



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 11:40 AM UTC

PDB ID : 6YI3 / pdb_00006yi3
BMRB ID : 34511
Title : The N-terminal RNA-binding domain of the SARS-CoV-2 nucleocapsid phosphoprotein
Authors : Veverka, V.; Boura, E.
Deposited on : 2020-03-31

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

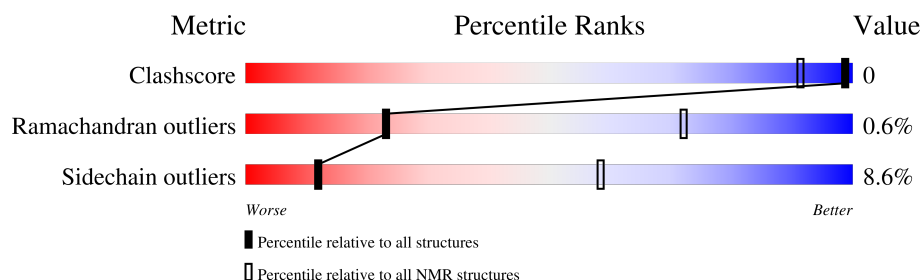
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	140	

2 Ensemble composition and analysis

This entry contains 40 models. Model 4 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:10-A:50, A:66-A:75, A:81-A:136 (107)	0.46	4
2	A:51-A:65 (15)	1.19	14

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 16, 20, 21, 23, 24, 25, 26, 29, 31, 32, 33, 35, 36, 38
2	2, 6, 17, 18, 22, 37, 39
3	15, 30, 40
Single-model clusters	19; 27; 28; 34

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2107 atoms, of which 1038 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	140	Total	C	H	N	O	S	0
			2107	671	1038	195	201	2	

There are 3 discrepancies between the modelled and reference sequences:

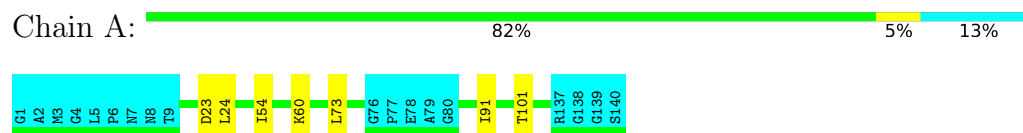
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0DTC9
A	2	ALA	-	expression tag	UNP P0DTC9
A	3	MET	-	expression tag	UNP P0DTC9

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: Nucleoprotein

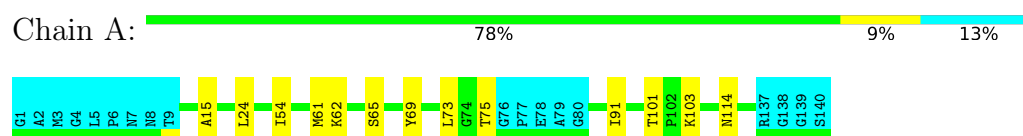


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

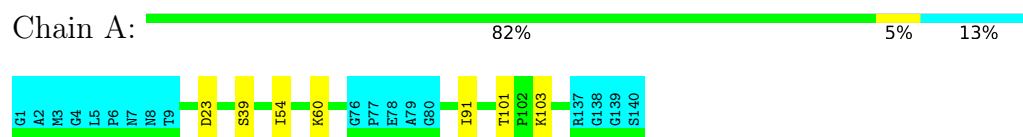
4.2.1 Score per residue for model 1

- Molecule 1: Nucleoprotein



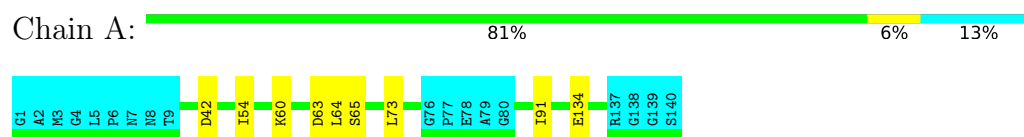
4.2.2 Score per residue for model 2

- Molecule 1: Nucleoprotein



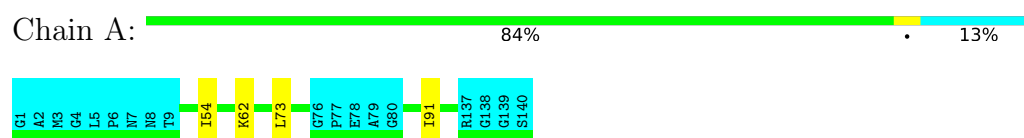
4.2.3 Score per residue for model 3

- Molecule 1: Nucleoprotein



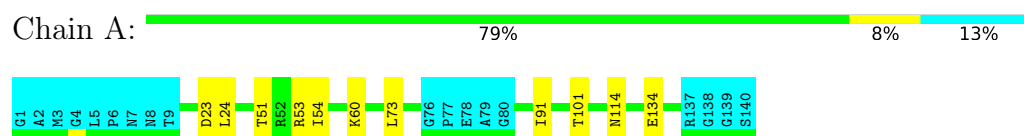
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Nucleoprotein



