



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 02:36 PM EST

PDB ID : 6RFM
BMRB ID : 34393
Title : Bordetella pertussis adenylate cyclase toxin transmembrane segment 411-490
in DPC micelles
Authors : Masin, J.; Bumba, L.; Veverka, V.
Deposited on : 2019-04-15

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

We welcome your comments at validation@mail.wwpdb.org

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<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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

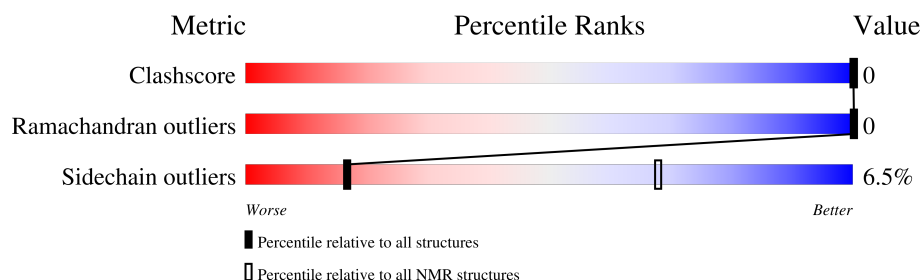
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	80	

2 Ensemble composition and analysis

This entry contains 50 models. Model 44 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:419-A:438 (20)	0.45	18
2	A:462-A:485 (24)	0.31	44

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 9 clusters. No single-model clusters were found.

Cluster number	Models
1	13, 20, 25, 26, 27, 35, 36, 41, 42, 47
2	6, 10, 14, 16, 32, 37, 39, 46, 48
3	4, 15, 17, 24, 29, 49
4	21, 31, 34, 43, 50
5	2, 11, 19, 22, 44
6	12, 23, 33, 40, 45
7	1, 7, 8, 28, 38
8	3, 9, 18
9	5, 30

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1135 atoms, of which 559 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bifunctional hemolysin/adenylate cyclase.

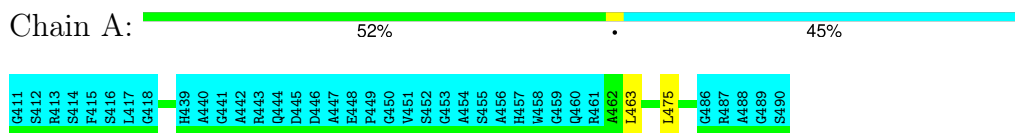
Mol	Chain	Residues	Atoms						Trace
1	A	80	Total	C	H	N	O	S	0
			1135	348	559	112	113	3	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Bifunctional hemolysin/adenylate cyclase

