39)	1:44:A:PRO:C	1:45:A:LEU:N	1:45:A:LEU:CA	1:45:A:LEU:C	2	1.48
(1,36)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:ARG:N	16	1.46
(1,26)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	9	1.42
(1,100)	1:76:A:ILE:N	1:76:A:ILE:CA	1:76:A:ILE:C	1:77:A:ARG:N	13	1.35
(1,30)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:LEU:N	27	1.3
(1,92)	1:72:A:GLU:N	1:72:A:GLU:CA	1:72:A:GLU:C	1:73:A:GLN:N	5	1.21
(1,26)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	21	1.16
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	8	1.13
(1,105)	1:85:A:ASP:C	1:86:A:LEU:N	1:86:A:LEU:CA	1:86:A:LEU:C	16	1.12
(1,85)	1:68:A:ARG:C	1:69:A:ALA:N	1:69:A:ALA:CA	1:69:A:ALA:C	29	1.12
(1,27)	1:35:A:LEU:C	1:36:A:SER:N	1:36:A:SER:CA	1:36:A:SER:C	2	1.08
(1,68)	1:60:A:VAL:N	1:60:A:VAL:CA	1:60:A:VAL:C	1:61:A:LEU:N	11	1.07
(1,36)	1:40:A:GLU:N	1:40:A:GLU:CA	1:40:A:GLU:C	1:41:A:ARG:N	2	1.07
(1,26)	1:35:A:LEU:N	1:35:A:LEU:CA	1:35:A:LEU:C	1:36:A:SER:N	27	1.02