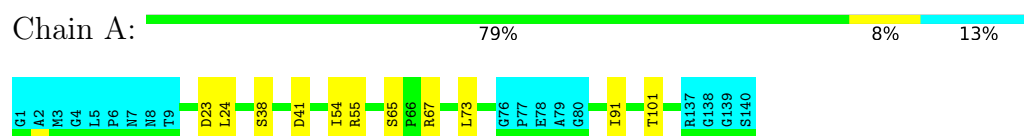
4.2.5 Score per residue for model 5

- Molecule 1: Nucleoprotein



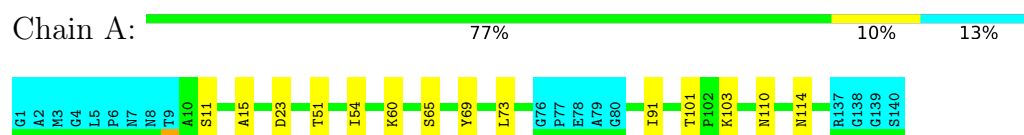
4.2.6 Score per residue for model 6

- Molecule 1: Nucleoprotein



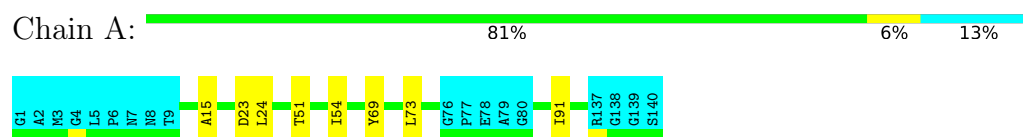
4.2.7 Score per residue for model 7

- Molecule 1: Nucleoprotein



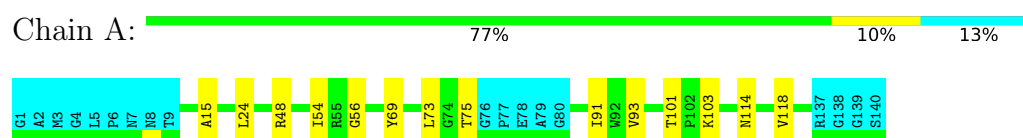
4.2.8 Score per residue for model 8

- Molecule 1: Nucleoprotein



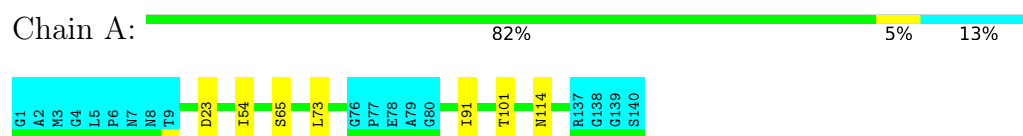
4.2.9 Score per residue for model 9

- Molecule 1: Nucleoprotein



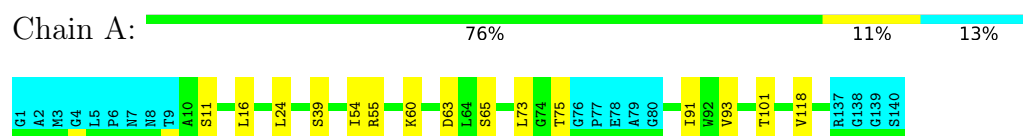
4.2.10 Score per residue for model 10

- Molecule 1: Nucleoprotein



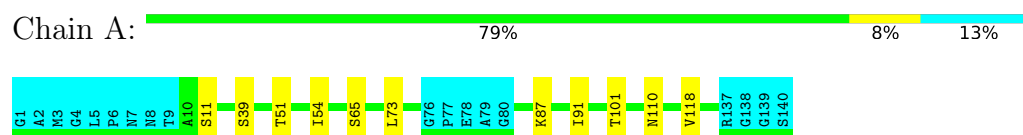
4.2.11 Score per residue for model 11

- Molecule 1: Nucleoprotein



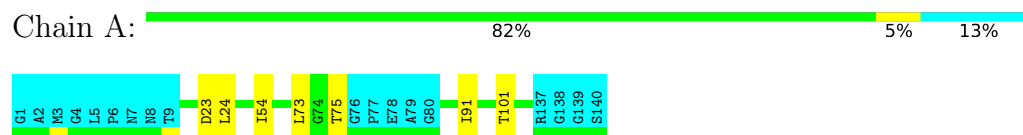
4.2.12 Score per residue for model 12

- Molecule 1: Nucleoprotein



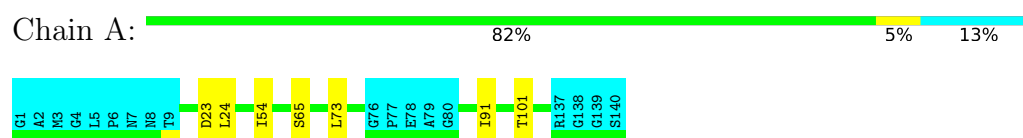
4.2.13 Score per residue for model 13

- Molecule 1: Nucleoprotein



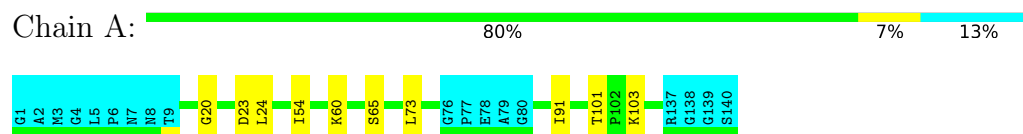
4.2.14 Score per residue for model 14

- Molecule 1: Nucleoprotein



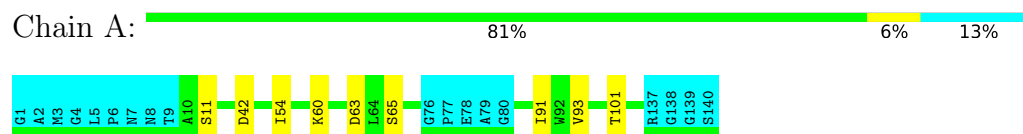
4.2.15 Score per residue for model 15

- Molecule 1: Nucleoprotein



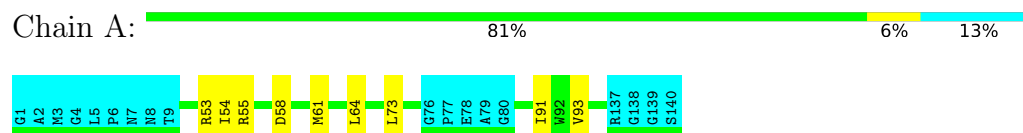
4.2.16 Score per residue for model 16

- Molecule 1: Nucleoprotein



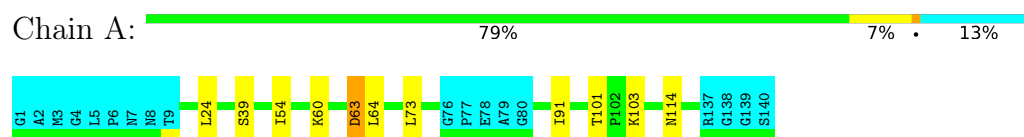
4.2.17 Score per residue for model 17

- Molecule 1: Nucleoprotein



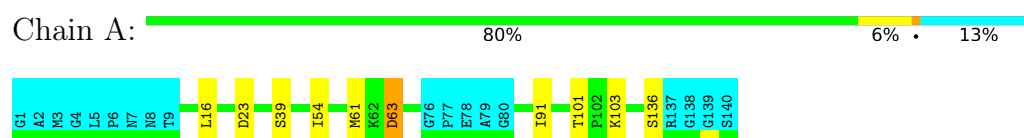
4.2.18 Score per residue for model 18

- Molecule 1: Nucleoprotein



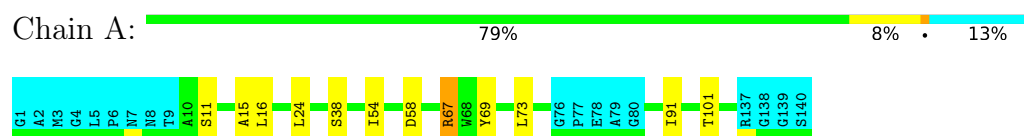
4.2.19 Score per residue for model 19

- Molecule 1: Nucleoprotein



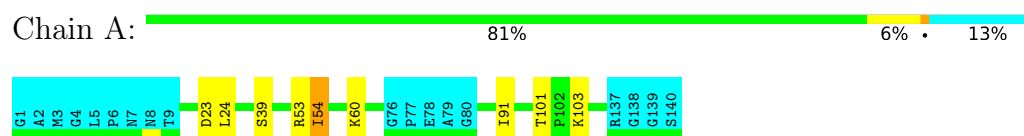
4.2.20 Score per residue for model 20

- Molecule 1: Nucleoprotein



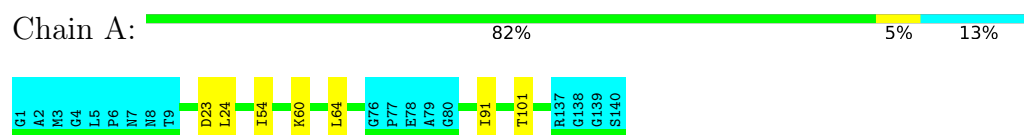
4.2.21 Score per residue for model 21

- Molecule 1: Nucleoprotein



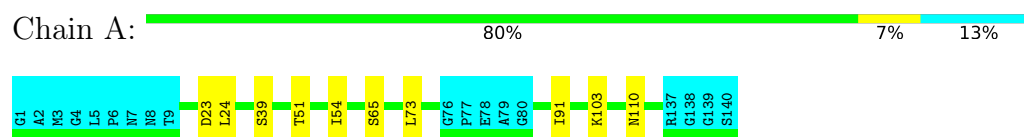
4.2.22 Score per residue for model 22

- Molecule 1: Nucleoprotein



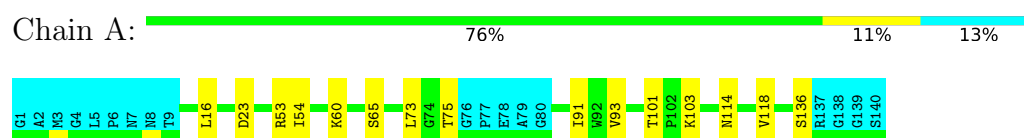
4.2.23 Score per residue for model 23

- Molecule 1: Nucleoprotein



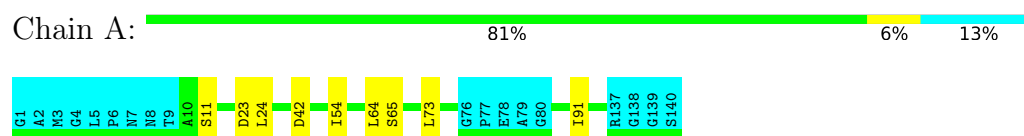
4.2.24 Score per residue for model 24

- Molecule 1: Nucleoprotein



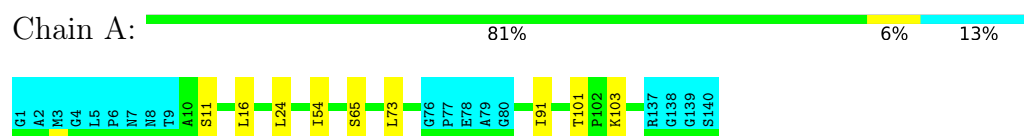
4.2.25 Score per residue for model 25

- Molecule 1: Nucleoprotein



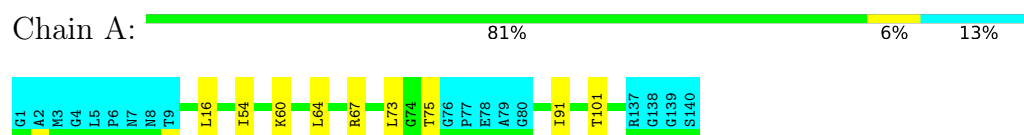
4.2.26 Score per residue for model 26