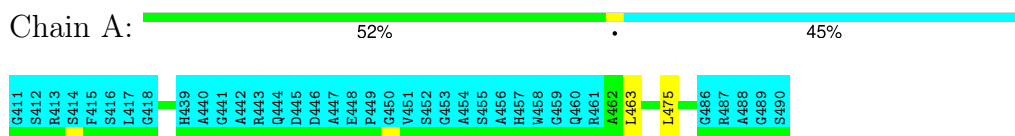


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

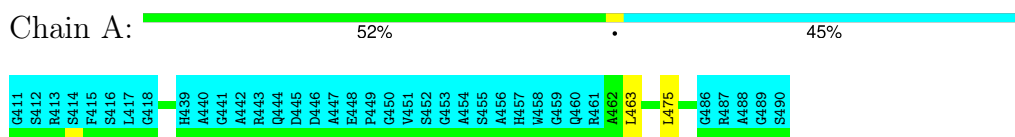
4.2.1 Score per residue for model 1

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



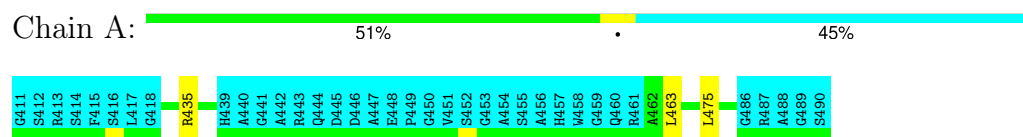
4.2.2 Score per residue for model 2

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



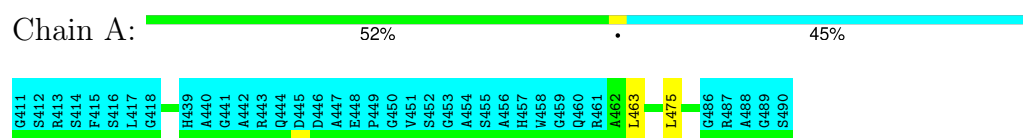
4.2.3 Score per residue for model 3

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



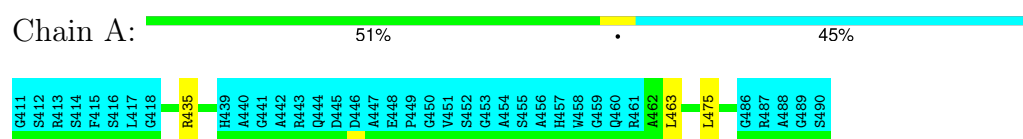
4.2.4 Score per residue for model 4

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



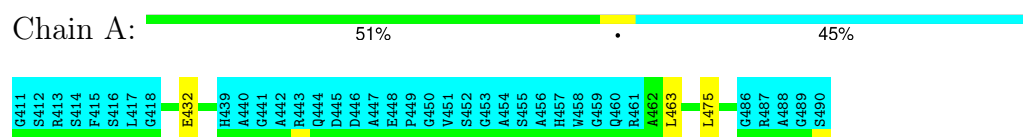
4.2.5 Score per residue for model 5

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



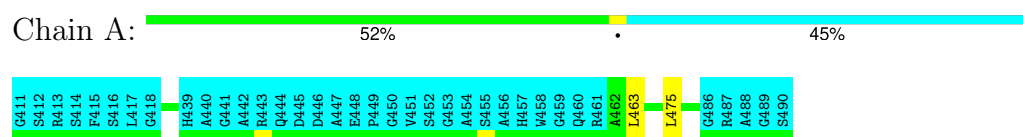
4.2.6 Score per residue for model 6

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



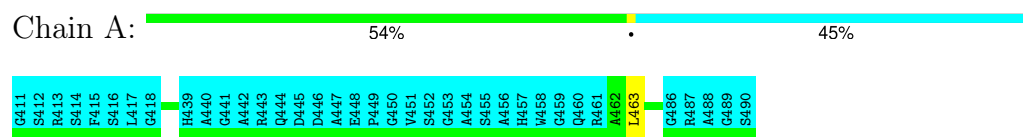
4.2.7 Score per residue for model 7

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



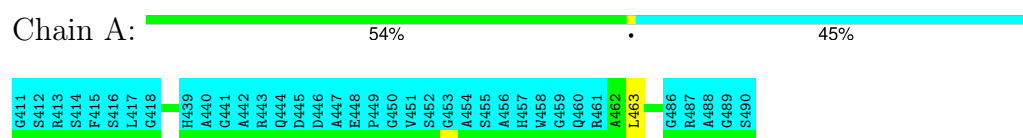
4.2.8 Score per residue for model 8

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



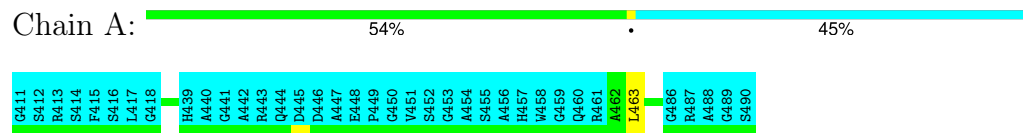
4.2.9 Score per residue for model 9

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



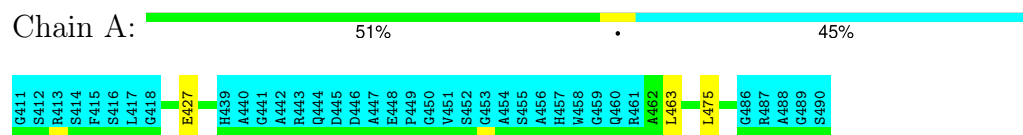
4.2.10 Score per residue for model 10

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



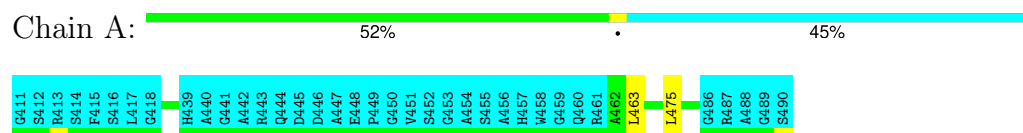
4.2.11 Score per residue for model 11

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



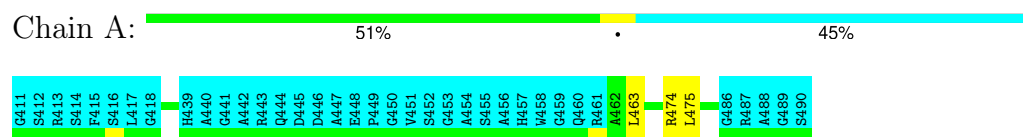
4.2.12 Score per residue for model 12

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



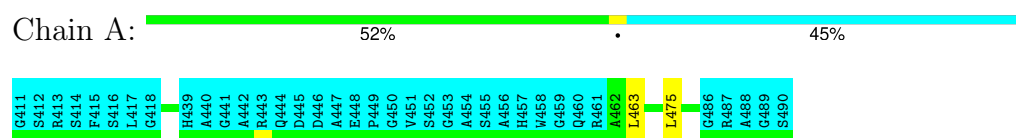
4.2.13 Score per residue for model 13

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



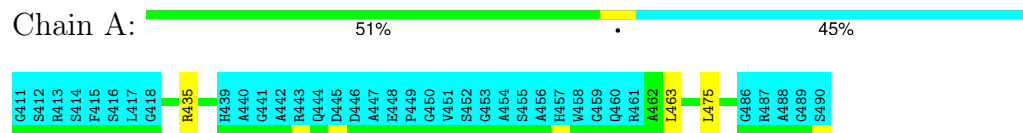
4.2.14 Score per residue for model 14

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



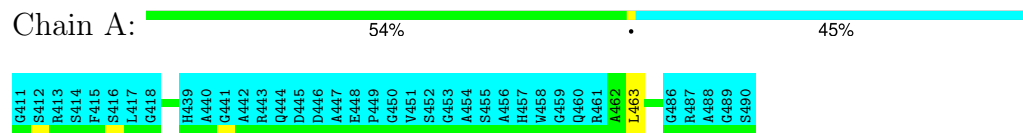
4.2.15 Score per residue for model 15

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



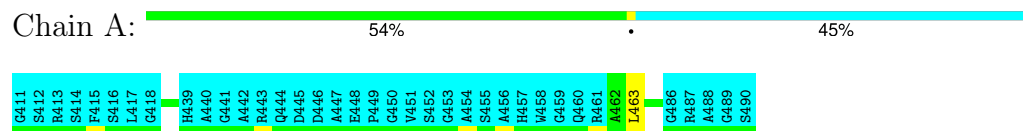
4.2.16 Score per residue for model 16

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



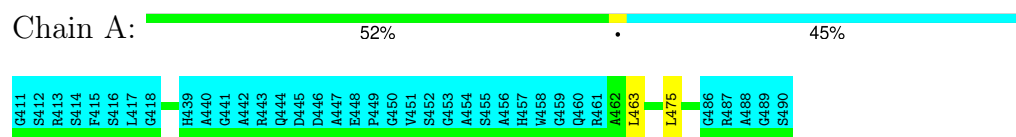
4.2.17 Score per residue for model 17

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



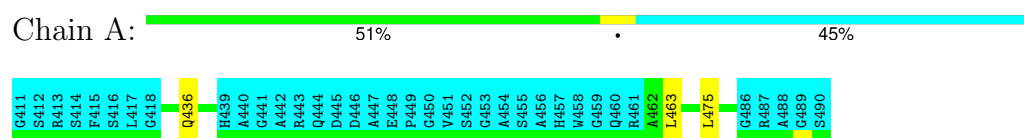
4.2.18 Score per residue for model 18

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



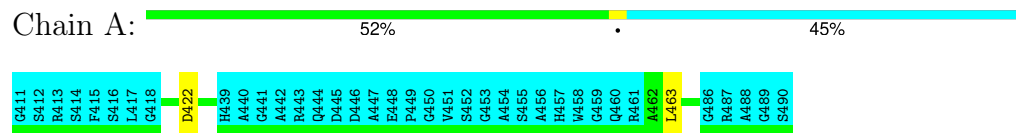
4.2.19 Score per residue for model 19

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



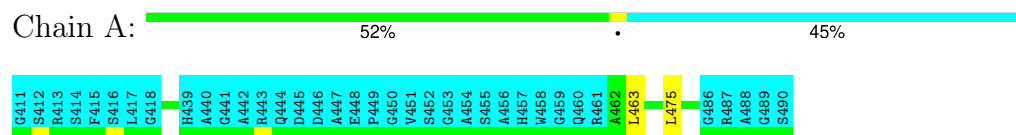
4.2.20 Score per residue for model 20

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



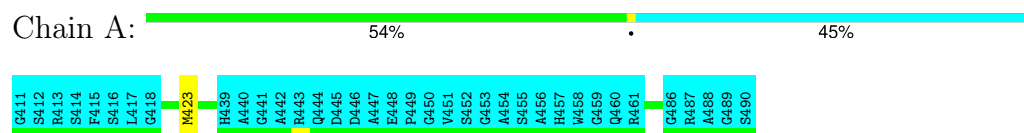
4.2.21 Score per residue for model 21

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



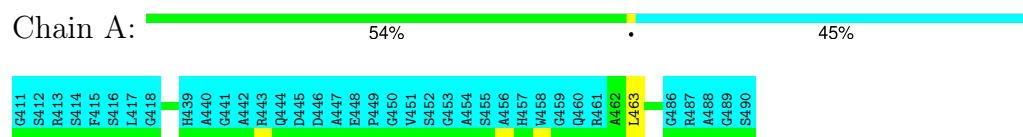
4.2.22 Score per residue for model 22

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



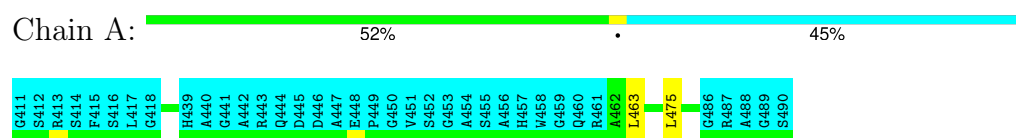
4.2.23 Score per residue for model 23

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



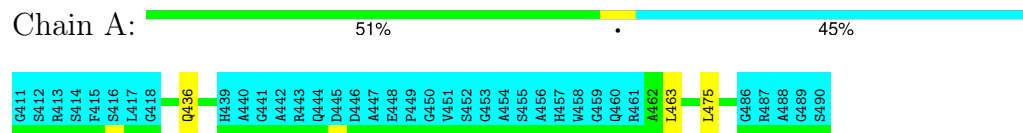
4.2.24 Score per residue for model 24

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



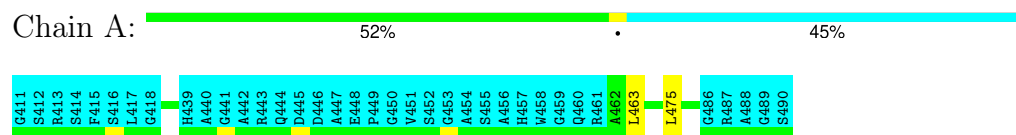
4.2.25 Score per residue for model 25

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



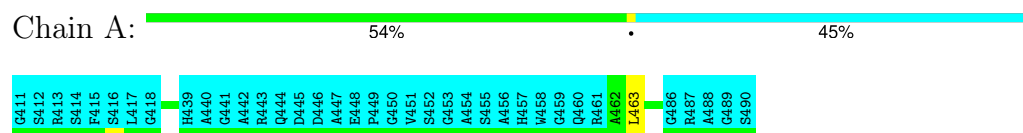
4.2.26 Score per residue for model 26

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



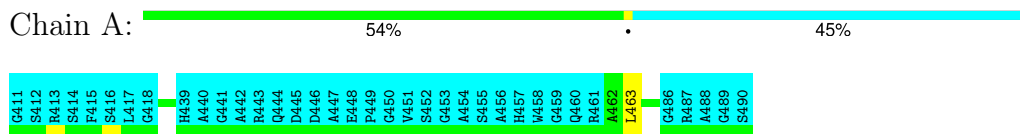
4.2.27 Score per residue for model 27

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



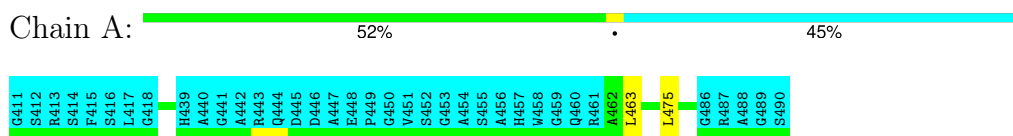
4.2.28 Score per residue for model 28

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



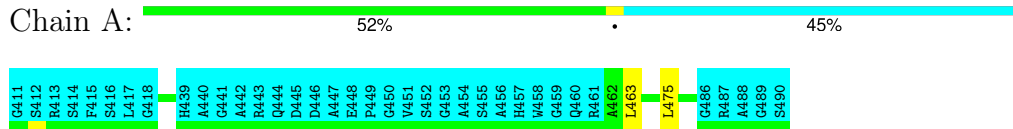
4.2.29 Score per residue for model 29

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



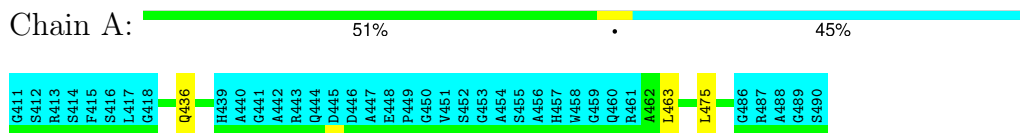
4.2.30 Score per residue for model 30

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



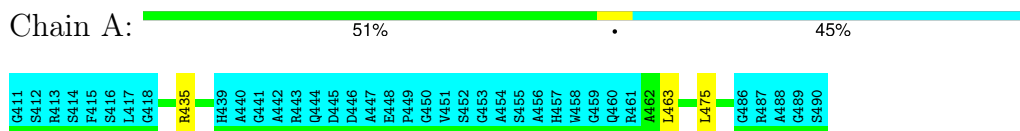
4.2.31 Score per residue for model 31

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



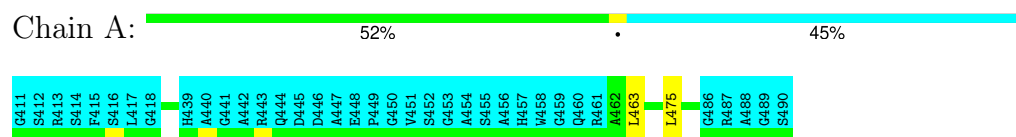
4.2.32 Score per residue for model 32

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



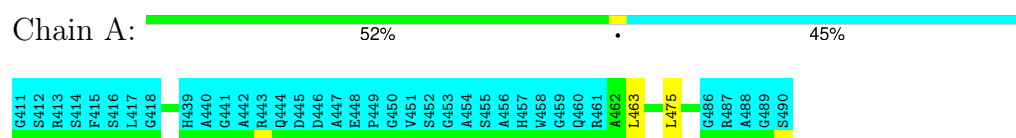
4.2.33 Score per residue for model 33

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



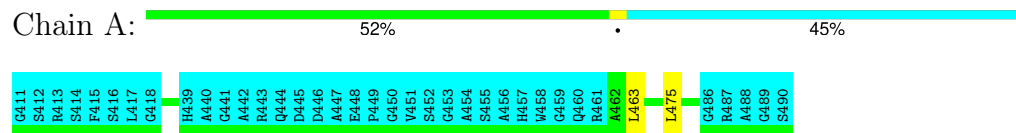
4.2.34 Score per residue for model 34

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



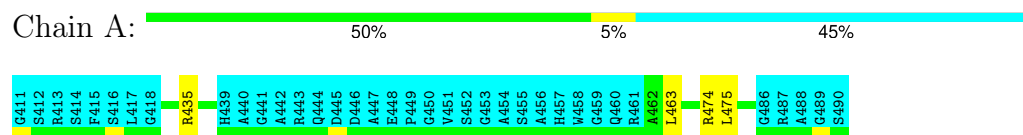
4.2.35 Score per residue for model 35

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



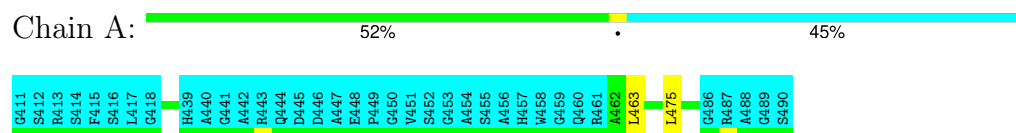
4.2.36 Score per residue for model 36

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



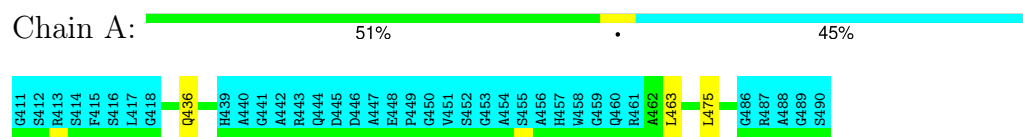
4.2.37 Score per residue for model 37

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



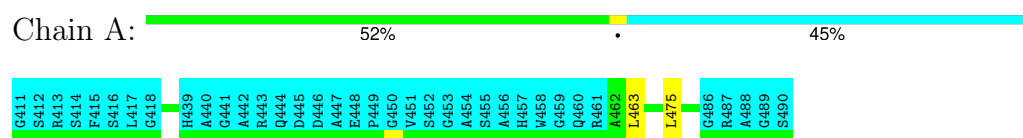
4.2.38 Score per residue for model 38

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



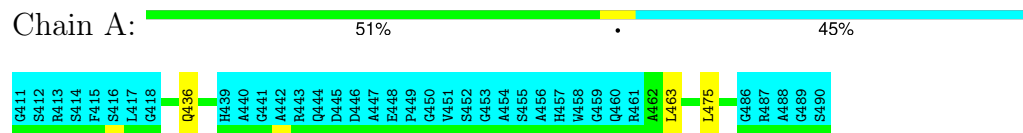
4.2.39 Score per residue for model 39

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



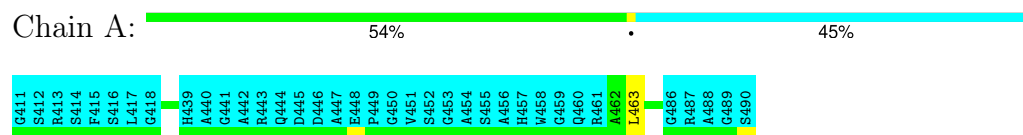
4.2.40 Score per residue for model 40

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



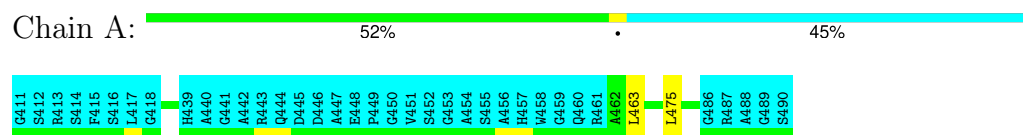
4.2.41 Score per residue for model 41

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



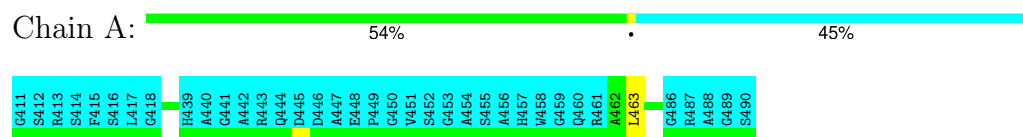
4.2.42 Score per residue for model 42

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



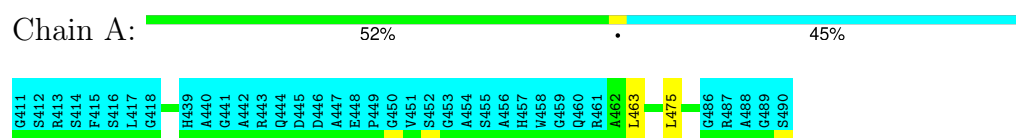
4.2.43 Score per residue for model 43

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



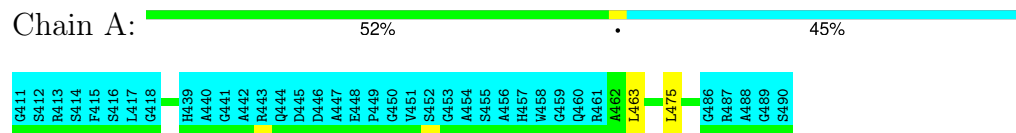
4.2.44 Score per residue for model 44 (medoid)

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



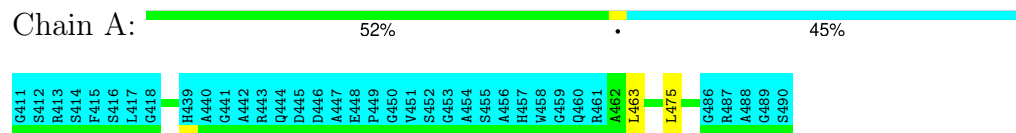
4.2.45 Score per residue for model 45

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



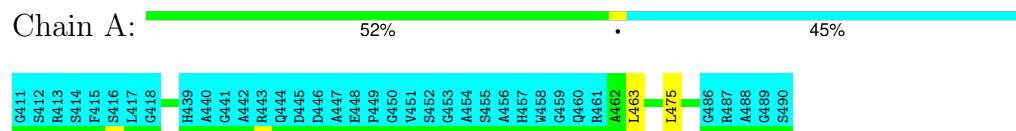
4.2.46 Score per residue for model 46

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



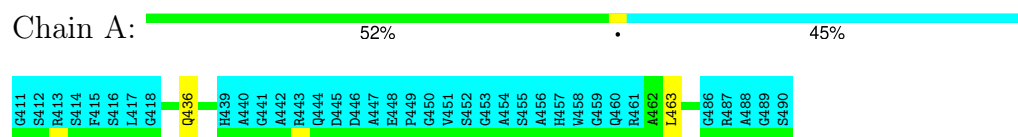
4.2.47 Score per residue for model 47

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



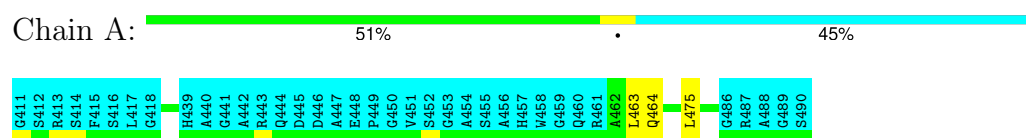
4.2.48 Score per residue for model 48

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



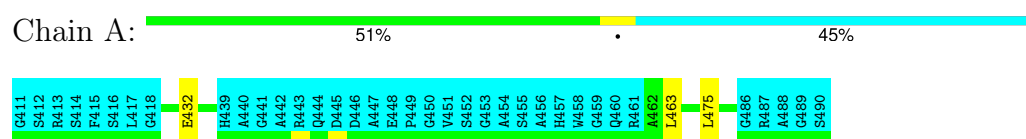
4.2.49 Score per residue for model 49

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



4.2.50 Score per residue for model 50

- Molecule 1: Bifunctional hemolysin/adenylate cyclase



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
YASARA	refinement	
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	885
Number of shifts mapped to atoms	885
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.54±0.02	0±0/325 (0.0± 0.0%)	0.66±0.02	0±0/441 (0.0± 0.1%)
All	All	0.54	0/16250 (0.0%)	0.66	5/22050 (0.0%)

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	474	ARG	NE-CZ-NH1	5.69	123.15	120.30	13	2
1	A	435	ARG	NE-CZ-NH1	5.64	123.12	120.30	32	3

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	323	330	330	0±0
All	All	16150	16500	16500	-

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is -.

There are no clashes.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	44/80 (55%)	44±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	2200/4000 (55%)	2200 (100%)	0 (0%)	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	31/53 (58%)	29±1 (94±2%)	2±1 (6±2%)	17	68
All	All	1550/2650 (58%)	1450 (94%)	100 (6%)	17	68

All 9 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	463	LEU	49
1	A	475	LEU	37
1	A	436	GLN	6
1	A	435	ARG	2
1	A	432	GLU	2
1	A	427	GLU	1
1	A	422	ASP	1
1	A	423	MET	1
1	A	464	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping

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

Total number of shifts	885
Number of shifts mapped to atoms	885
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	78	0.12 ± 0.30	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	70	-0.10 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	78	0.03 ± 0.16	None needed (< 0.5 ppm)
^{15}N	76	-0.13 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 546 atoms were assigned a chemical shift out of a possible 583. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	221/221 (100%)	89/89 (100%)	88/88 (100%)	44/44 (100%)
Sidechain	317/345 (92%)	220/230 (96%)	92/104 (88%)	5/11 (45%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	8/17 (47%)	5/9 (56%)	3/7 (43%)	0/1 (0%)
Overall	546/583 (94%)	314/328 (96%)	183/199 (92%)	49/56 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 885 atoms were assigned a chemical shift out of a possible 998. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	394/407 (97%)	162/168 (96%)	156/160 (98%)	76/79 (96%)
Sidechain	461/538 (86%)	320/354 (90%)	135/159 (85%)	6/25 (24%)
Aromatic	30/53 (57%)	17/28 (61%)	12/21 (57%)	1/4 (25%)
Overall	885/998 (89%)	499/550 (91%)	303/340 (89%)	83/108 (77%)

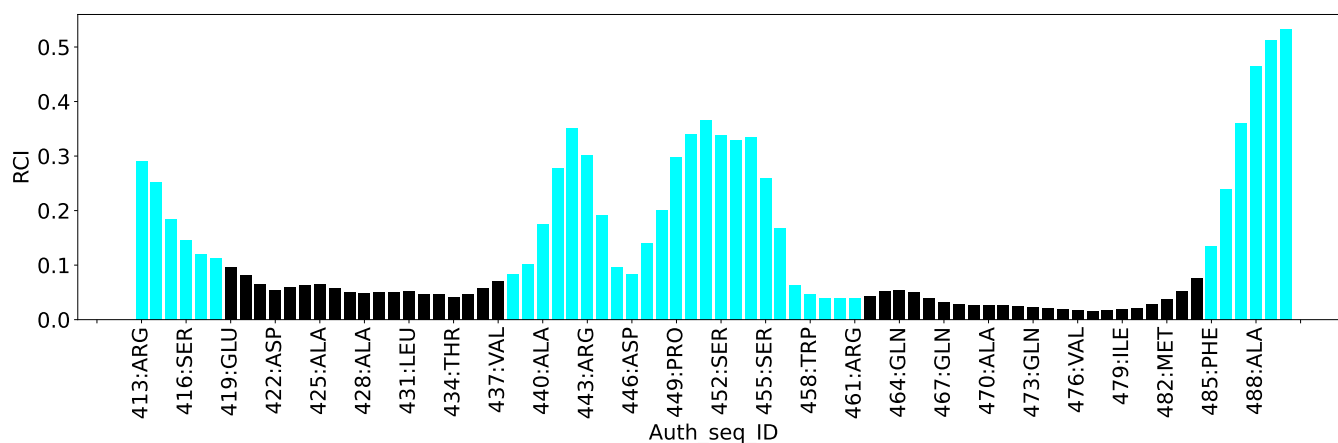
7.1.4 Statistically unusual chemical shifts [i](#)

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	1170
Intra-residue ($ i-j =0$)	315
Sequential ($ i-j =1$)	412
Medium range ($ i-j >1$ and $ i-j <5$)	434
Long range ($ i-j \geq 5$)	9
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	98
Number of unmapped restraints	0
Number of restraints per residue	15.8
Number of long range restraints per residue ¹	0.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	4.0	0.2
0.2-0.5 (Medium)	0.5	0.43
>0.5 (Large)	0.0	0.52

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)	2.7	4.99
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

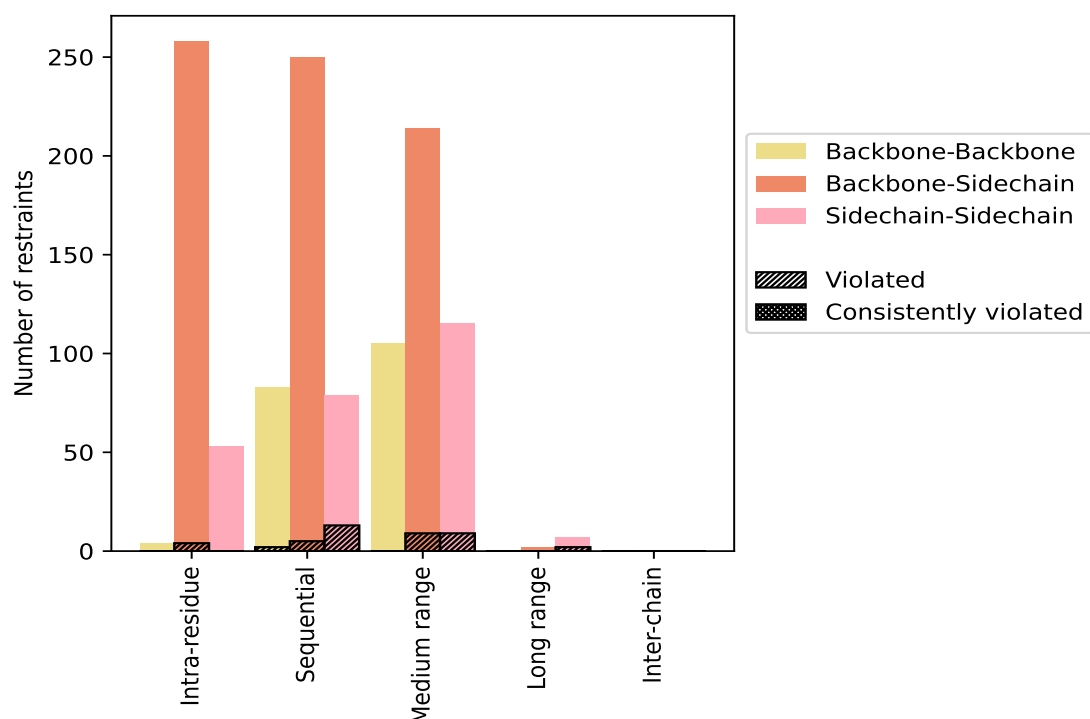
9.1 Summary of distance violations ⓘ

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)	315	26.9	4	1.3	0.3	0	0.0	0.0
Backbone-Backbone	4	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	258	22.1	4	1.6	0.3	0	0.0	0.0
Sidechain-Sidechain	53	4.5	0	0.0	0.0	0	0.0	0.0
Sequential (i-j =1)	412	35.2	20	4.9	1.7	0	0.0	0.0
Backbone-Backbone	83	7.1	2	2.4	0.2	0	0.0	0.0
Backbone-Sidechain	250	21.4	5	2.0	0.4	0	0.0	0.0
Sidechain-Sidechain	79	6.8	13	16.5	1.1	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	434	37.1	18	4.1	1.5	0	0.0	0.0
Backbone-Backbone	105	9.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	214	18.3	9	4.2	0.8	0	0.0	0.0
Sidechain-Sidechain	115	9.8	9	7.8	0.8	0	0.0	0.0
Long range (i-j ≥5)	9	0.8	2	22.2	0.2	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	0.2	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	0.6	2	28.6	0.2	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	1170	100.0	44	3.8	3.8	0	0.0	0.0
Backbone-Backbone	192	16.4	2	1.0	0.2	0	0.0	0.0
Backbone-Sidechain	724	61.9	18	2.5	1.5	0	0.0	0.0
Sidechain-Sidechain	254	21.7	24	9.4	2.1	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	1	1	0	2	0.12	0.13	0.02	0.12
2	1	3	6	0	0	10	0.15	0.23	0.05	0.12
3	0	1	3	0	0	4	0.13	0.18	0.03	0.12
4	1	3	5	1	0	10	0.14	0.19	0.02	0.12
5	0	0	1	0	0	1	0.19	0.19	0.0	0.19
6	0	0	1	0	0	1	0.12	0.12	0.0	0.12
7	0	3	6	0	0	9	0.14	0.17	0.03	0.13
8	0	1	2	0	0	3	0.12	0.14	0.02	0.11
9	1	1	4	0	0	6	0.14	0.18	0.02	0.13
10	1	1	7	0	0	9	0.15	0.23	0.04	0.15

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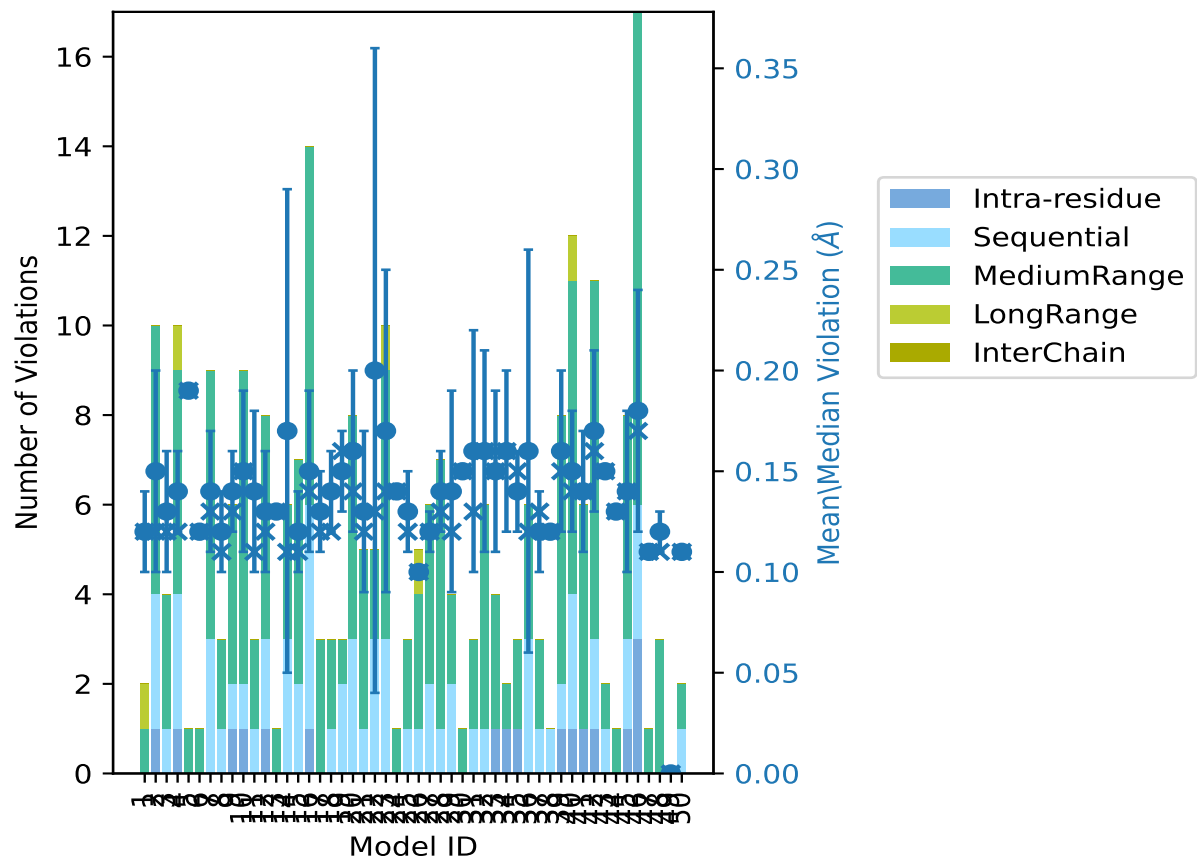
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	2	0	0	3	0.14	0.2	0.04	0.11
12	1	2	5	0	0	8	0.13	0.18	0.03	0.12
13	0	0	1	0	0	1	0.13	0.13	0.0	0.13
14	0	3	3	0	0	6	0.17	0.43	0.12	0.11
15	0	2	5	0	0	7	0.12	0.17	0.02	0.11
16	1	5	8	0	0	14	0.15	0.25	0.04	0.14
17	0	0	3	0	0	3	0.13	0.15	0.02	0.12
18	0	1	2	0	0	3	0.14	0.17	0.02	0.12
19	0	2	1	0	0	3	0.15	0.16	0.02	0.16
20	0	3	5	0	0	8	0.16	0.23	0.04	0.14
21	0	1	4	0	0	5	0.13	0.21	0.04	0.12
22	0	3	2	0	0	5	0.2	0.52	0.16	0.13
23	0	3	6	1	0	10	0.17	0.38	0.08	0.14
24	0	0	1	0	0	1	0.14	0.14	0.0	0.14
25	0	1	2	0	0	3	0.13	0.16	0.02	0.12
26	0	1	3	1	0	5	0.1	0.11	0.0	0.1
27	0	2	4	0	0	6	0.12	0.14	0.01	0.12
28	0	1	6	0	0	7	0.14	0.17	0.02	0.13
29	0	2	2	0	0	4	0.14	0.22	0.05	0.12
30	0	0	1	0	0	1	0.15	0.15	0.0	0.15
31	0	1	2	0	0	3	0.16	0.24	0.06	0.13
32	0	1	5	0	0	6	0.16	0.26	0.05	0.16
33	1	0	3	0	0	4	0.15	0.2	0.04	0.15
34	1	0	1	0	0	2	0.16	0.2	0.04	0.16
35	1	0	2	0	0	3	0.14	0.17	0.02	0.15
36	0	3	3	0	0	6	0.16	0.38	0.1	0.12
37	0	1	2	0	0	3	0.12	0.14	0.02	0.13
38	0	1	0	0	0	1	0.12	0.12	0.0	0.12
39	1	1	6	0	0	8	0.16	0.22	0.04	0.15
40	1	3	7	1	0	12	0.15	0.2	0.03	0.14
41	1	0	5	0	0	6	0.14	0.2	0.03	0.14
42	1	2	8	0	0	11	0.17	0.24	0.04	0.16
43	0	1	1	0	0	2	0.15	0.15	0.0	0.15
44	0	0	1	0	0	1	0.13	0.13	0.0	0.13
45	1	2	5	0	0	8	0.14	0.23	0.04	0.14
46	3	3	11	0	0	17	0.18	0.36	0.06	0.17
47	0	0	1	0	0	1	0.11	0.11	0.0	0.11
48	0	0	3	0	0	3	0.12	0.13	0.01	0.11
49	0	0	0	0	0	0	0.0	0.0	0.0	0.0
50	0	1	1	0	0	2	0.11	0.11	0.0	0.11

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble ⓘ

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1126(IR:311, SQ:392, MR:416, LR:7, 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	%
2	11	3	0	0	16	1	2.0
0	1	4	1	0	6	2	4.0
0	1	2	1	0	4	3	6.0
1	2	1	0	0	4	4	8.0

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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	2	1	0	0	3	5	10.0
0	1	0	0	0	1	6	12.0
0	0	1	0	0	1	7	14.0
0	0	1	0	0	1	8	16.0
0	1	0	0	0	1	9	18.0
0	0	0	0	0	0	10	20.0
1	0	0	0	0	1	11	22.0
0	0	0	0	0	0	12	24.0
0	0	0	0	0	0	13	26.0
0	0	0	0	0	0	14	28.0
0	0	0	0	0	0	15	30.0
0	0	0	0	0	0	16	32.0
0	1	0	0	0	1	17	34.0
0	0	0	0	0	0	18	36.0
0	0	1	0	0	1	19	38.0
0	0	1	0	0	1	20	40.0
0	0	0	0	0	0	21	42.0
0	0	1	0	0	1	22	44.0
0	0	0	0	0	0	23	46.0
0	0	0	0	0	0	24	48.0
0	0	1	0	0	1	25	50.0
0	0	0	0	0	0	26	52.0
0	0	0	0	0	0	27	54.0
0	0	0	0	0	0	28	56.0
0	0	0	0	0	0	29	58.0
0	0	0	0	0	0	30	60.0
0	0	0	0	0	0	31	62.0
0	0	0	0	0	0	32	64.0
0	0	0	0	0	0	33	66.0
0	0	0	0	0	0	34	68.0
0	0	0	0	0	0	35	70.0
0	0	0	0	0	0	36	72.0
0	0	0	0	0	0	37	74.0
0	0	0	0	0	0	38	76.0
0	0	0	0	0	0	39	78.0
0	0	0	0	0	0	40	80.0
0	0	0	0	0	0	41	82.0
0	0	1	0	0	1	42	84.0
0	0	0	0	0	0	43	86.0
0	0	0	0	0	0	44	88.0
0	0	0	0	0	0	45	90.0