- Molecule 1: Nucleoprotein



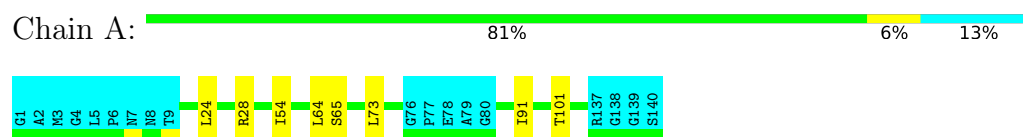
4.2.27 Score per residue for model 27

- Molecule 1: Nucleoprotein



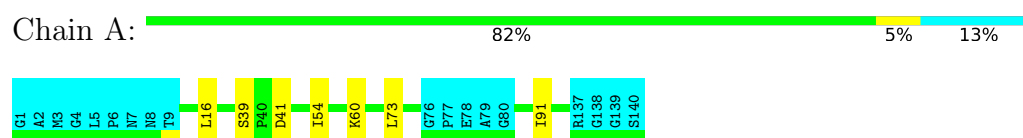
4.2.28 Score per residue for model 28

- Molecule 1: Nucleoprotein



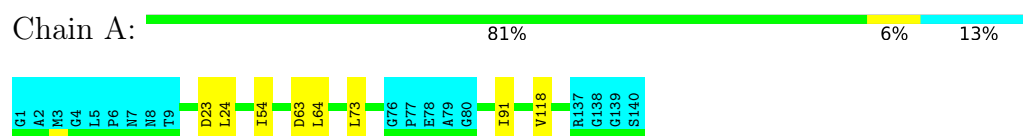
4.2.29 Score per residue for model 29

- Molecule 1: Nucleoprotein



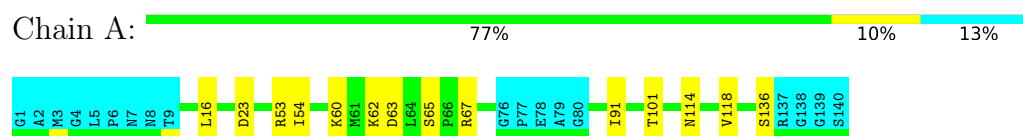
4.2.30 Score per residue for model 30

- Molecule 1: Nucleoprotein



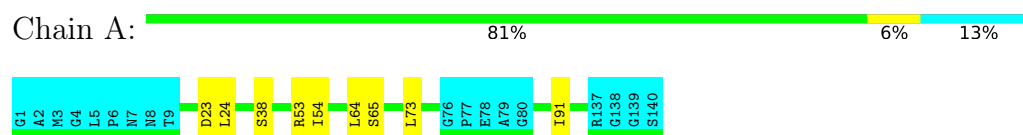
4.2.31 Score per residue for model 31

- Molecule 1: Nucleoprotein



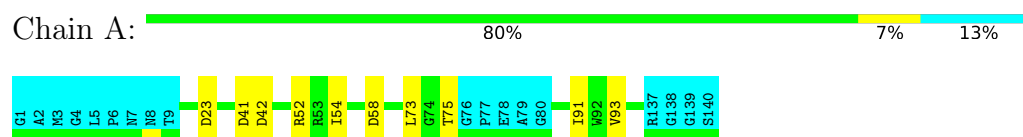
4.2.32 Score per residue for model 32

- Molecule 1: Nucleoprotein



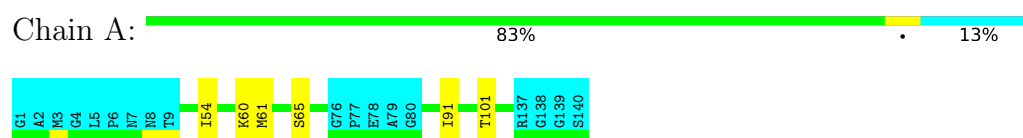
4.2.33 Score per residue for model 33

- Molecule 1: Nucleoprotein



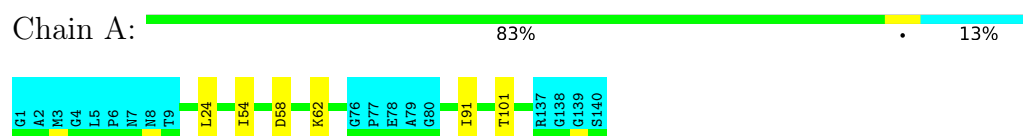
4.2.34 Score per residue for model 34

- Molecule 1: Nucleoprotein



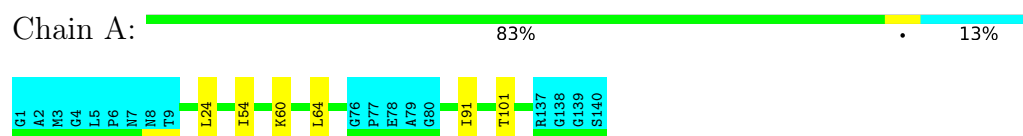
4.2.35 Score per residue for model 35

- Molecule 1: Nucleoprotein



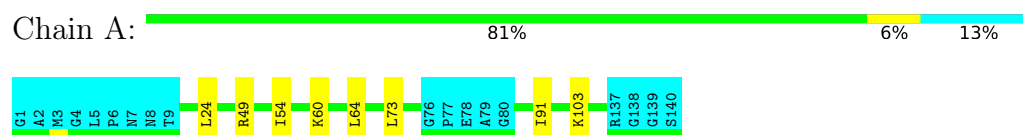
4.2.36 Score per residue for model 36

- Molecule 1: Nucleoprotein



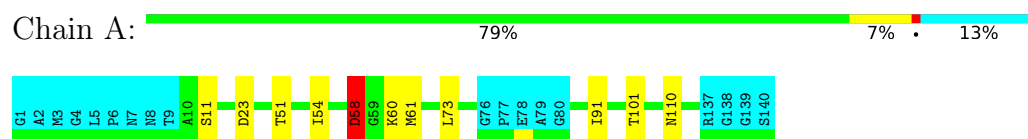
4.2.37 Score per residue for model 37

- Molecule 1: Nucleoprotein



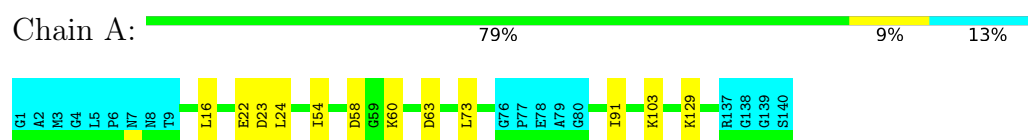
4.2.38 Score per residue for model 38

- Molecule 1: Nucleoprotein



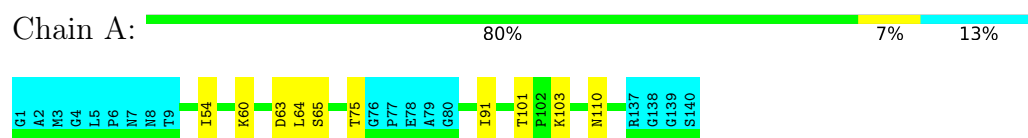
4.2.39 Score per residue for model 39

- Molecule 1: Nucleoprotein



4.2.40 Score per residue for model 40

- Molecule 1: Nucleoprotein



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 40 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
CYANA	structure calculation	
YASARA	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	1665
Number of shifts mapped to atoms	1665
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	0.72±0.01	0±0/983 (0.0± 0.0%)	0.86±0.03	0±0/1337 (0.0± 0.0%)
All	All	0.72	0/39320 (0.0%)	0.86	12/53480 (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	64	LEU	N-CA-C	-6.67	104.31	113.18	22	2
1	A	58	ASP	N-CA-C	-6.41	105.21	113.16	38	1
1	A	16	LEU	N-CA-C	-5.36	102.55	110.48	19	4
1	A	63	ASP	N-CA-C	5.31	119.05	112.47	31	2
1	A	54	ILE	N-CA-C	-5.25	102.12	108.53	21	1
1	A	56	GLY	N-CA-C	-5.21	105.08	112.37	9	1
1	A	101	THR	N-CA-C	-5.20	102.22	108.25	7	1

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	955	931	931	0±0
All	All	38200	37240	37240	8