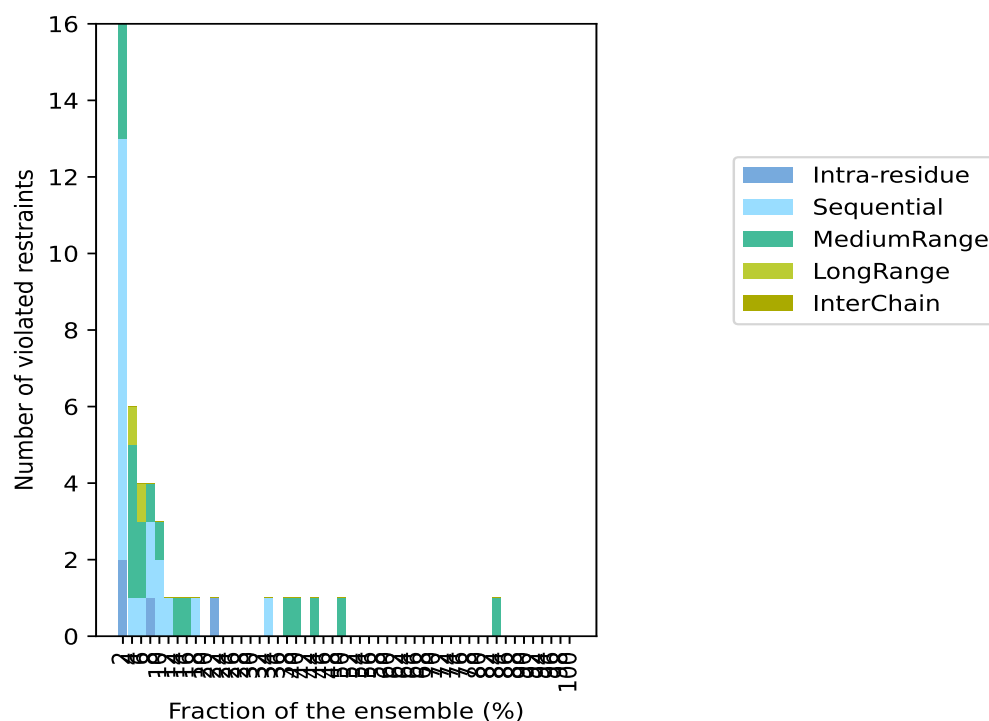
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	46	92.0
0	0	0	0	0	0	47	94.0
0	0	0	0	0	0	48	96.0
0	0	0	0	0	0	49	98.0
0	0	0	0	0	0	50	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶ Number of models with violations

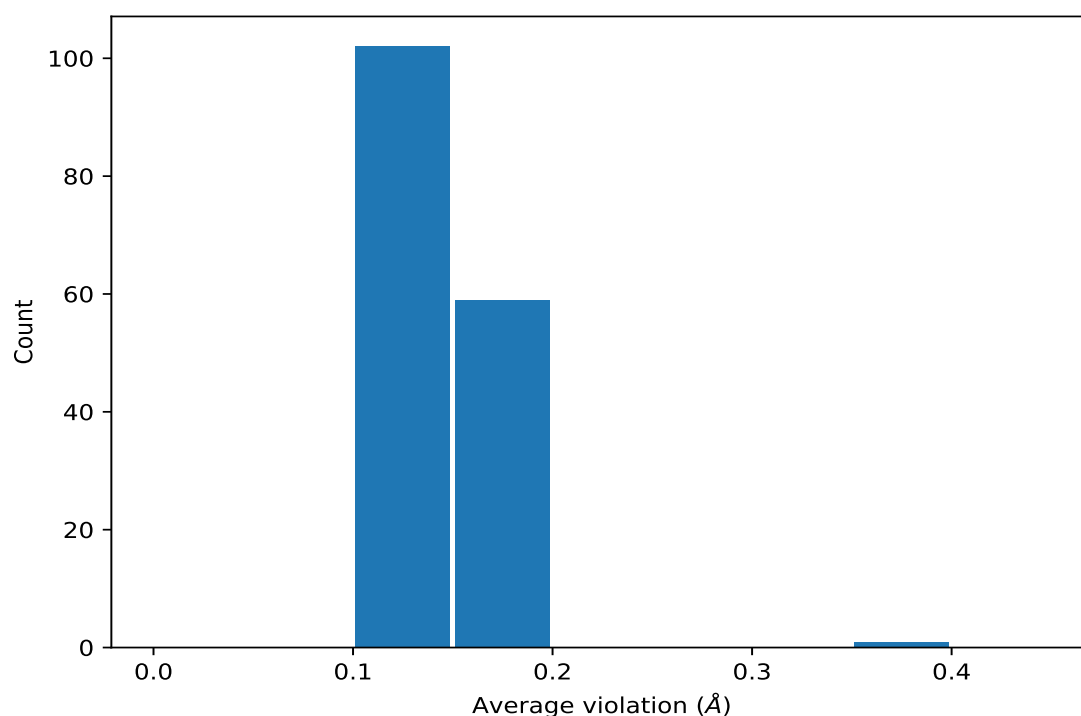
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	42	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	42	0.16	0.04	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	42	0.16	0.04	0.15
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	25	0.15	0.04	0.12
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	25	0.15	0.04	0.12
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	25	0.15	0.04	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	22	0.12	0.02	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	22	0.12	0.02	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	22	0.12	0.02	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	22	0.12	0.02	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	22	0.12	0.02	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	22	0.12	0.02	0.12
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	20	0.18	0.05	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	20	0.18	0.05	0.17
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	19	0.13	0.02	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	19	0.13	0.02	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	19	0.13	0.02	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	17	0.14	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	17	0.14	0.03	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	17	0.14	0.03	0.13
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	11	0.16	0.03	0.15
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	11	0.16	0.03	0.15
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	9	0.19	0.09	0.16
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	9	0.19	0.09	0.16
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	9	0.19	0.09	0.16
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	9	0.19	0.09	0.16
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	9	0.19	0.09	0.16
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	9	0.19	0.09	0.16
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	8	0.13	0.02	0.12
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	8	0.13	0.02	0.12
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	8	0.13	0.02	0.12
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	7	0.14	0.05	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	7	0.14	0.05	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	7	0.14	0.05	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG21	6	0.15	0.02	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG22	6	0.15	0.02	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG23	6	0.15	0.02	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG21	6	0.15	0.02	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG22	6	0.15	0.02	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG23	6	0.15	0.02	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE1	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE2	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE3	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE1	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE2	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE3	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE1	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE2	5	0.14	0.02	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE3	5	0.14	0.02	0.14
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG21	5	0.12	0.01	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG22	5	0.12	0.01	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG23	5	0.12	0.01	0.12
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG11	5	0.11	0.0	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG12	5	0.11	0.0	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG13	5	0.11	0.0	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG21	5	0.11	0.0	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG22	5	0.11	0.0	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG23	5	0.11	0.0	0.11
(1,801)	1:467:A:GLN:HG2	1:468:A:ALA:H	4	0.37	0.13	0.4
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE1	4	0.18	0.1	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE2	4	0.18	0.1	0.14
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE3	4	0.18	0.1	0.14
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE1	4	0.18	0.1	0.14
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE2	4	0.18	0.1	0.14
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE3	4	0.18	0.1	0.14
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE1	4	0.18	0.1	0.14
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE2	4	0.18	0.1	0.14
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE3	4	0.18	0.1	0.14
(1,479)	1:443:A:ARG:H	1:443:A:ARG:HB3	4	0.14	0.02	0.15
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE21	4	0.12	0.01	0.12
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE22	4	0.12	0.01	0.12
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE21	4	0.12	0.01	0.12
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE22	4	0.12	0.01	0.12
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE21	4	0.12	0.01	0.12
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE22	4	0.12	0.01	0.12
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD11	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD12	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD13	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD21	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD22	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD23	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD11	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD12	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD13	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD21	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD22	3	0.17	0.04	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD23	3	0.17	0.04	0.15
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG11	3	0.13	0.03	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG12	3	0.13	0.03	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG13	3	0.13	0.03	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG21	3	0.13	0.03	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG22	3	0.13	0.03	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG23	3	0.13	0.03	0.12
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE1	3	0.12	0.03	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE2	3	0.12	0.03	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE3	3	0.12	0.03	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE1	3	0.12	0.03	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE2	3	0.12	0.03	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE3	3	0.12	0.03	0.1
(1,478)	1:442:A:ALA:HB1	1:443:A:ARG:H	3	0.12	0.01	0.12
(1,478)	1:442:A:ALA:HB2	1:443:A:ARG:H	3	0.12	0.01	0.12
(1,478)	1:442:A:ALA:HB3	1:443:A:ARG:H	3	0.12	0.01	0.12