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ALA:HB2	1:A:69:TYR:CZ	0.47	2.44	9	5
1:A:58:ASP:C	1:A:60:LYS:H	0.41	2.21	38	1
1:A:61:MET:HA	1:A:61:MET:HE2	0.41	1.92	19	1
1:A:15:ALA:HB1	1:A:67:ARG:HB2	0.40	1.94	20	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/140 (87%)	116±2 (95±1%)	5±2 (4±1%)	1±1 (1±1%)	23	72
All	All	4880/5600 (87%)	4646 (95%)	204 (4%)	30 (1%)	23	72

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	24	LEU	23
1	A	63	ASP	4
1	A	64	LEU	2
1	A	20	GLY	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/107 (91%)	89±2 (91±2%)	8±2 (9±2%)	12	58
All	All	3880/4280 (91%)	3548 (91%)	332 (9%)	12	58

All 37 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	54	ILE	40
1	A	91	ILE	40
1	A	73	LEU	30
1	A	101	THR	27
1	A	23	ASP	21
1	A	65	SER	19
1	A	60	LYS	19
1	A	103	LYS	14
1	A	75	THR	8
1	A	114	ASN	8
1	A	39	SER	8
1	A	64	LEU	8
1	A	11	SER	8
1	A	51	THR	6
1	A	53	ARG	6
1	A	93	VAL	6
1	A	118	VAL	6
1	A	58	ASP	6
1	A	63	ASP	5
1	A	110	ASN	5
1	A	16	LEU	5
1	A	61	MET	4
1	A	62	LYS	4
1	A	42	ASP	4
1	A	67	ARG	4
1	A	38	SER	3
1	A	41	ASP	3
1	A	55	ARG	3
1	A	136	SER	3
1	A	134	GLU	2
1	A	48	ARG	1
1	A	87	LYS	1
1	A	28	ARG	1
1	A	52	ARG	1
1	A	49	ARG	1
1	A	22	GLU	1
1	A	129	LYS	1

6.3.3 RNA ⓘ

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 91% for the well-defined parts and 91% 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	1665
Number of shifts mapped to atoms	1665
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	24

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	0.17 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.03 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	0.10 ± 0.15	None needed (< 0.5 ppm)
^{15}N	127	-0.56 ± 0.42	None needed (imprecise)

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 91%, i.e. 1493 atoms were assigned a chemical shift out of a possible 1635. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	603/607 (99%)	249/250 (100%)	242/244 (99%)	112/113 (99%)
Sidechain	786/875 (90%)	532/566 (94%)	234/266 (88%)	20/43 (47%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	104/153 (68%)	63/74 (85%)	38/74 (51%)	3/5 (60%)
Overall	1493/1635 (91%)	844/890 (95%)	514/584 (88%)	135/161 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 91%, i.e. 1660 atoms were assigned a chemical shift out of a possible 1824. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	691/699 (99%)	287/290 (99%)	277/280 (99%)	127/129 (98%)
Sidechain	865/972 (89%)	585/629 (93%)	259/295 (88%)	21/48 (44%)
Aromatic	104/153 (68%)	63/74 (85%)	38/74 (51%)	3/5 (60%)
Overall	1660/1824 (91%)	935/993 (94%)	574/649 (88%)	151/182 (83%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	72	TYR	CE1	182.76	111.24 – 124.66	48.3
1	A	14	THR	HG1	6.34	0.08 – 2.19	24.6
1	A	125	THR	HG1	5.79	0.08 – 2.19	22.1
1	A	101	THR	HG1	5.78	0.08 – 2.19	22.0
1	A	47	TYR	CE1	129.73	111.24 – 124.66	8.8
1	A	109	ARG	HB3	-0.55	0.43 – 3.11	-8.6
1	A	49	ARG	HB3	-0.51	0.43 – 3.11	-8.5
1	A	47	TYR	HE1	5.00	5.59 – 7.82	-7.6
1	A	47	TYR	HE2	5.00	5.58 – 7.83	-7.5
1	A	24	LEU	HD11	-1.21	-0.61 – 2.12	-7.2
1	A	24	LEU	HD12	-1.21	-0.61 – 2.12	-7.2
1	A	24	LEU	HD13	-1.21	-0.61 – 2.12	-7.2
1	A	33	PRO	HD3	0.96	1.76 – 5.48	-7.1
1	A	24	LEU	HB3	-0.85	-0.26 – 3.31	-6.7
1	A	78	GLU	HB2	0.69	1.00 – 3.05	-6.5
1	A	33	PRO	HG3	-0.10	0.33 – 3.48	-6.3
1	A	31	GLY	HA2	1.75	2.15 – 5.77	-6.1
1	A	24	LEU	HB2	-0.33	-0.07 – 3.30	-5.8
1	A	83	TYR	HA	1.62	1.87 – 7.33	-5.5
1	A	47	TYR	HD1	5.43	5.49 – 8.39	-5.2
1	A	47	TYR	HD2	5.43	5.48 – 8.39	-5.2
1	A	24	LEU	HD21	-0.67	-0.65 – 2.13	-5.1

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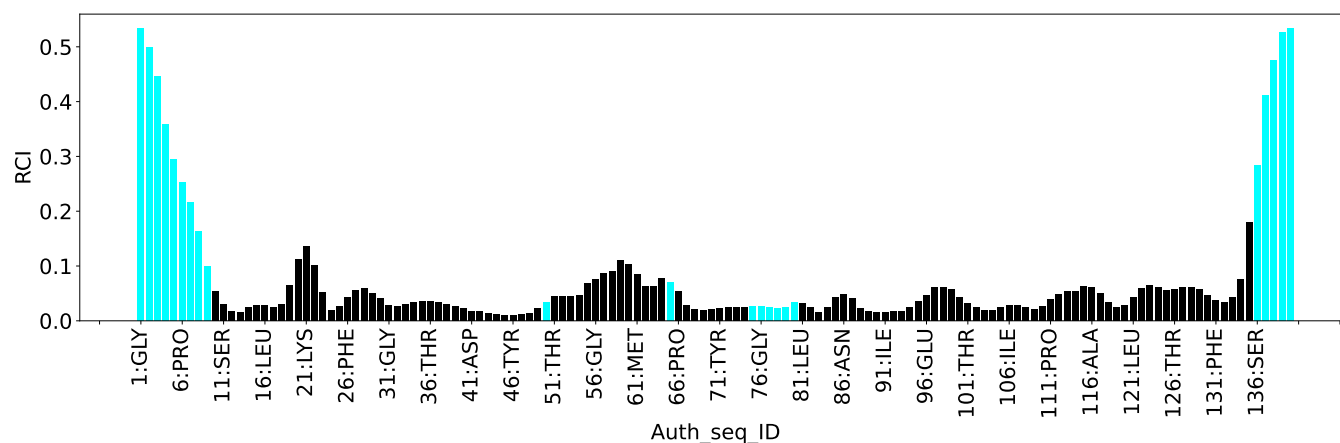
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	24	LEU	HD22	-0.67	-0.65 – 2.13	-5.1
1	A	24	LEU	HD23	-0.67	-0.65 – 2.13	-5.1

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	2405
Intra-residue ($ i-j =0$)	573
Sequential ($ i-j =1$)	708
Medium range ($ i-j >1$ and $ i-j <5$)	252
Long range ($ i-j \geq 5$)	872
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	176
Number of unmapped restraints	0
Number of restraints per residue	18.4
Number of long range restraints per residue ¹	6.2

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)	6.0	0.2
0.2-0.5 (Medium)	9.7	0.5
>0.5 (Large)	10.9	1.51

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)	1.8	9.88
10.0-20.0 (Medium)	0.1	14.68
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

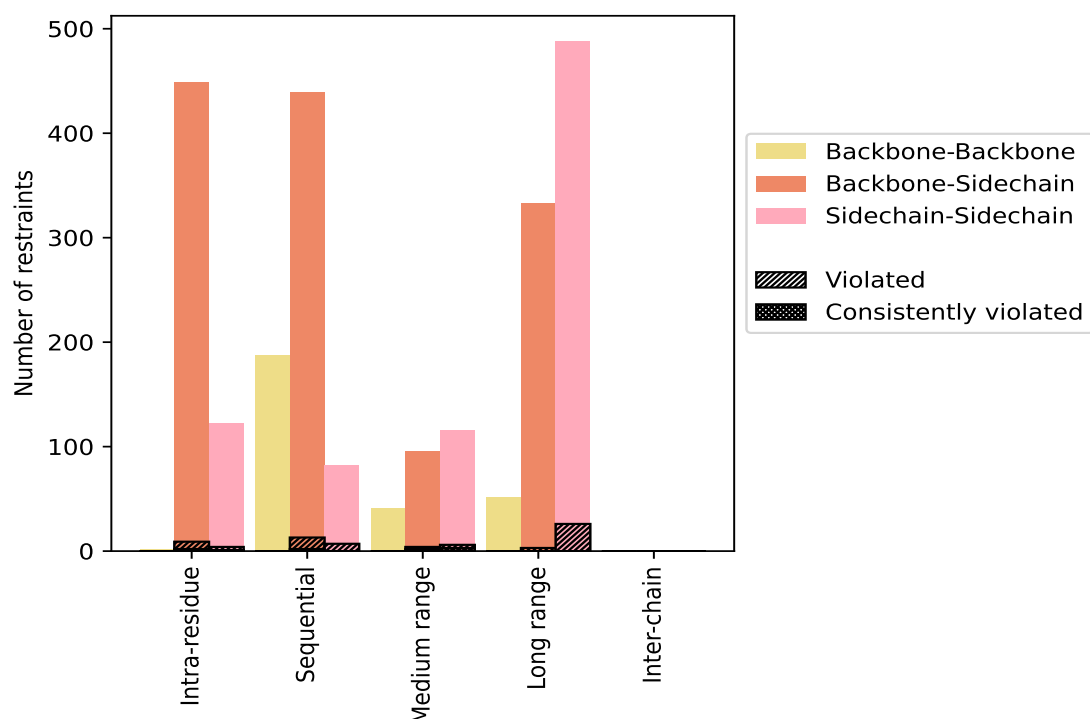
9.1 Summary of distance violations ⓘ

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$)	573	23.8	13	2.3	0.5	3	0.5	0.1
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	449	18.7	9	2.0	0.4	2	0.4	0.1
Sidechain-Sidechain	122	5.1	4	3.3	0.2	1	0.8	0.0
Sequential ($ i-j =1$)	708	29.4	20	2.8	0.8	2	0.3	0.1
Backbone-Backbone	187	7.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	439	18.3	13	3.0	0.5	2	0.5	0.1
Sidechain-Sidechain	82	3.4	7	8.5	0.3	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	252	10.5	10	4.0	0.4	5	2.0	0.2
Backbone-Backbone	41	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	95	4.0	4	4.2	0.2	2	2.1	0.1
Sidechain-Sidechain	116	4.8	6	5.2	0.2	3	2.6	0.1
Long range ($ i-j \geq 5$)	872	36.3	29	3.3	1.2	0	0.0	0.0
Backbone-Backbone	51	2.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	333	13.8	3	0.9	0.1	0	0.0	0.0
Sidechain-Sidechain	488	20.3	26	5.3	1.1	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	2405	100.0	72	3.0	3.0	10	0.4	0.4
Backbone-Backbone	281	11.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1316	54.7	29	2.2	1.2	6	0.5	0.2
Sidechain-Sidechain	808	33.6	43	5.3	1.8	4	0.5	0.2

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	5	6	6	6	0	23	0.44	1.32	0.31	0.38
2	7	7	6	5	0	25	0.44	1.18	0.28	0.44
3	7	7	7	7	0	28	0.51	1.35	0.38	0.42
4	7	6	7	5	0	25	0.55	1.32	0.33	0.46
5	4	6	7	8	0	25	0.59	1.43	0.36	0.51
6	6	8	6	8	0	28	0.55	1.35	0.36	0.48
7	5	5	7	9	0	26	0.56	1.32	0.36	0.48
8	7	6	7	6	0	26	0.54	1.28	0.35	0.47
9	5	3	7	7	0	22	0.65	1.47	0.35	0.51
10	5	7	7	10	0	29	0.52	1.44	0.36	0.51

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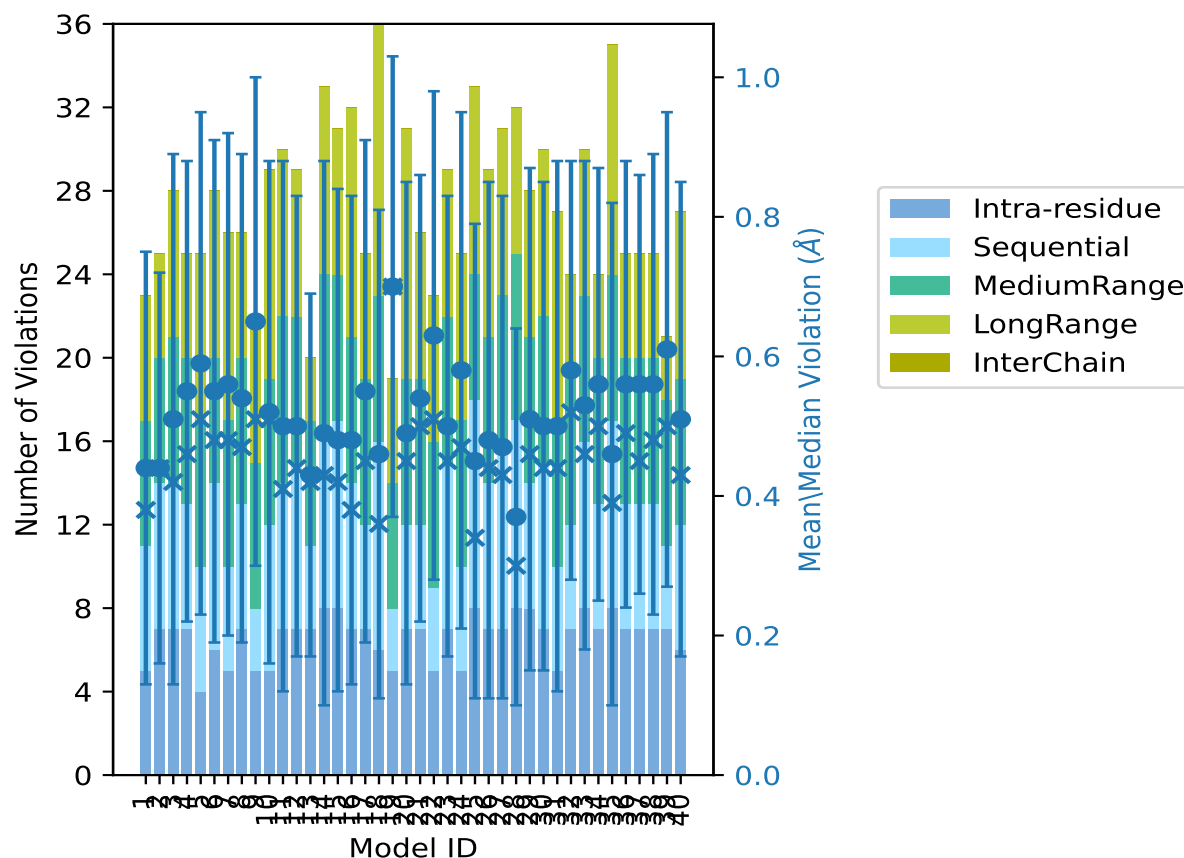
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	7	7	8	8	0	30	0.5	1.51	0.38	0.41
12	7	8	7	7	0	29	0.5	1.33	0.33	0.44
13	7	4	6	3	0	20	0.43	1.23	0.26	0.42
14	8	8	8	9	0	33	0.49	1.42	0.39	0.43
15	8	9	7	7	0	31	0.48	1.38	0.36	0.42
16	7	7	7	11	0	32	0.48	1.42	0.35	0.38
17	7	5	7	6	0	25	0.55	1.49	0.36	0.45
18	6	10	7	13	0	36	0.46	1.38	0.35	0.36
19	5	3	6	5	0	19	0.7	1.21	0.33	0.7
20	7	5	7	12	0	31	0.49	1.43	0.36	0.45
21	7	5	7	7	0	26	0.54	1.31	0.32	0.5
22	5	4	7	7	0	23	0.63	1.4	0.35	0.51
23	7	8	7	7	0	29	0.5	1.35	0.33	0.45
24	5	5	7	8	0	25	0.58	1.42	0.37	0.47
25	8	10	6	9	0	33	0.45	1.29	0.34	0.34
26	7	7	7	8	0	29	0.48	1.35	0.37	0.44
27	7	9	7	8	0	31	0.47	1.38	0.36	0.43
28	8	9	8	7	0	32	0.37	1.08	0.27	0.3
29	8	6	7	7	0	28	0.51	1.49	0.36	0.46
30	7	8	7	8	0	30	0.5	1.37	0.35	0.44
31	5	5	7	10	0	27	0.5	1.36	0.38	0.44
32	7	5	7	5	0	24	0.58	1.18	0.3	0.52
33	8	8	7	7	0	30	0.53	1.5	0.35	0.46
34	7	6	7	4	0	24	0.56	1.19	0.31	0.5
35	8	9	7	11	0	35	0.46	1.33	0.36	0.39
36	7	6	7	5	0	25	0.56	1.32	0.32	0.49
37	7	6	7	5	0	25	0.56	1.19	0.3	0.45
38	7	6	7	5	0	25	0.56	1.32	0.33	0.48
39	7	4	7	3	0	21	0.61	1.32	0.34	0.5
40	6	6	7	8	0	27	0.51	1.29	0.34	0.43