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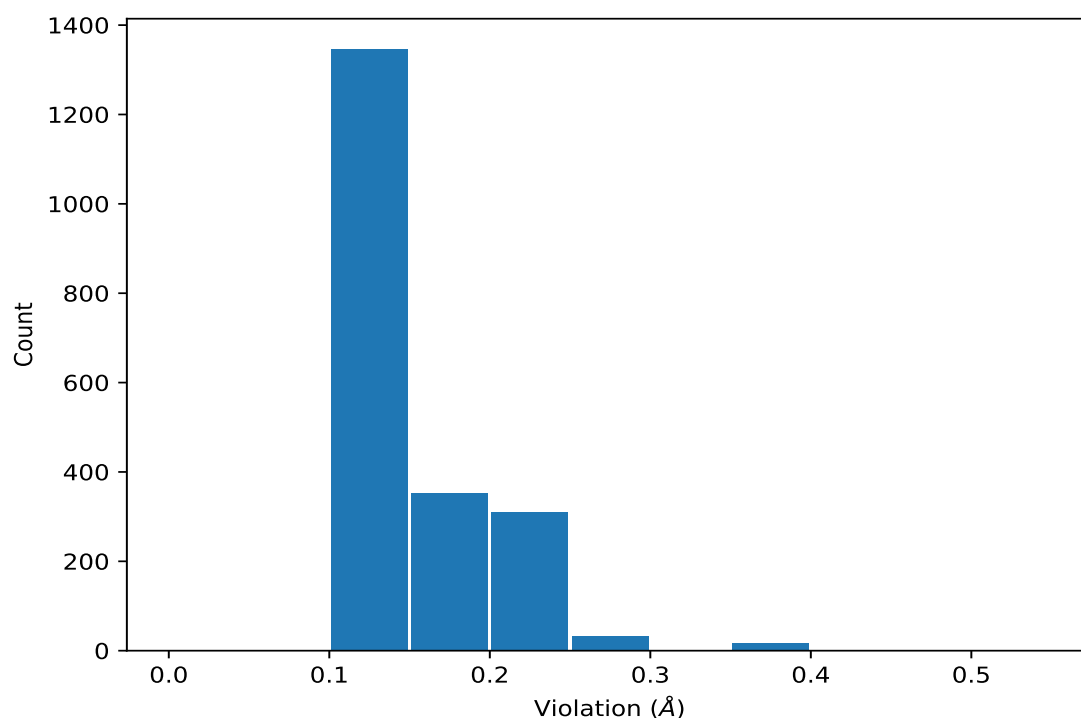
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,349)	1:414:A:SER:HB2	1:415:A:PHE:HD1	2	0.14	0.02	0.14
(1,349)	1:414:A:SER:HB2	1:415:A:PHE:HD2	2	0.14	0.02	0.14
(1,349)	1:414:A:SER:HB3	1:415:A:PHE:HD1	2	0.14	0.02	0.14
(1,349)	1:414:A:SER:HB3	1:415:A:PHE:HD2	2	0.14	0.02	0.14
(1,238)	1:456:A:ALA:HB1	1:460:A:GLN:HB3	2	0.12	0.01	0.12
(1,238)	1:456:A:ALA:HB2	1:460:A:GLN:HB3	2	0.12	0.01	0.12
(1,238)	1:456:A:ALA:HB3	1:460:A:GLN:HB3	2	0.12	0.01	0.12
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE1	2	0.12	0.02	0.12
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE2	2	0.12	0.02	0.12
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE3	2	0.12	0.02	0.12
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE1	2	0.12	0.02	0.12
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE2	2	0.12	0.02	0.12
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE3	2	0.12	0.02	0.12
(1,555)	1:469:A:VAL:HG21	1:473:A:GLN:HE22	2	0.11	0.0	0.11
(1,555)	1:469:A:VAL:HG22	1:473:A:GLN:HE22	2	0.11	0.0	0.11
(1,555)	1:469:A:VAL:HG23	1:473:A:GLN:HE22	2	0.11	0.0	0.11
(1,867)	1:481:A:LEU:HG	1:483:A:THR:H	2	0.11	0.0	0.11
(1,844)	1:475:A:LEU:HD11	1:478:A:ALA:H	2	0.1	0.0	0.1
(1,844)	1:475:A:LEU:HD12	1:478:A:ALA:H	2	0.1	0.0	0.1
(1,844)	1:475:A:LEU:HD13	1:478:A:ALA:H	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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)
(1,801)	1:467:A:GLN:HG2	1:468:A:ALA:H	22	0.52
(1,801)	1:467:A:GLN:HG2	1:468:A:ALA:H	14	0.43
(1,801)	1:467:A:GLN:HG2	1:468:A:ALA:H	36	0.38
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	23	0.38
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	23	0.38
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	23	0.38
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	23	0.38
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	23	0.38
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	23	0.38
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE1	46	0.36
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE2	46	0.36
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE3	46	0.36
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE1	46	0.36
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE2	46	0.36
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE3	46	0.36
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE1	46	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE2	46	0.36
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE3	46	0.36
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	46	0.29
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	46	0.29
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	46	0.29
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	46	0.29
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	46	0.29
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	46	0.29
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	46	0.29
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	46	0.29
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	46	0.29
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	46	0.29
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	46	0.29
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	46	0.29
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	46	0.26
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	46	0.26
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	46	0.26
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	32	0.26
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	32	0.26
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	32	0.26
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	32	0.26
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	32	0.26
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	32	0.26
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	16	0.25
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	16	0.25
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	16	0.25
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	16	0.25
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	16	0.25
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	16	0.25
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	16	0.25
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	16	0.25
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	16	0.25
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	16	0.25
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	16	0.25
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	16	0.25
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	42	0.24
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	42	0.24
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	42	0.24
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	42	0.24
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	42	0.24
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	42	0.24
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	42	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	42	0.24
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	42	0.24
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	42	0.24
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	42	0.24
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	42	0.24
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	42	0.24
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	42	0.24
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	42	0.24
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	42	0.24
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	42	0.24
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	42	0.24
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	23	0.24
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	23	0.24
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	23	0.24
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	23	0.24
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	23	0.24
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	23	0.24
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	23	0.24
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	23	0.24
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	23	0.24
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	23	0.24
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	23	0.24
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	23	0.24
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	31	0.24
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	31	0.24
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	31	0.24
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	31	0.24
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	31	0.24
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	31	0.24
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD11	45	0.23
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD12	45	0.23
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD13	45	0.23
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD21	45	0.23
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD22	45	0.23
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD23	45	0.23
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD11	45	0.23
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD12	45	0.23
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD13	45	0.23
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD21	45	0.23
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD22	45	0.23
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD23	45	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	2	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	2	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	2	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	2	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	2	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	2	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	2	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	2	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	2	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	2	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	2	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	20	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	20	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	20	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	20	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	20	0.23
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	20	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	20	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	20	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	20	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	20	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	20	0.23
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	20	0.23
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	10	0.23
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	10	0.23
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	10	0.23
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	2	0.22
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	2	0.22
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	16	0.22
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	16	0.22
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	16	0.22
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	16	0.22
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	16	0.22
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	16	0.22
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	16	0.22
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	16	0.22
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	16	0.22
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	16	0.22
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	16	0.22
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	16	0.22
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	16	0.22
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	16	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	16	0.22
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	16	0.22
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	16	0.22
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	16	0.22
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	29	0.22
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	29	0.22
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	29	0.22
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	29	0.22
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	29	0.22
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	29	0.22
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	29	0.22
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	29	0.22
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	29	0.22
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	29	0.22
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	29	0.22
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	29	0.22
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	29	0.22
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	29	0.22
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	29	0.22
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	29	0.22
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	29	0.22
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	29	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	39	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	39	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	39	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	39	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	39	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	39	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	39	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	39	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	39	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	39	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	39	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	39	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	42	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	42	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	42	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	42	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	42	0.22
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	42	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	42	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	42	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	42	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	42	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	42	0.22
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	42	0.22
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	16	0.22
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	16	0.22
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	16	0.22
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	20	0.22
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	20	0.22
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	20	0.22
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	21	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	21	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	21	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	21	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	21	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	21	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	21	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	21	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	21	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	21	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	21	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	21	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	21	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	21	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	21	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	21	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	21	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	21	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	39	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	39	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	39	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	39	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	39	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	39	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	39	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	39	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	39	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	39	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	39	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	39	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	39	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	39	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	39	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	39	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	39	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	39	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	46	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	46	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	46	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	46	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	46	0.21
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	46	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	46	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	46	0.21
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	46	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	46	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	46	0.21
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	46	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	46	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	46	0.21
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	46	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	46	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	46	0.21
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	46	0.21
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	2	0.21
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	2	0.21
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	2	0.21
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	2	0.21
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	2	0.21
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	2	0.21
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	2	0.21
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	2	0.21
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	2	0.21
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	2	0.21
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	2	0.21
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	2	0.21
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	2	0.21
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	2	0.21
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	2	0.21
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	2	0.21
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	2	0.21
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	2	0.21
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	23	0.21
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	23	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	23	0.21
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	11	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	11	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	11	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	11	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	11	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	11	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	11	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	11	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	11	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	11	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	11	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	11	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	11	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	11	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	11	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	11	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	11	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	11	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	34	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	34	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	34	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	34	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	34	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	34	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	34	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	34	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	34	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	34	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	34	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	34	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	34	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	34	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	34	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	34	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	34	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	34	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	40	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	40	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	40	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	40	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	40	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	40	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	40	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	40	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	40	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	40	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	40	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	40	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	40	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	40	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	40	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	40	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	40	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	40	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	41	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	41	0.2
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	41	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	41	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	41	0.2
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	41	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	41	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	41	0.2
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	41	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	41	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	41	0.2
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	41	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	41	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	41	0.2
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	41	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	41	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	41	0.2
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	41	0.2
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	33	0.2
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	33	0.2
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	33	0.2
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	33	0.2
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	33	0.2
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	33	0.2
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	33	0.2
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	33	0.2
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	33	0.2
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	33	0.2
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	33	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	33	0.2
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	40	0.2
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	40	0.2
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	40	0.2
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	42	0.2
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	42	0.2
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	42	0.2
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	46	0.2
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	46	0.2
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	46	0.2
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	46	0.19
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	46	0.19
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	5	0.19
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	5	0.19
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	5	0.19
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	5	0.19
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	5	0.19
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	5	0.19
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	5	0.19
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	5	0.19
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	5	0.19
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	5	0.19
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	5	0.19
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	5	0.19
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	5	0.19
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	5	0.19
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	5	0.19
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	5	0.19
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	5	0.19
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	5	0.19
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	32	0.19
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	32	0.19
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	32	0.19
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	32	0.19
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	32	0.19
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	32	0.19
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	32	0.19
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	32	0.19
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	32	0.19
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	32	0.19
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	32	0.19
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	32	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	32	0.19
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	32	0.19
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	32	0.19
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	32	0.19
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	32	0.19
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	32	0.19
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	32	0.19
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	32	0.19
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	32	0.19
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	32	0.19
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	32	0.19
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	32	0.19
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	32	0.19
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	32	0.19
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	32	0.19
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	32	0.19
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	32	0.19
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	32	0.19
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG21	4	0.19
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG22	4	0.19
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG23	4	0.19
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG21	4	0.19
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG22	4	0.19
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG23	4	0.19
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	39	0.18
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	39	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	3	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	3	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	3	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	3	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	3	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	3	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	3	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	3	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	3	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	3	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	3	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	3	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	3	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	3	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	3	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	3	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	3	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	10	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	10	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	10	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	10	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	10	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	10	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	10	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	10	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	10	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	10	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	10	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	10	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	10	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	10	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	10	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	10	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	10	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	10	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	12	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	12	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	12	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	12	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	12	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	12	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	12	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	12	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	12	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	12	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	12	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	12	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	12	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	12	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	12	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	12	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	12	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	12	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	14	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	14	0.18
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	14	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	14	0.18
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	14	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	14	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	14	0.18
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	14	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	14	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	14	0.18
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	14	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	14	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	14	0.18
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	14	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	14	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	14	0.18
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	14	0.18
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	42	0.18
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	42	0.18
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	42	0.18
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	42	0.18
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	42	0.18
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	42	0.18
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	42	0.18
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	42	0.18
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	42	0.18
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	42	0.18
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	42	0.18
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	42	0.18
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	42	0.18
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	42	0.18
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	42	0.18
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	42	0.18
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	42	0.18
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	42	0.18
(1,502)	1:450:A:GLY:HA2	1:451:A:VAL:H	46	0.18
(1,502)	1:450:A:GLY:HA3	1:451:A:VAL:H	46	0.18
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	9	0.18
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	9	0.18
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	9	0.18
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE1	10	0.18
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE2	10	0.18
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE3	10	0.18
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE1	10	0.18
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE2	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE3	10	0.18
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE1	10	0.18
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE2	10	0.18
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE3	10	0.18
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	35	0.17
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	35	0.17
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	18	0.17
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	18	0.17
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	18	0.17
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	18	0.17
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	18	0.17
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	18	0.17
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	18	0.17
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	18	0.17
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	18	0.17
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	18	0.17
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	18	0.17
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	18	0.17
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	18	0.17
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	18	0.17
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	18	0.17
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	18	0.17
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	18	0.17
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	18	0.17
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	33	0.17
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	33	0.17
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	33	0.17
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	33	0.17
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	33	0.17
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	33	0.17
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	33	0.17
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	33	0.17
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	33	0.17
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	33	0.17
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	33	0.17
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	33	0.17
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	33	0.17
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	33	0.17
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	33	0.17
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	33	0.17
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	33	0.17
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	33	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	7	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	7	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	7	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	7	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	7	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	7	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	7	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	7	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	7	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	7	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	7	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	7	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	15	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	15	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	15	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	15	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	15	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	15	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	15	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	15	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	15	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	15	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	15	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	15	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	28	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	28	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	28	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	28	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	28	0.17
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	28	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	28	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	28	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	28	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	28	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	28	0.17
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	28	0.17
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG11	46	0.17
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG12	46	0.17
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG13	46	0.17
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG21	46	0.17
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG22	46	0.17
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG23	46	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	46	0.17
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	46	0.17
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	46	0.17
(1,554)	1:472:A:ALA:HB1	1:473:A:GLN:HE22	20	0.17
(1,554)	1:472:A:ALA:HB2	1:473:A:GLN:HE22	20	0.17
(1,554)	1:472:A:ALA:HB3	1:473:A:GLN:HE22	20	0.17
(1,522)	1:456:A:ALA:HB1	1:460:A:GLN:HE22	41	0.17
(1,522)	1:456:A:ALA:HB2	1:460:A:GLN:HE22	41	0.17
(1,522)	1:456:A:ALA:HB3	1:460:A:GLN:HE22	41	0.17
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG21	40	0.17
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG22	40	0.17
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG23	40	0.17
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG21	40	0.17
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG22	40	0.17
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG23	40	0.17
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	7	0.17
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	7	0.17
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	7	0.17
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	7	0.17
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	7	0.17
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	7	0.17
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	46	0.17
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	46	0.17
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	46	0.17
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	28	0.17
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	28	0.17
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	28	0.17
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	12	0.16
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	12	0.16
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	7	0.16
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	7	0.16
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	7	0.16
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	7	0.16
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	7	0.16
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	7	0.16
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	7	0.16
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	7	0.16
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	7	0.16
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	7	0.16
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	7	0.16
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	7	0.16
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	7	0.16
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	7	0.16
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	7	0.16
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	7	0.16
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	7	0.16
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	19	0.16
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	19	0.16
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	19	0.16
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	19	0.16
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	19	0.16
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	19	0.16
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	19	0.16
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	19	0.16
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	19	0.16
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	19	0.16
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	19	0.16
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	19	0.16
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	19	0.16
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	19	0.16
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	19	0.16
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	19	0.16
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	19	0.16
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	19	0.16
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	39	0.16
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	39	0.16
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	39	0.16
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	39	0.16
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	39	0.16
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	39	0.16
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	39	0.16
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	39	0.16
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	39	0.16
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	39	0.16
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	39	0.16
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	39	0.16
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	39	0.16
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	39	0.16
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	39	0.16
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	39	0.16
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	39	0.16
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	39	0.16
(1,801)	1:467:A:GLN:HG2	1:468:A:ALA:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	1:446:A:ASP:HA	1:447:A:ALA:H	25	0.16
(1,479)	1:443:A:ARG:H	1:443:A:ARG:HB3	10	0.16
(1,479)	1:443:A:ARG:H	1:443:A:ARG:HB3	42	0.16
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	19	0.16
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	19	0.16
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	19	0.16
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	19	0.16
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	19	0.16
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	19	0.16
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE1	4	0.16
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE2	4	0.16
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE3	4	0.16
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE1	4	0.16
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE2	4	0.16
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE3	4	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	16	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	16	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	16	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	40	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	40	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	40	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	42	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	42	0.16
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	42	0.16
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	2	0.16
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	2	0.16
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	2	0.16
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	4	0.15
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	4	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	17	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	17	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	17	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	17	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	17	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	17	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	17	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	17	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	17	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	17	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	17	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	17	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	17	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	17	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	17	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	17	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	17	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	30	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	30	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	30	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	30	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	30	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	30	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	30	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	30	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	30	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	30	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	30	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	30	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	30	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	30	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	30	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	30	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	30	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	30	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	35	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	35	0.15
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	35	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	35	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	35	0.15
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	35	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	35	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	35	0.15
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	35	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	35	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	35	0.15
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	35	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	35	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	35	0.15
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	35	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	35	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	35	0.15
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	35	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	16	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	16	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	16	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	16	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	16	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	46	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	46	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	46	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	46	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	46	0.15
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	46	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD11	43	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD12	43	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD13	43	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD21	43	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD22	43	0.15
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD23	43	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD11	43	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD12	43	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD13	43	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD21	43	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD22	43	0.15
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD23	43	0.15
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	41	0.15
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	41	0.15
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	41	0.15
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	41	0.15
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	41	0.15
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	41	0.15
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	41	0.15
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	41	0.15
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	41	0.15
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	41	0.15
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	41	0.15
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	41	0.15
(1,979)	1:426:A:VAL:HG11	1:430:A:GLU:HB2	46	0.15
(1,979)	1:426:A:VAL:HG11	1:430:A:GLU:HB3	46	0.15
(1,979)	1:426:A:VAL:HG12	1:430:A:GLU:HB2	46	0.15
(1,979)	1:426:A:VAL:HG12	1:430:A:GLU:HB3	46	0.15
(1,979)	1:426:A:VAL:HG13	1:430:A:GLU:HB2	46	0.15
(1,979)	1:426:A:VAL:HG13	1:430:A:GLU:HB3	46	0.15
(1,979)	1:426:A:VAL:HG21	1:430:A:GLU:HB2	46	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:426:A:VAL:HG21	1:430:A:GLU:HB3	46	0.15
(1,979)	1:426:A:VAL:HG22	1:430:A:GLU:HB2	46	0.15
(1,979)	1:426:A:VAL:HG22	1:430:A:GLU:HB3	46	0.15
(1,979)	1:426:A:VAL:HG23	1:430:A:GLU:HB2	46	0.15
(1,979)	1:426:A:VAL:HG23	1:430:A:GLU:HB3	46	0.15
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	28	0.15
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	28	0.15
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	28	0.15
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	28	0.15
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	28	0.15
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	28	0.15
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	28	0.15
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	28	0.15
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	28	0.15
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	28	0.15
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	28	0.15
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	28	0.15
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	28	0.15
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	28	0.15
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	28	0.15
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	28	0.15
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	28	0.15
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	28	0.15
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	42	0.15
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	42	0.15
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	42	0.15
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	23	0.15
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	23	0.15
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	23	0.15
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE1	40	0.15
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE2	40	0.15
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE3	40	0.15
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE1	40	0.15
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE2	40	0.15
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE3	40	0.15
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE1	40	0.15
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE2	40	0.15
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE3	40	0.15
(1,349)	1:414:A:SER:HB2	1:415:A:PHE:HD1	16	0.15
(1,349)	1:414:A:SER:HB2	1:415:A:PHE:HD2	16	0.15
(1,349)	1:414:A:SER:HB3	1:415:A:PHE:HD1	16	0.15
(1,349)	1:414:A:SER:HB3	1:415:A:PHE:HD2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	10	0.15
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	10	0.15
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	10	0.15
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	40	0.14
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	40	0.14
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	45	0.14
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	45	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	4	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	4	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	4	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	4	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	4	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	4	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	4	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	4	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	4	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	4	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	4	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	4	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	4	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	4	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	4	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	4	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	4	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	4	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	8	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	8	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	8	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	8	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	8	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	8	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	8	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	8	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	8	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	8	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	8	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	8	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	8	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	8	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	8	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	8	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	8	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	22	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	22	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	22	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	22	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	22	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	22	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	22	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	22	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	22	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	22	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	22	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	22	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	22	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	22	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	22	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	22	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	22	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	22	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	24	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	24	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	24	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	24	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	24	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	24	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	24	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	24	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	24	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	24	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	24	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	24	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	24	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	24	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	24	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	24	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	24	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	24	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	45	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	45	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	45	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	45	0.14
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	45	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	45	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	45	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	45	0.14
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	45	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	45	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	45	0.14
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	45	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	45	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	45	0.14
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	45	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	45	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	45	0.14
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	45	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	10	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	10	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	10	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	10	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	10	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	10	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	40	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	40	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	40	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	40	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	40	0.14
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	40	0.14
(1,1027)	1:437:A:VAL:HB	1:438:A:LEU:HD11	16	0.14
(1,1027)	1:437:A:VAL:HB	1:438:A:LEU:HD12	16	0.14
(1,1027)	1:437:A:VAL:HB	1:438:A:LEU:HD13	16	0.14
(1,1027)	1:437:A:VAL:HB	1:438:A:LEU:HD21	16	0.14
(1,1027)	1:437:A:VAL:HB	1:438:A:LEU:HD22	16	0.14
(1,1027)	1:437:A:VAL:HB	1:438:A:LEU:HD23	16	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	21	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	21	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	21	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	21	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	21	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	21	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	21	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	21	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	21	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	21	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	21	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	21	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	21	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	21	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	21	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	21	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	21	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	21	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	27	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	27	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	27	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	27	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	27	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	27	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	27	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	27	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	27	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	27	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	27	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	27	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	27	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	27	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	27	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	27	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	27	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	27	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	36	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	36	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	36	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	36	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	36	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	36	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	36	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	36	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	36	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	36	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	36	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	36	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	36	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	36	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	36	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	36	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	36	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	36	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	37	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	37	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	37	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	37	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	37	0.14
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	37	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	37	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	37	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	37	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	37	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	37	0.14
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	37	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	37	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	37	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	37	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	37	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	37	0.14
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	37	0.14
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	40	0.14
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	40	0.14
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	40	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	9	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	9	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	9	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	42	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	42	0.14
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	42	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG21	12	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG22	12	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG23	12	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG21	12	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG22	12	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG23	12	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG21	43	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG22	43	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG23	43	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG21	43	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG22	43	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG23	43	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG21	45	0.14
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG22	45	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG23	45	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG21	45	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG22	45	0.14
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG23	45	0.14
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE1	23	0.14
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE2	23	0.14
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE3	23	0.14
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE1	23	0.14
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE2	23	0.14
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE3	23	0.14
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	2	0.14
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	2	0.14
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	2	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE1	16	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE2	16	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE3	16	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE1	16	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE2	16	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE3	16	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE1	16	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE2	16	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE3	16	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE1	42	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE2	42	0.14
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE3	42	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE1	42	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE2	42	0.14
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE3	42	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE1	42	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE2	42	0.14
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE3	42	0.14
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG21	20	0.14
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG22	20	0.14
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG23	20	0.14
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	1	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	1	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	1	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	1	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	1	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	1	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	1	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	1	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	1	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	1	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	1	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	1	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	1	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	1	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	1	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	1	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	1	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	13	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	13	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	13	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	13	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	13	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	13	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	13	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	13	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	13	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	13	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	13	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	13	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	13	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	13	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	13	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	13	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	13	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	13	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	23	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	23	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	23	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	23	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	23	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	23	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	23	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	23	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	23	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	23	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	23	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	23	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	23	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	23	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	23	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	23	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	23	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	31	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	31	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	31	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	31	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	31	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	31	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	31	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	31	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	31	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	31	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	31	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	31	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	31	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	31	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	31	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	31	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	31	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	31	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	44	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	44	0.13
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	44	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	44	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	44	0.13
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	44	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	44	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	44	0.13
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	44	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	44	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	44	0.13
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	44	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	44	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	44	0.13
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	44	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	44	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	44	0.13
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	44	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	9	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	9	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	9	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	9	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	9	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	23	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	23	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	23	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	23	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	23	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	23	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	42	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	42	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	42	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	42	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	42	0.13
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	42	0.13
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE21	7	0.13
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE22	7	0.13
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE21	7	0.13
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE22	7	0.13
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE21	7	0.13
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE22	7	0.13
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD11	7	0.13
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD12	7	0.13
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD13	7	0.13
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD21	7	0.13
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD22	7	0.13
(1,1076)	1:460:A:GLN:HE21	1:463:A:LEU:HD23	7	0.13
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD11	7	0.13
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD12	7	0.13
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD13	7	0.13
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD21	7	0.13
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD22	7	0.13
(1,1076)	1:460:A:GLN:HE22	1:463:A:LEU:HD23	7	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	36	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	36	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	36	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	36	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	36	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	36	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	36	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	36	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	36	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	36	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	36	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	36	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	37	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	37	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	37	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	37	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	37	0.13
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	37	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	37	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	37	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	37	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	37	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	37	0.13
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	37	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	3	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	3	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	3	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	3	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	3	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	3	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	3	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	3	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	3	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	3	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	3	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	3	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	3	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	3	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	3	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	3	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	3	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	3	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	4	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	4	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	4	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	4	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	4	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	4	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	4	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	4	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	4	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	4	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	4	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	4	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	4	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	4	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	4	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	4	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	4	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	15	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	15	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	15	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	15	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	15	0.13
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	15	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	15	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	15	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	15	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	15	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	15	0.13
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	15	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	15	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	15	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	15	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	15	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	15	0.13
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	15	0.13
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	10	0.13
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	10	0.13
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	10	0.13
(1,501)	1:451:A:VAL:H	1:451:A:VAL:HB	46	0.13
(1,483)	1:445:A:ASP:H	1:445:A:ASP:HB3	46	0.13
(1,479)	1:443:A:ARG:H	1:443:A:ARG:HB3	16	0.13
(1,478)	1:442:A:ALA:HB1	1:443:A:ARG:H	45	0.13
(1,478)	1:442:A:ALA:HB2	1:443:A:ARG:H	45	0.13
(1,478)	1:442:A:ALA:HB3	1:443:A:ARG:H	45	0.13
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG21	29	0.13
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG22	29	0.13
(1,388)	1:433:A:MET:HB2	1:434:A:THR:HG23	29	0.13
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG21	29	0.13
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG22	29	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,388)	1:433:A:MET:HB3	1:434:A:THR:HG23	29	0.13
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	27	0.13
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	27	0.13
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	27	0.13
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	27	0.13
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	27	0.13
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	27	0.13
(1,238)	1:456:A:ALA:HB1	1:460:A:GLN:HB3	20	0.13
(1,238)	1:456:A:ALA:HB2	1:460:A:GLN:HB3	20	0.13
(1,238)	1:456:A:ALA:HB3	1:460:A:GLN:HB3	20	0.13
(1,224)	1:466:A:ALA:HB1	1:467:A:GLN:HG2	22	0.13
(1,224)	1:466:A:ALA:HB2	1:467:A:GLN:HG2	22	0.13
(1,224)	1:466:A:ALA:HB3	1:467:A:GLN:HG2	22	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	9	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	9	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	9	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	20	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	20	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	20	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	23	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	23	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	23	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	28	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	28	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	28	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	39	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	39	0.13
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	39	0.13
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	39	0.13
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	39	0.13
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	39	0.13
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	48	0.13
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	48	0.13
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	48	0.13
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE1	40	0.13
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE2	40	0.13
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE3	40	0.13
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE1	40	0.13
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE2	40	0.13
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE3	40	0.13
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE1	40	0.13
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE2	40	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE3	40	0.13
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG21	46	0.13
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG22	46	0.13
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG23	46	0.13
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	33	0.12
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	33	0.12
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	34	0.12
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	34	0.12
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB2	41	0.12
(1,1168)	1:487:A:ARG:H	1:487:A:ARG:HB3	41	0.12
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	6	0.12
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	6	0.12
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	6	0.12
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	6	0.12
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	6	0.12
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	6	0.12
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	6	0.12
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	6	0.12
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	6	0.12
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	6	0.12
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	6	0.12
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	6	0.12
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	6	0.12
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	6	0.12
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	6	0.12
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	6	0.12
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	6	0.12
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	6	0.12
(1,1143)	1:476:A:VAL:HG11	1:477:A:HIS:HD2	20	0.12
(1,1143)	1:476:A:VAL:HG12	1:477:A:HIS:HD2	20	0.12
(1,1143)	1:476:A:VAL:HG13	1:477:A:HIS:HD2	20	0.12
(1,1143)	1:476:A:VAL:HG21	1:477:A:HIS:HD2	20	0.12
(1,1143)	1:476:A:VAL:HG22	1:477:A:HIS:HD2	20	0.12
(1,1143)	1:476:A:VAL:HG23	1:477:A:HIS:HD2	20	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	21	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	21	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	21	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	21	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	21	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	21	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	27	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	27	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	27	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	27	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	27	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	27	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	32	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	32	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	32	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	32	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	32	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	32	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	41	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	41	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	41	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	41	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	41	0.12
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	41	0.12
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE21	22	0.12
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE22	22	0.12
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE21	22	0.12
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE22	22	0.12
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE21	22	0.12
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE22	22	0.12
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE21	36	0.12
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE22	36	0.12
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE21	36	0.12
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE22	36	0.12
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE21	36	0.12
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE22	36	0.12
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	18	0.12
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	18	0.12
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	18	0.12
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	18	0.12
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	18	0.12
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	18	0.12
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	18	0.12
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	18	0.12
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	18	0.12
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	18	0.12
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	18	0.12
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	18	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	18	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	18	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	18	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	18	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	18	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	18	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	18	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	18	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	18	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	18	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	18	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	18	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	18	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	18	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	18	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	18	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	18	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	19	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	19	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	19	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	19	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	19	0.12
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	19	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	19	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	19	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	19	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	19	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	19	0.12
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	19	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	19	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	19	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	19	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	19	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	19	0.12
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	19	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG11	16	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG12	16	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG13	16	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG21	16	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG22	16	0.12
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG23	16	0.12
(1,725)	1:437:A:VAL:H	1:440:A:ALA:HB1	4	0.12
(1,725)	1:437:A:VAL:H	1:440:A:ALA:HB2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,725)	1:437:A:VAL:H	1:440:A:ALA:HB3	4	0.12
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	28	0.12
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	28	0.12
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	28	0.12
(1,479)	1:443:A:ARG:H	1:443:A:ARG:HB3	9	0.12
(1,478)	1:442:A:ALA:HB1	1:443:A:ARG:H	4	0.12
(1,478)	1:442:A:ALA:HB2	1:443:A:ARG:H	4	0.12
(1,478)	1:442:A:ALA:HB3	1:443:A:ARG:H	4	0.12
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE1	16	0.12
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE2	16	0.12
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE3	16	0.12
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE1	16	0.12
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE2	16	0.12
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE3	16	0.12
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE1	16	0.12
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE2	16	0.12
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE3	16	0.12
(1,349)	1:414:A:SER:HB2	1:415:A:PHE:HD1	38	0.12
(1,349)	1:414:A:SER:HB2	1:415:A:PHE:HD2	38	0.12
(1,349)	1:414:A:SER:HB3	1:415:A:PHE:HD1	38	0.12
(1,349)	1:414:A:SER:HB3	1:415:A:PHE:HD2	38	0.12
(1,238)	1:456:A:ALA:HB1	1:460:A:GLN:HB3	40	0.12
(1,238)	1:456:A:ALA:HB2	1:460:A:GLN:HB3	40	0.12
(1,238)	1:456:A:ALA:HB3	1:460:A:GLN:HB3	40	0.12
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	4	0.12
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	4	0.12
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	4	0.12
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	4	0.12
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	4	0.12
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	4	0.12
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	12	0.12
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	12	0.12
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	12	0.12
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	17	0.12
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	17	0.12
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	17	0.12
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	25	0.12
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	25	0.12
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	25	0.12
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	27	0.12
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	27	0.12
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	27	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	32	0.12
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	32	0.12
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	32	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG21	16	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG22	16	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG23	16	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG21	40	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG22	40	0.12
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG23	40	0.12
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	26	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	26	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	26	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	26	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	26	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	26	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	26	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	26	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	26	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	26	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	26	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	26	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	26	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	26	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	26	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	26	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	26	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	26	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	28	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	28	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	28	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	28	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	28	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	28	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	28	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	28	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	28	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	28	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	28	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	28	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	28	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	28	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	28	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	28	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	28	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	28	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	47	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	47	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	47	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	47	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	47	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	47	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	47	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	47	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	47	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	47	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	47	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	47	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	47	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	47	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	47	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	47	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	47	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	47	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	48	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	48	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	48	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	48	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	48	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	48	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	48	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	48	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	48	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	48	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	48	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	48	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	48	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	48	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	48	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	48	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	48	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	48	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	50	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	50	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	50	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	50	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	50	0.11
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	50	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	50	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	50	0.11
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	50	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	50	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	50	0.11
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	50	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	50	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	50	0.11
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	50	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	50	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	50	0.11
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	50	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	8	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	8	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	8	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	8	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	8	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	8	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	12	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	12	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	12	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	12	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	12	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	12	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	17	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	17	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	17	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	17	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	17	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	17	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	35	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	35	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	35	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	35	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	35	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	35	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	39	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	39	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	39	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	39	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	39	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	39	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	45	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	45	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	45	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	45	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	45	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	45	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	48	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	48	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	48	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	48	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	48	0.11
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	48	0.11
(1,1052)	1:448:A:GLU:HB2	1:449:A:PRO:HD2	50	0.11
(1,1052)	1:448:A:GLU:HB2	1:449:A:PRO:HD3	50	0.11
(1,1052)	1:448:A:GLU:HB3	1:449:A:PRO:HD2	50	0.11
(1,1052)	1:448:A:GLU:HB3	1:449:A:PRO:HD3	50	0.11
(1,1026)	1:437:A:VAL:HA	1:438:A:LEU:HD11	15	0.11
(1,1026)	1:437:A:VAL:HA	1:438:A:LEU:HD12	15	0.11
(1,1026)	1:437:A:VAL:HA	1:438:A:LEU:HD13	15	0.11
(1,1026)	1:437:A:VAL:HA	1:438:A:LEU:HD21	15	0.11
(1,1026)	1:437:A:VAL:HA	1:438:A:LEU:HD22	15	0.11
(1,1026)	1:437:A:VAL:HA	1:438:A:LEU:HD23	15	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	3	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	3	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	3	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	3	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	3	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	3	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	3	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	3	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	3	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	3	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	3	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	3	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	11	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	11	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	11	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	11	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	11	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	11	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	11	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	11	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	11	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	11	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	11	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	14	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	14	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	14	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	14	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	14	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	14	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	14	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	14	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	14	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	14	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	14	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	14	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG11	25	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG12	25	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG13	25	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG21	25	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG22	25	0.11
(1,1008)	1:433:A:MET:HG2	1:437:A:VAL:HG23	25	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG11	25	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG12	25	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG13	25	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG21	25	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG22	25	0.11
(1,1008)	1:433:A:MET:HG3	1:437:A:VAL:HG23	25	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	11	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	11	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	11	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	11	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	11	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	11	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	11	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	11	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	11	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	11	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	11	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	11	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	11	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	11	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	11	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	11	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	11	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	26	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	26	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	26	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	26	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	26	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	26	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	26	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	26	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	26	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	26	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	26	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	26	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	26	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	26	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	26	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	26	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	26	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	26	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	29	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	29	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	29	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	29	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	29	0.11
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	29	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	29	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	29	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	29	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	29	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	29	0.11
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	29	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	29	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	29	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	29	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	29	0.11
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	29	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	29	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG11	4	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG12	4	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG13	4	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG21	4	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG22	4	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG23	4	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG11	28	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG12	28	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG13	28	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG21	28	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG22	28	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG23	28	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG11	39	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG12	39	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG13	39	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG21	39	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG22	39	0.11
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG23	39	0.11
(1,867)	1:481:A:LEU:HG	1:483:A:THR:H	16	0.11
(1,867)	1:481:A:LEU:HG	1:483:A:THR:H	46	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	2	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	2	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	2	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	15	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	15	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	15	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	20	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	20	0.11
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	20	0.11
(1,555)	1:469:A:VAL:HG21	1:473:A:GLN:HE22	2	0.11
(1,555)	1:469:A:VAL:HG22	1:473:A:GLN:HE22	2	0.11
(1,555)	1:469:A:VAL:HG23	1:473:A:GLN:HE22	2	0.11
(1,555)	1:469:A:VAL:HG21	1:473:A:GLN:HE22	10	0.11
(1,555)	1:469:A:VAL:HG22	1:473:A:GLN:HE22	10	0.11
(1,555)	1:469:A:VAL:HG23	1:473:A:GLN:HE22	10	0.11
(1,486)	1:446:A:ASP:H	1:447:A:ALA:HB1	23	0.11
(1,486)	1:446:A:ASP:H	1:447:A:ALA:HB2	23	0.11
(1,486)	1:446:A:ASP:H	1:447:A:ALA:HB3	23	0.11
(1,478)	1:442:A:ALA:HB1	1:443:A:ARG:H	9	0.11
(1,478)	1:442:A:ALA:HB2	1:443:A:ARG:H	9	0.11
(1,478)	1:442:A:ALA:HB3	1:443:A:ARG:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:426:A:VAL:HG21	1:427:A:GLU:H	2	0.11
(1,438)	1:426:A:VAL:HG22	1:427:A:GLU:H	2	0.11
(1,438)	1:426:A:VAL:HG23	1:427:A:GLU:H	2	0.11
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE1	40	0.11
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE2	40	0.11
(1,383)	1:415:A:PHE:HE1	1:423:A:MET:HE3	40	0.11
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE1	40	0.11
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE2	40	0.11
(1,383)	1:415:A:PHE:HE2	1:423:A:MET:HE3	40	0.11
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE1	12	0.11
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE2	12	0.11
(1,382)	1:420:A:VAL:HG11	1:423:A:MET:HE3	12	0.11
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE1	12	0.11
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE2	12	0.11
(1,382)	1:420:A:VAL:HG12	1:423:A:MET:HE3	12	0.11
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE1	12	0.11
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE2	12	0.11
(1,382)	1:420:A:VAL:HG13	1:423:A:MET:HE3	12	0.11
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	12	0.11
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	12	0.11
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	12	0.11
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	12	0.11
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	12	0.11
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	12	0.11
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	14	0.11
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	14	0.11
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	14	0.11
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	14	0.11
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	14	0.11
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	14	0.11
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD2	16	0.11
(1,366)	1:442:A:ALA:HB1	1:443:A:ARG:HD3	16	0.11
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD2	16	0.11
(1,366)	1:442:A:ALA:HB2	1:443:A:ARG:HD3	16	0.11
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD2	16	0.11
(1,366)	1:442:A:ALA:HB3	1:443:A:ARG:HD3	16	0.11
(1,225)	1:466:A:ALA:HB1	1:467:A:GLN:HG3	46	0.11
(1,225)	1:466:A:ALA:HB2	1:467:A:GLN:HG3	46	0.11
(1,225)	1:466:A:ALA:HB3	1:467:A:GLN:HG3	46	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	7	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	7	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	27	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	27	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	27	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	32	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	32	0.11
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	32	0.11
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	7	0.11
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	7	0.11
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	7	0.11
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	45	0.11
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	45	0.11
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	45	0.11
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE1	23	0.11
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE2	23	0.11
(1,52)	1:481:A:LEU:HD11	1:482:A:MET:HE3	23	0.11
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE1	23	0.11
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE2	23	0.11
(1,52)	1:481:A:LEU:HD12	1:482:A:MET:HE3	23	0.11
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE1	23	0.11
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE2	23	0.11
(1,52)	1:481:A:LEU:HD13	1:482:A:MET:HE3	23	0.11
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	15	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	15	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	15	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	15	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	15	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	15	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	15	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	15	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	15	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	15	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	15	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	15	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	15	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	15	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	15	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	15	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	15	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	15	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	36	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	36	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	36	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	36	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	36	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	36	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	36	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	36	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	36	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	36	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	36	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	36	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	36	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	36	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	36	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	36	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	36	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	36	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB1	37	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB2	37	0.1
(1,1148)	1:476:A:VAL:HG11	1:480:A:ALA:HB3	37	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB1	37	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB2	37	0.1
(1,1148)	1:476:A:VAL:HG12	1:480:A:ALA:HB3	37	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB1	37	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB2	37	0.1
(1,1148)	1:476:A:VAL:HG13	1:480:A:ALA:HB3	37	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB1	37	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB2	37	0.1
(1,1148)	1:476:A:VAL:HG21	1:480:A:ALA:HB3	37	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB1	37	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB2	37	0.1
(1,1148)	1:476:A:VAL:HG22	1:480:A:ALA:HB3	37	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB1	37	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB2	37	0.1
(1,1148)	1:476:A:VAL:HG23	1:480:A:ALA:HB3	37	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	3	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	3	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	3	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	3	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	3	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	3	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	7	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	7	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	7	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	7	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	7	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	7	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	29	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	29	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	29	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	29	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	29	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	29	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG11	33	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG12	33	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG13	33	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG21	33	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG22	33	0.1
(1,1125)	1:473:A:GLN:H	1:476:A:VAL:HG23	33	0.1
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE21	14	0.1
(1,1109)	1:466:A:ALA:HB1	1:467:A:GLN:HE22	14	0.1
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE21	14	0.1
(1,1109)	1:466:A:ALA:HB2	1:467:A:GLN:HE22	14	0.1
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE21	14	0.1
(1,1109)	1:466:A:ALA:HB3	1:467:A:GLN:HE22	14	0.1
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG11	8	0.1
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG12	8	0.1
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG13	8	0.1
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG21	8	0.1
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG22	8	0.1
(1,970)	1:425:A:ALA:HB1	1:426:A:VAL:HG23	8	0.1
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG11	8	0.1
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG12	8	0.1
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG13	8	0.1
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG21	8	0.1
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG22	8	0.1
(1,970)	1:425:A:ALA:HB2	1:426:A:VAL:HG23	8	0.1
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG11	8	0.1
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG12	8	0.1
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG13	8	0.1
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG21	8	0.1
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG22	8	0.1
(1,970)	1:425:A:ALA:HB3	1:426:A:VAL:HG23	8	0.1
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG11	12	0.1
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG12	12	0.1
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG13	12	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG21	12	0.1
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG22	12	0.1
(1,967)	1:424:A:ALA:H	1:426:A:VAL:HG23	12	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG11	2	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG12	2	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG13	2	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG21	2	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG22	2	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG23	2	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG11	26	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG12	26	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG13	26	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG21	26	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG22	26	0.1
(1,957)	1:422:A:ASP:HA	1:426:A:VAL:HG23	26	0.1
(1,844)	1:475:A:LEU:HD11	1:478:A:ALA:H	10	0.1
(1,844)	1:475:A:LEU:HD12	1:478:A:ALA:H	10	0.1
(1,844)	1:475:A:LEU:HD13	1:478:A:ALA:H	10	0.1
(1,844)	1:475:A:LEU:HD11	1:478:A:ALA:H	42	0.1
(1,844)	1:475:A:LEU:HD12	1:478:A:ALA:H	42	0.1
(1,844)	1:475:A:LEU:HD13	1:478:A:ALA:H	42	0.1
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG11	26	0.1
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG12	26	0.1
(1,751)	1:465:A:GLY:H	1:469:A:VAL:HG13	26	0.1
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	15	0.1
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	15	0.1
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	15	0.1
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG11	27	0.1
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG12	27	0.1
(1,710)	1:435:A:ARG:H	1:437:A:VAL:HG13	27	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE1	1	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE2	1	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE3	1	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE1	1	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE2	1	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE3	1	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE1	26	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE2	26	0.1
(1,306)	1:415:A:PHE:HD1	1:423:A:MET:HE3	26	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE1	26	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE2	26	0.1
(1,306)	1:415:A:PHE:HD2	1:423:A:MET:HE3	26	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	14	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	14	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	14	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	15	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	15	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	15	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	21	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	21	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	21	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG21	45	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG22	45	0.1
(1,201)	1:467:A:GLN:HB2	1:469:A:VAL:HG23	45	0.1
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	21	0.1
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	21	0.1
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	21	0.1
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	22	0.1
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	22	0.1
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	22	0.1
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	31	0.1
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	31	0.1
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	31	0.1
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	36	0.1
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	36	0.1
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	36	0.1
(1,108)	1:479:A:ILE:HD11	1:481:A:LEU:H	41	0.1
(1,108)	1:479:A:ILE:HD12	1:481:A:LEU:H	41	0.1
(1,108)	1:479:A:ILE:HD13	1:481:A:LEU:H	41	0.1
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG21	2	0.1
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG22	2	0.1
(1,34)	1:482:A:MET:HG2	1:483:A:THR:HG23	2	0.1