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2333(IR:560, SQ:688, MR:242, LR:843, 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	%
4	6	2	6	0	18	1	2.5
0	2	0	5	0	7	2	5.0
0	1	1	4	0	6	3	7.5
1	2	0	1	0	4	4	10.0
0	0	0	1	0	1	5	12.5
0	0	0	1	0	1	6	15.0

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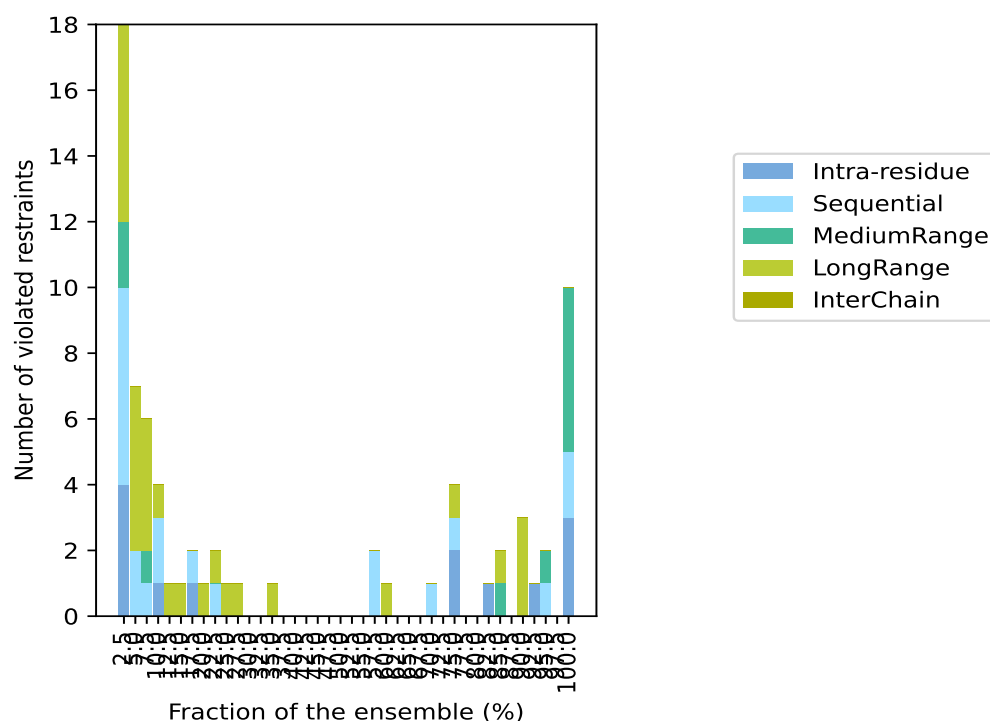
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	1	0	0	0	2	7	17.5
0	0	0	1	0	1	8	20.0
0	1	0	1	0	2	9	22.5
0	0	0	1	0	1	10	25.0
0	0	0	1	0	1	11	27.5
0	0	0	0	0	0	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	1	0	1	14	35.0
0	0	0	0	0	0	15	37.5
0	0	0	0	0	0	16	40.0
0	0	0	0	0	0	17	42.5
0	0	0	0	0	0	18	45.0
0	0	0	0	0	0	19	47.5
0	0	0	0	0	0	20	50.0
0	0	0	0	0	0	21	52.5
0	0	0	0	0	0	22	55.0
0	2	0	0	0	2	23	57.5
0	0	0	1	0	1	24	60.0
0	0	0	0	0	0	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	1	0	0	0	1	28	70.0
0	0	0	0	0	0	29	72.5
2	1	0	1	0	4	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
1	0	0	0	0	1	33	82.5
0	0	1	1	0	2	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	3	0	3	36	90.0
1	0	0	0	0	1	37	92.5
0	1	1	0	0	2	38	95.0
0	0	0	0	0	0	39	97.5
3	2	5	0	0	10	40	100.0

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

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

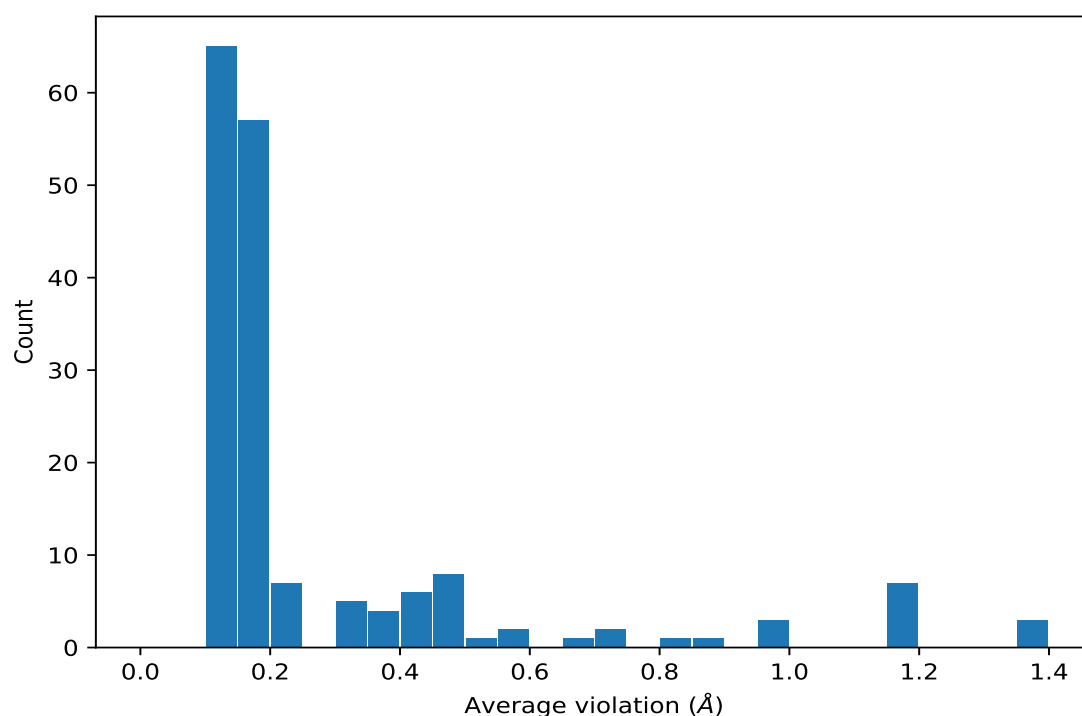
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	40	1.16	0.12	1.13
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	40	0.85	0.18	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	40	0.81	0.06	0.82
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	40	0.7	0.14	0.78
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	40	0.69	0.06	0.68
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	40	0.5	0.02	0.51
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	40	0.48	0.04	0.48
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	40	0.47	0.33	0.3
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	40	0.42	0.05	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	40	0.42	0.05	0.44
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	40	0.19	0.03	0.2
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	40	0.19	0.03	0.2
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	38	0.48	0.1	0.45
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	38	0.19	0.04	0.18
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	37	0.35	0.32	0.2
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	36	1.35	0.09	1.35

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	36	1.35	0.09	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	36	1.35	0.09	1.35
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	36	1.17	0.07	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	36	1.17	0.07	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	36	1.17	0.07	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	36	1.17	0.07	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	36	1.17	0.07	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	36	1.17	0.07	1.16
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	36	0.96	0.08	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	36	0.96	0.08	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	36	0.96	0.08	0.95
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	34	0.74	0.09	0.7
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	34	0.22	0.08	0.18
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	33	0.49	0.04	0.5
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	30	0.46	0.01	0.46
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	30	0.4	0.03	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	30	0.4	0.03	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	30	0.4	0.03	0.4
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	30	0.32	0.01	0.32
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	30	0.16	0.03	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	30	0.16	0.03	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	30	0.16	0.03	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	30	0.16	0.03	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	30	0.16	0.03	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	30	0.16	0.03	0.16
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	28	0.49	0.05	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	28	0.49	0.05	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	28	0.49	0.05	0.51
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	24	0.39	0.12	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	24	0.39	0.12	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	24	0.39	0.12	0.4
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	23	0.19	0.06	0.17
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	23	0.19	0.06	0.17
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	23	0.19	0.06	0.17
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	23	0.12	0.02	0.12
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	23	0.12	0.02	0.12
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	23	0.12	0.02	0.12
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	23	0.12	0.02	0.12
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	23	0.12	0.02	0.12
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	23	0.12	0.02	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	14	0.14	0.04	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	14	0.14	0.04	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	14	0.14	0.04	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	14	0.14	0.04	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	14	0.14	0.04	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	14	0.14	0.04	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	14	0.14	0.04	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	14	0.14	0.04	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	14	0.14	0.04	0.12
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	11	0.19	0.07	0.2
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	11	0.19	0.07	0.2
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	10	0.15	0.04	0.13
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	10	0.15	0.04	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	10	0.15	0.04	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	10	0.15	0.04	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	10	0.15	0.04	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	10	0.15	0.04	0.13
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	9	0.34	0.1	0.36
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	9	0.1	0.0	0.1
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	9	0.1	0.0	0.1
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	9	0.1	0.0	0.1
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	8	0.32	0.05	0.32
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	7	0.42	0.01	0.41
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	7	0.12	0.0	0.12
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	7	0.12	0.0	0.12
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	7	0.12	0.0	0.12
(1,802)	1:13:A:PHE:HE1	1:37:A:ASN:HD22	6	0.34	0.12	0.37
(1,802)	1:13:A:PHE:HE2	1:37:A:ASN:HD22	6	0.34	0.12	0.37
(1,1056)	1:44:A:ILE:HD11	1:73:A:LEU:HG	5	0.16	0.01	0.16
(1,1056)	1:44:A:ILE:HD12	1:73:A:LEU:HG	5	0.16	0.01	0.16
(1,1056)	1:44:A:ILE:HD13	1:73:A:LEU:HG	5	0.16	0.01	0.16
(1,2106)	1:42:A:ASP:HB2	1:43:A:GLN:HE21	4	0.59	0.35	0.63
(1,2106)	1:42:A:ASP:HB3	1:43:A:GLN:HE21	4	0.59	0.35	0.63
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG21	4	0.15	0.03	0.14
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG22	4	0.15	0.03	0.14
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG23	4	0.15	0.03	0.14
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG21	4	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG22	4	0.15	0.03	0.14
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG23	4	0.15	0.03	0.14
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG2	4	0.13	0.01	0.13
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG3	4	0.13	0.01	0.13
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG2	4	0.13	0.01	0.13
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG3	4	0.13	0.01	0.13
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG2	4	0.13	0.01	0.13
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG3	4	0.13	0.01	0.13
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD2	4	0.13	0.01	0.12
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD3	4	0.13	0.01	0.12
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD11	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD12	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD13	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD21	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD22	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD23	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD11	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD12	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD13	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD21	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD22	3	0.16	0.04	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD23	3	0.16	0.04	0.16
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD11	3	0.15	0.03	0.16
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD12	3	0.15	0.03	0.16
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD13	3	0.15	0.03	0.16
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB1	3	0.15	0.02	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB2	3	0.15	0.02	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB3	3	0.15	0.02	0.13
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD11	3	0.12	0.0	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD12	3	0.12	0.0	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD13	3	0.12	0.0	0.12
(1,1979)	1:16:A:LEU:HD11	1:134:A:GLU:H	3	0.11	0.0	0.11
(1,1979)	1:16:A:LEU:HD12	1:134:A:GLU:H	3	0.11	0.0	0.11
(1,1979)	1:16:A:LEU:HD13	1:134:A:GLU:H	3	0.11	0.0	0.11
(1,1979)	1:16:A:LEU:HD21	1:134:A:GLU:H	3	0.11	0.0	0.11
(1,1979)	1:16:A:LEU:HD22	1:134:A:GLU:H	3	0.11	0.0	0.11
(1,1979)	1:16:A:LEU:HD23	1:134:A:GLU:H	3	0.11	0.0	0.11
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD1	3	0.1	0.0	0.1
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD2	3	0.1	0.0	0.1
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD1	3	0.1	0.0	0.1
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD2	3	0.1	0.0	0.1
(1,1119)	1:54:A:ILE:HD11	1:62:A:LYS:HE2	2	0.21	0.06	0.21