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

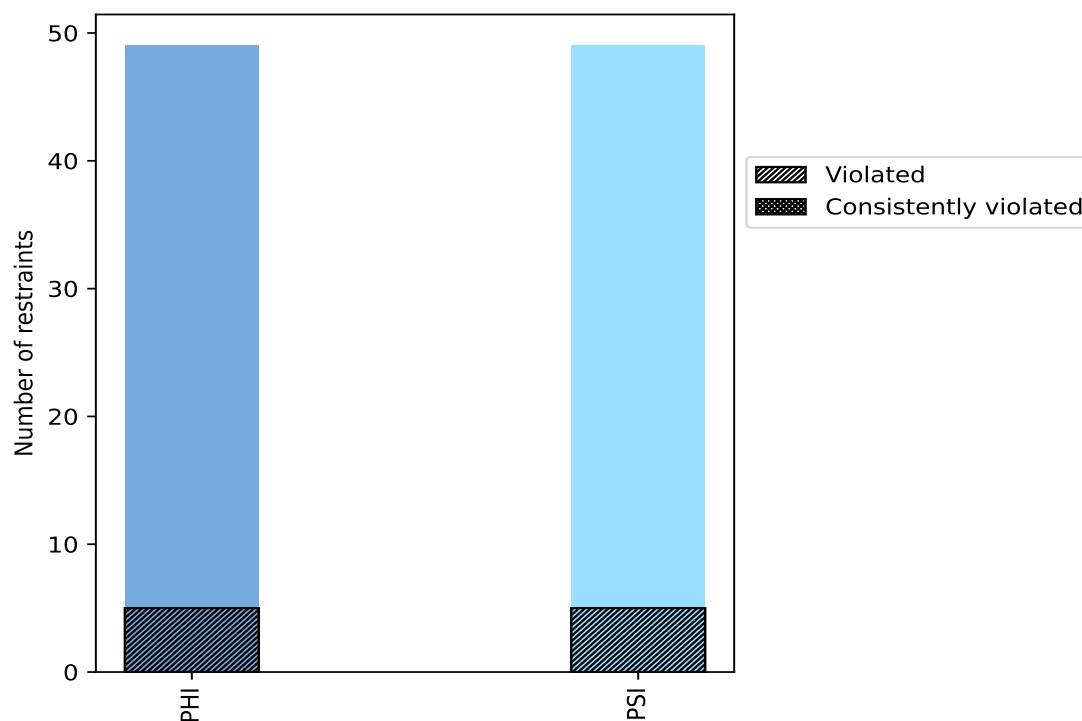
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	49	50.0	5	10.2	5.1	0	0.0	0.0
PSI	49	50.0	5	10.2	5.1	0	0.0	0.0
Total	98	100.0	10	10.2	10.2	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 [i](#)

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

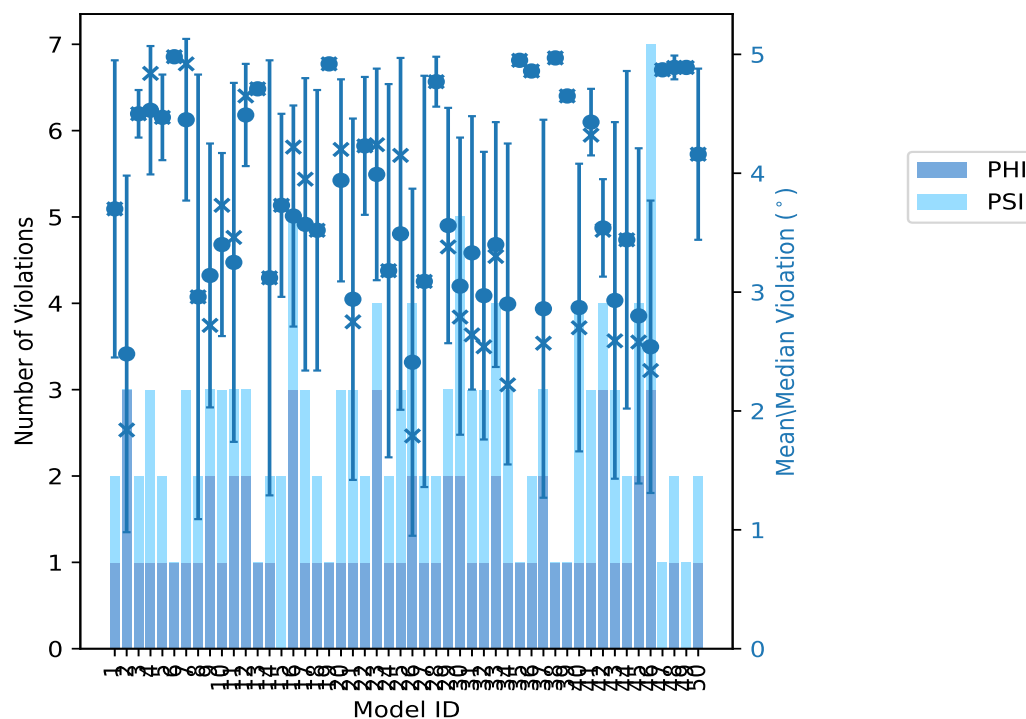
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	1	2	3.7	4.94	1.25	3.7
2	3	0	3	2.48	4.55	1.5	1.84
3	1	1	2	4.5	4.69	0.2	4.5
4	1	2	3	4.53	4.98	0.54	4.84
5	1	1	2	4.47	4.83	0.36	4.47
6	1	0	1	4.98	4.98	0.0	4.98
7	1	2	3	4.45	4.94	0.68	4.92
8	1	1	2	2.96	4.82	1.87	2.96
9	2	1	3	3.14	4.66	1.11	2.72
10	1	2	3	3.4	4.13	0.77	3.73
11	2	1	3	3.25	4.99	1.51	3.46
12	2	1	3	4.49	4.91	0.43	4.65
13	1	0	1	4.71	4.71	0.0	4.71
14	1	1	2	3.12	4.95	1.83	3.12
15	0	2	2	3.73	4.5	0.77	3.73
16	3	2	5	3.64	4.45	0.93	4.22
17	1	2	3	3.57	4.85	1.23	3.95
18	1	1	2	3.52	4.7	1.18	3.52
19	1	0	1	4.92	4.92	0.0	4.92
20	1	2	3	3.94	4.83	0.85	4.2
21	1	2	3	2.94	4.9	1.52	2.75
22	1	1	2	4.23	4.81	0.58	4.23
23	3	1	4	3.99	4.91	0.89	4.24
24	1	1	2	3.18	4.76	1.57	3.18
25	1	2	3	3.49	4.88	1.48	4.15
26	2	2	4	2.41	4.82	1.46	1.79
27	1	1	2	3.09	4.82	1.73	3.09
28	1	1	2	4.77	4.98	0.21	4.77
29	2	1	3	3.56	4.85	0.99	3.38
30	2	3	5	3.05	4.88	1.25	2.79
31	1	2	3	3.33	4.95	1.15	2.64
32	1	2	3	2.97	4.62	1.21	2.54
33	2	2	4	3.4	4.92	1.03	3.3
34	1	2	3	2.9	4.79	1.35	2.22
35	1	0	1	4.95	4.95	0.0	4.95
36	1	1	2	4.86	4.91	0.04	4.86
37	2	1	3	2.86	4.94	1.59	2.57
38	1	0	1	4.97	4.97	0.0	4.97

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	1	0	1	4.65	4.65	0.0	4.65
40	1	3	4	2.87	4.59	1.21	2.7
41	1	2	3	4.43	4.81	0.28	4.32
42	3	1	4	3.54	4.08	0.41	3.52
43	1	2	3	2.93	4.91	1.5	2.59
44	1	1	2	3.44	4.86	1.42	3.44
45	2	2	4	2.8	4.95	1.41	2.58
46	3	4	7	2.54	4.43	1.23	2.34
47	0	1	1	4.87	4.87	0.0	4.87
48	1	1	2	4.89	4.99	0.1	4.89
49	0	1	1	4.89	4.89	0.0	4.89
50	1	1	2	4.16	4.89	0.72	4.16

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	1	2.0
0	1	1	2	4.0
0	1	1	3	6.0
2	0	2	4	8.0
0	0	0	5	10.0
1	0	1	6	12.0
0	0	0	7	14.0
0	0	0	8	16.0
0	0	0	9	18.0
0	0	0	10	20.0
0	0	0	11	22.0
0	0	0	12	24.0
1	0	1	13	26.0
0	0	0	14	28.0
0	0	0	15	30.0
0	0	0	16	32.0
0	0	0	17	34.0
0	0	0	18	36.0
0	0	0	19	38.0
0	0	0	20	40.0
0	0	0	21	42.0
0	0	0	22	44.0
0	0	0	23	46.0
0	0	0	24	48.0
0	1	1	25	50.0
0	0	0	26	52.0
0	0	0	27	54.0
0	0	0	28	56.0
0	0	0	29	58.0
0	0	0	30	60.0
0	0	0	31	62.0
0	0	0	32	64.0
0	0	0	33	66.0
0	0	0	34	68.0
0	0	0	35	70.0
0	1	1	36	72.0
0	0	0	37	74.0

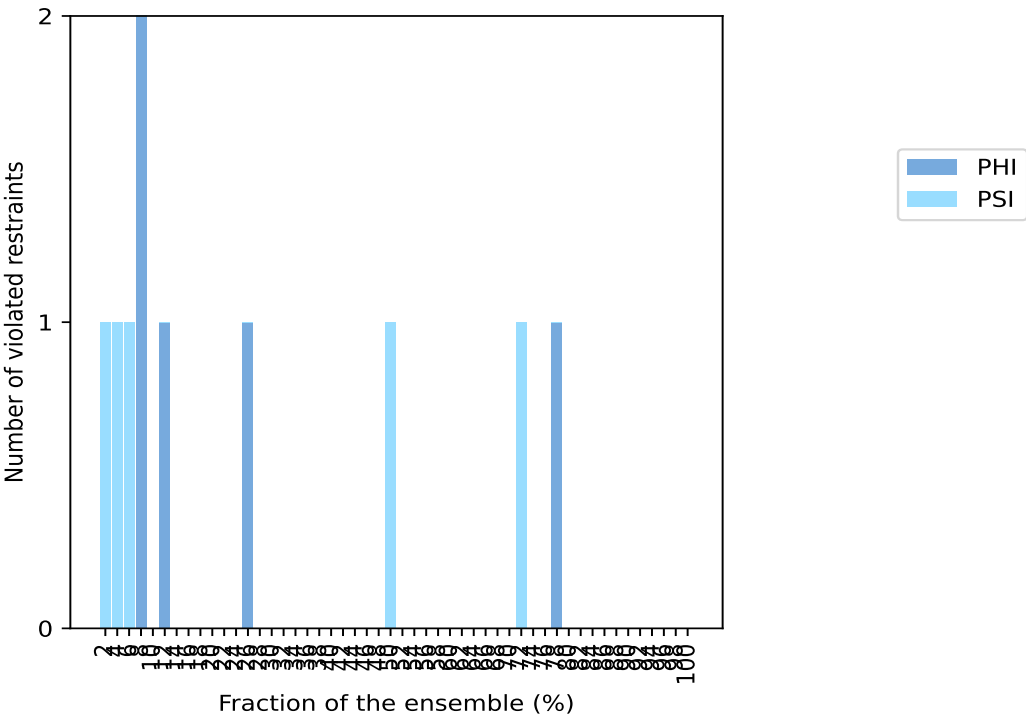
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	38	76.0
1	0	1	39	78.0
0	0	0	40	80.0
0	0	0	41	82.0
0	0	0	42	84.0
0	0	0	43	86.0
0	0	0	44	88.0
0	0	0	45	90.0
0	0	0	46	92.0
0	0	0	47	94.0
0	0	0	48	96.0
0	0	0	49	98.0
0	0	0	50	100.0

¹ Number of models with violations

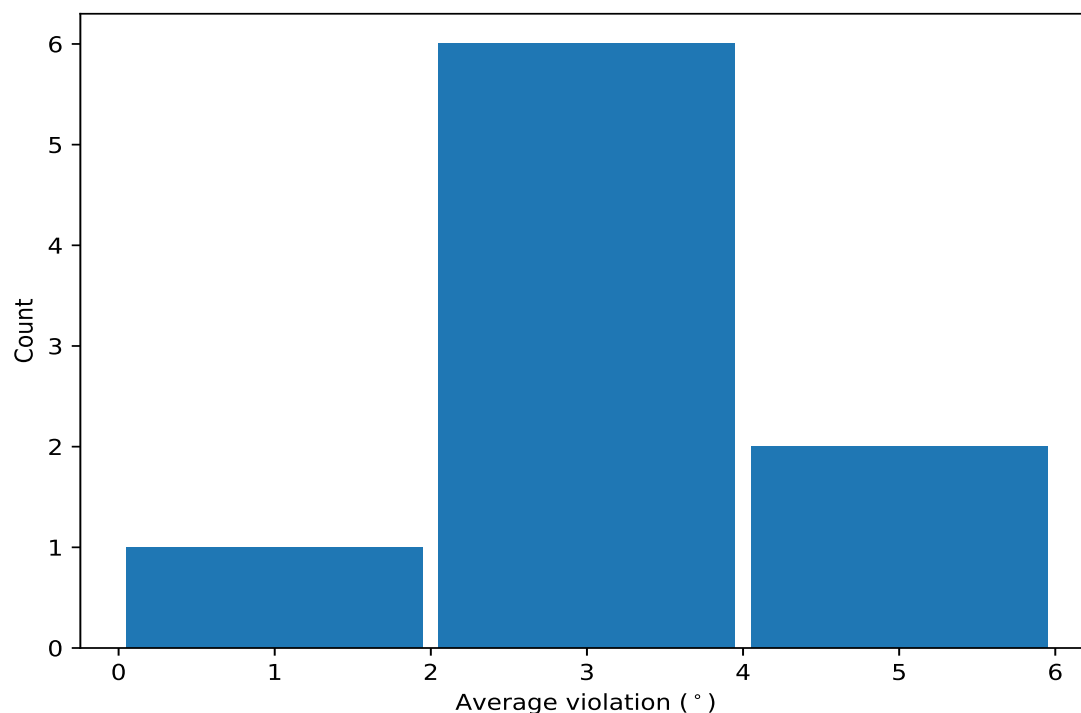
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



10.4 Most violated dihedral-angle restraints in the ensemble [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.

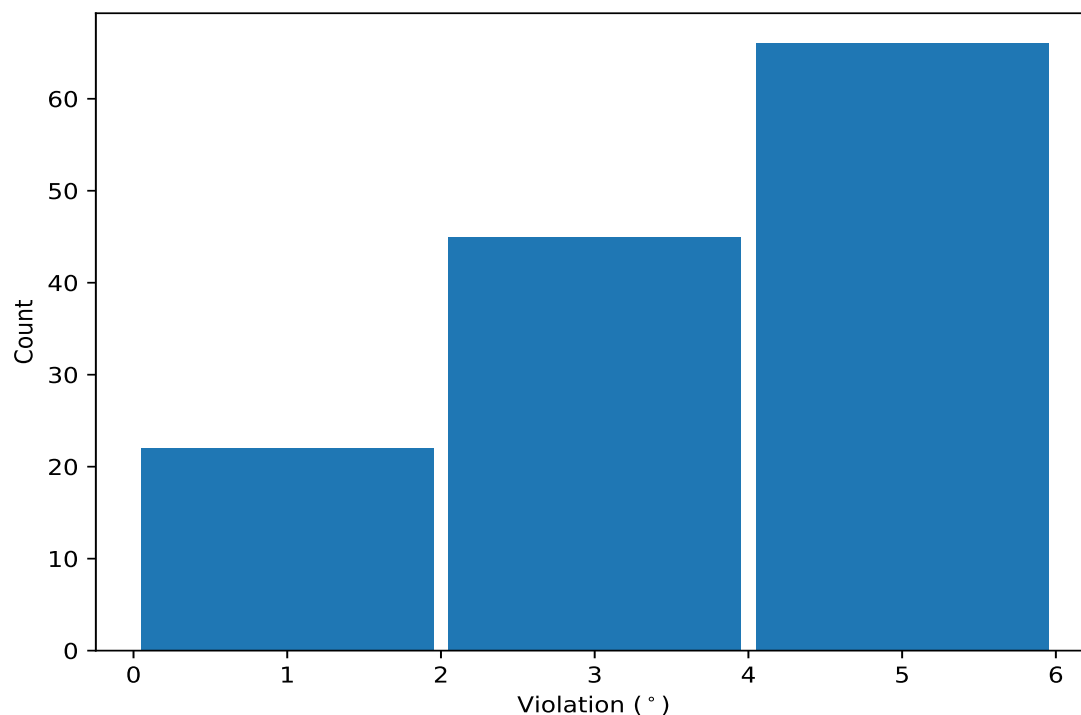
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	39	3.65	1.31	4.15
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	36	4.12	1.0	4.7
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	25	3.6	1.42	4.45
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	13	2.27	1.1	2.1
(1,43)	1:456:A:ALA:C	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	6	4.27	0.61	4.49
(1,35)	1:435:A:ARG:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	4	3.31	0.87	3.12
(1,73)	1:471:A:ALA:C	1:472:A:ALA:N	1:472:A:ALA:CA	1:472:A:ALA:C	4	2.82	0.96	2.68
(1,28)	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	1:433:A:MET:N	3	2.07	0.67	1.9
(1,90)	1:480:A:ALA:N	1:480:A:ALA:CA	1:480:A:ALA:C	1:481:A:LEU:N	2	1.4	0.09	1.4

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 (°)
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	11	4.99
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	48	4.99
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	6	4.98
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	28	4.98
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	4	4.98
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	38	4.97
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	14	4.95
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	35	4.95
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	31	4.95
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	45	4.95
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	7	4.94
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	1	4.94
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	37	4.94
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	19	4.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	7	4.92
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	33	4.92
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	36	4.91
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	43	4.91
(1,43)	1:456:A:ALA:C	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	23	4.91
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	12	4.91
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	21	4.9
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	49	4.89
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	50	4.89
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	25	4.88
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	30	4.88
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	47	4.87
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	44	4.86
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	17	4.85
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	29	4.85
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	4	4.84
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	5	4.83
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	20	4.83
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	8	4.82
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	26	4.82
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	27	4.82
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	36	4.82
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	22	4.81
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	41	4.81
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	34	4.79
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	48	4.79
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	24	4.76
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	13	4.71
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	18	4.7
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	3	4.69
(1,35)	1:435:A:ARG:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	9	4.66
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	12	4.65
(1,43)	1:456:A:ALA:C	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	39	4.65
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	32	4.62
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	40	4.59
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	28	4.56
(1,43)	1:456:A:ALA:C	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	2	4.55
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	23	4.5
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	15	4.5
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	16	4.45
(1,43)	1:456:A:ALA:C	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	46	4.43
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	16	4.41
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	41	4.32
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	3	4.3
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	46	4.3
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	16	4.22
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	20	4.2
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	41	4.15
(1,73)	1:471:A:ALA:C	1:472:A:ALA:N	1:472:A:ALA:CA	1:472:A:ALA:C	25	4.15
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	10	4.13
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	5	4.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:456:A:ALA:C	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	42	4.08
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	30	3.97
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	23	3.97
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	17	3.95
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	12	3.9
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	4	3.78
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	42	3.76
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	10	3.73
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	22	3.65
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	33	3.58
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	7	3.49
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	11	3.46
(1,35)	1:435:A:ARG:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	50	3.44
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	40	3.39
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	29	3.38
(1,73)	1:471:A:ALA:C	1:472:A:ALA:N	1:472:A:ALA:CA	1:472:A:ALA:C	42	3.29
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	33	3.03
(1,43)	1:456:A:ALA:C	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	16	3.02
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	42	3.02
(1,28)	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	1:433:A:MET:N	15	2.96
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	45	2.93
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	20	2.79
(1,35)	1:435:A:ARG:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	30	2.79
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	21	2.75
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	9	2.72
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	31	2.64
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	43	2.59
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	37	2.57
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	23	2.56
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	32	2.54
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	1	2.45
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	29	2.45
(1,44)	1:457:A:HIS:N	1:457:A:HIS:CA	1:457:A:HIS:C	1:458:A:TRP:N	46	2.44
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	31	2.41
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	10	2.34
(1,35)	1:435:A:ARG:C	1:436:A:GLN:N	1:436:A:GLN:CA	1:436:A:GLN:C	46	2.34
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	18	2.33
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	26	2.29
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	30	2.27
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	34	2.22
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	45	2.22
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	16	2.1
(1,73)	1:471:A:ALA:C	1:472:A:ALA:N	1:472:A:ALA:CA	1:472:A:ALA:C	33	2.07
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	9	2.04
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	44	2.03
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	40	2.0
(1,28)	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	1:433:A:MET:N	17	1.9
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	2	1.84
(1,73)	1:471:A:ALA:C	1:472:A:ALA:N	1:472:A:ALA:CA	1:472:A:ALA:C	32	1.76
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	34	1.69
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	46	1.68

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	24	1.61
(1,90)	1:480:A:ALA:N	1:480:A:ALA:CA	1:480:A:ALA:C	1:481:A:LEU:N	40	1.49
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	25	1.45
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	27	1.36
(1,28)	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	1:433:A:MET:N	30	1.34
(1,90)	1:480:A:ALA:N	1:480:A:ALA:CA	1:480:A:ALA:C	1:481:A:LEU:N	46	1.31
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	11	1.31
(1,68)	1:469:A:VAL:N	1:469:A:VAL:CA	1:469:A:VAL:C	1:470:A:ALA:N	14	1.3
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	26	1.29
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	43	1.28
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	46	1.26
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	26	1.23
(1,48)	1:459:A:GLY:N	1:459:A:GLY:CA	1:459:A:GLY:C	1:460:A:GLN:N	21	1.18
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	8	1.09
(1,91)	1:480:A:ALA:C	1:481:A:LEU:N	1:481:A:LEU:CA	1:481:A:LEU:C	45	1.09
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	37	1.08
(1,27)	1:431:A:LEU:C	1:432:A:GLU:N	1:432:A:GLU:CA	1:432:A:GLU:C	2	1.06