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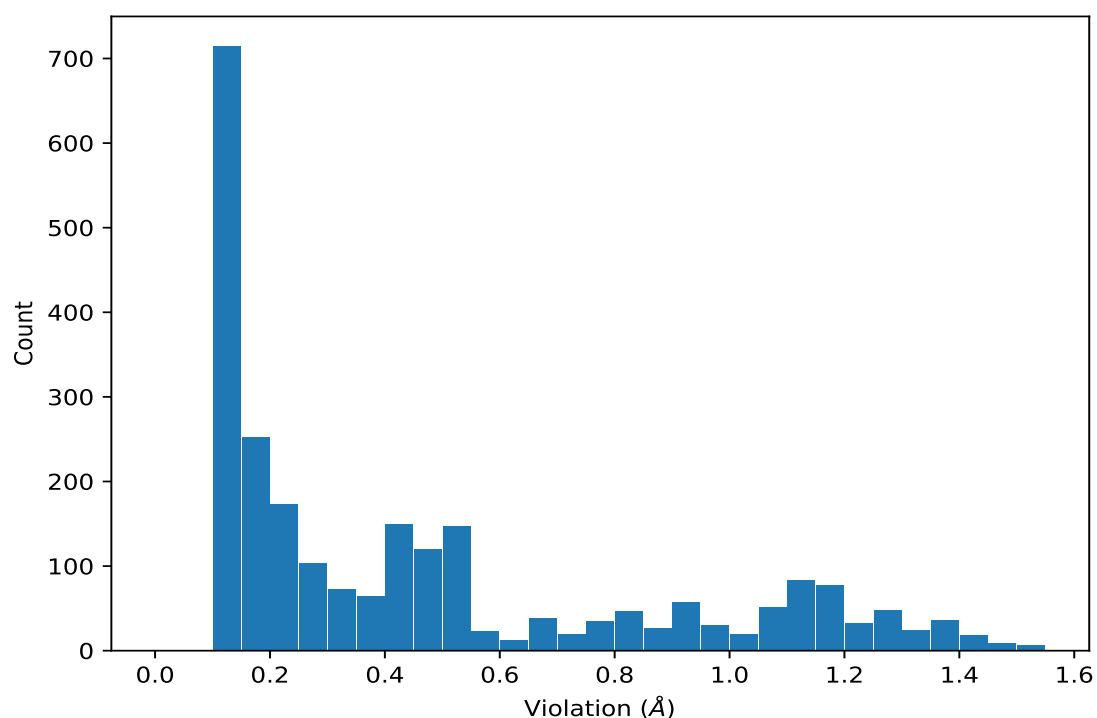
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1119)	1:54:A:ILE:HD11	1:62:A:LYS:HE3	2	0.21	0.06	0.21
(1,1119)	1:54:A:ILE:HD12	1:62:A:LYS:HE2	2	0.21	0.06	0.21
(1,1119)	1:54:A:ILE:HD12	1:62:A:LYS:HE3	2	0.21	0.06	0.21
(1,1119)	1:54:A:ILE:HD13	1:62:A:LYS:HE2	2	0.21	0.06	0.21
(1,1119)	1:54:A:ILE:HD13	1:62:A:LYS:HE3	2	0.21	0.06	0.21
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD11	2	0.15	0.01	0.15
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD12	2	0.15	0.01	0.15
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD13	2	0.15	0.01	0.15
(1,1110)	1:54:A:ILE:HG21	1:55:A:ARG:H	2	0.14	0.02	0.14
(1,1110)	1:54:A:ILE:HG22	1:55:A:ARG:H	2	0.14	0.02	0.14
(1,1110)	1:54:A:ILE:HG23	1:55:A:ARG:H	2	0.14	0.02	0.14
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD11	2	0.14	0.01	0.14
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD12	2	0.14	0.01	0.14
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD13	2	0.14	0.01	0.14
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD11	2	0.14	0.01	0.14
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD12	2	0.14	0.01	0.14
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD13	2	0.14	0.01	0.14
(1,272)	1:59:A:GLY:H	1:60:A:LYS:HB2	2	0.13	0.01	0.13
(1,272)	1:59:A:GLY:H	1:60:A:LYS:HB3	2	0.13	0.01	0.13
(1,1104)	1:54:A:ILE:HG21	1:62:A:LYS:HG2	2	0.11	0.0	0.11
(1,1104)	1:54:A:ILE:HG21	1:62:A:LYS:HG3	2	0.11	0.0	0.11
(1,1104)	1:54:A:ILE:HG22	1:62:A:LYS:HG2	2	0.11	0.0	0.11
(1,1104)	1:54:A:ILE:HG22	1:62:A:LYS:HG3	2	0.11	0.0	0.11
(1,1104)	1:54:A:ILE:HG23	1:62:A:LYS:HG2	2	0.11	0.0	0.11
(1,1104)	1:54:A:ILE:HG23	1:62:A:LYS:HG3	2	0.11	0.0	0.11
(1,2210)	1:73:A:LEU:HD11	1:92:A:TRP:HE3	2	0.11	0.0	0.11
(1,2210)	1:73:A:LEU:HD12	1:92:A:TRP:HE3	2	0.11	0.0	0.11
(1,2210)	1:73:A:LEU:HD13	1:92:A:TRP:HE3	2	0.11	0.0	0.11
(1,2210)	1:73:A:LEU:HD21	1:92:A:TRP:HE3	2	0.11	0.0	0.11
(1,2210)	1:73:A:LEU:HD22	1:92:A:TRP:HE3	2	0.11	0.0	0.11
(1,2210)	1:73:A:LEU:HD23	1:92:A:TRP:HE3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	11	1.51
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	11	1.51
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	11	1.51
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	33	1.5
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	33	1.5
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	33	1.5
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	17	1.49
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	17	1.49
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	17	1.49
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	29	1.49
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	29	1.49
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	29	1.49
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	9	1.47
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	9	1.47
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	9	1.47
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	10	1.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	10	1.44
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	10	1.44
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	5	1.43
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	5	1.43
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	5	1.43
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	20	1.43
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	20	1.43
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	20	1.43
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	14	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	14	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	14	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	16	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	16	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	16	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	24	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	24	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	24	1.42
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	22	1.4
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	22	1.4
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	22	1.4
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	15	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	15	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	15	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	18	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	18	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	18	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	27	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	27	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	27	1.38
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	30	1.37
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	30	1.37
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	30	1.37
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	11	1.36
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	11	1.36
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	11	1.36
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	11	1.36
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	11	1.36
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	11	1.36
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	31	1.36
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	31	1.36
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	31	1.36
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	3	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	3	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	3	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	6	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	6	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	6	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	23	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	23	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	23	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	26	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	26	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	26	1.35
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	12	1.33
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	12	1.33
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	12	1.33
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	35	1.33
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	35	1.33
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	35	1.33
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	1	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	3	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	4	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	7	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	9	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	22	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	30	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	36	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	38	1.32
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	39	1.32
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	7	1.31
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	7	1.31
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	7	1.31
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	21	1.31
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	21	1.31
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	21	1.31
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	5	1.31
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	27	1.31
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	29	1.29
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	29	1.29
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	29	1.29
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	29	1.29
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	29	1.29
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	29	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	4	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	4	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	4	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	25	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	25	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	25	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	40	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	40	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	40	1.29
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	8	1.28
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	8	1.28
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	8	1.28
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	16	1.27
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	16	1.27
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	16	1.27
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	16	1.27
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	16	1.27
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	16	1.27
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	9	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	9	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	9	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	9	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	9	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	9	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	14	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	14	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	14	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	14	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	14	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	14	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	20	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	20	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	20	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	20	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	20	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	20	1.26
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	24	1.25
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	24	1.25
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	24	1.25
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	24	1.25
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	24	1.25
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	24	1.25
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	36	1.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	36	1.24
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	36	1.24
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	38	1.23
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	38	1.23
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	38	1.23
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	13	1.23
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	14	1.23
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	33	1.22
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	33	1.22
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	33	1.22
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	33	1.22
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	33	1.22
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	33	1.22
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	11	1.22
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	11	1.22
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	11	1.22
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	35	1.22
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	10	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	10	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	10	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	10	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	10	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	10	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	17	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	17	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	17	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	17	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	17	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	17	1.21
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	19	1.21
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	19	1.21
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	19	1.21
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	18	1.2
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	18	1.2
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	18	1.2
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	18	1.2
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	18	1.2
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	18	1.2
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	39	1.2
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	39	1.2
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	39	1.2
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	33	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	15	1.2
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	30	1.19
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	30	1.19
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	30	1.19
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	30	1.19
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	30	1.19
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	30	1.19
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	34	1.19
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	34	1.19
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	34	1.19
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	37	1.19
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	37	1.19
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	37	1.19
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	15	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	15	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	15	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	15	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	15	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	15	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	26	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	26	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	26	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	26	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	26	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	26	1.18
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	32	1.18
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	32	1.18
(1,1822)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	32	1.18
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	2	1.18
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	27	1.17
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	27	1.17
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	27	1.17
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	27	1.17
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	27	1.17
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	27	1.17
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	26	1.17
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	3	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	3	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	3	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	3	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	3	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	3	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	6	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	6	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	6	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	6	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	6	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	6	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	23	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	23	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	23	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	23	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	23	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	23	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	31	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	31	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	31	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	31	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	31	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	31	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	35	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	35	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	35	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	35	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	35	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	35	1.16
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	6	1.16
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	5	1.15
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	5	1.15
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	5	1.15
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	5	1.15
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	5	1.15
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	5	1.15
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	17	1.15
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	25	1.14
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	37	1.14
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	4	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	4	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	4	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	4	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	4	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	4	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	7	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	7	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	7	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	7	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	7	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	7	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	8	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	8	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	8	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	8	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	8	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	8	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	12	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	12	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	12	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	12	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	12	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	12	1.13
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	8	1.13
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	11	1.13
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	39	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	39	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	39	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	39	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	39	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	39	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	40	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	40	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	40	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	40	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	40	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	40	1.12
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	14	1.12
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	21	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	21	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	21	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	21	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	21	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	21	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	34	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	34	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	34	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	34	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	34	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	34	1.11
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	16	1.11
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	16	1.11
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	16	1.11
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	12	1.11
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	19	1.11
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	23	1.11
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	25	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	25	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	25	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	25	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	25	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	25	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	36	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	36	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	36	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	36	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	36	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	36	1.1
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	29	1.1
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	29	1.1
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	29	1.1
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	31	1.1
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	21	1.1
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	19	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	19	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	19	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	19	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	19	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	19	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	37	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	37	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	37	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	37	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	37	1.09
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	37	1.09
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	14	1.09
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	14	1.09
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	14	1.09
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	5	1.09
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	24	1.09
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	18	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	22	1.08
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	22	1.08
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	22	1.08
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	22	1.08
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	22	1.08
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	22	1.08
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	20	1.08
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	20	1.08
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	20	1.08
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	18	1.08
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	2	1.08
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	16	1.08
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	28	1.08
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	19	1.08
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	32	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	32	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	32	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	32	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	32	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	32	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	38	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	38	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	38	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD21	38	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD22	38	1.07
(1,2036)	1:30:A:GLN:HE21	1:121:A:LEU:HD23	38	1.07
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	24	1.07
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	24	1.07
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	24	1.07
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	10	1.07
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	26	1.07
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	7	1.06
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	20	1.05
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	24	1.05
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	9	1.04
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	9	1.04
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	9	1.04
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	28	1.04
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	38	1.04
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	20	1.04
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	35	1.04
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	19	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	22	1.03
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	19	1.03
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	22	1.03
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	32	1.03
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	33	1.03
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	5	1.02
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	31	1.02
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	32	1.02
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	34	1.02
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	10	1.01
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	31	1.01
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	9	1.0
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	18	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	18	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	18	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	26	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	26	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	26	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	30	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	30	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	30	0.99
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	29	0.99
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	39	0.98
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	39	0.98
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	39	0.98
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	1	0.98
(1,173)	1:42:A:ASP:H	1:43:A:GLN:HE21	40	0.98
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	17	0.98
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	10	0.97
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	10	0.97
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	10	0.97
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	15	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	15	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	15	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	33	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	33	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	33	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	35	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	35	0.96
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	35	0.96
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	16	0.96
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	25	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	17	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	17	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	17	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	27	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	27	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	27	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	31	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	31	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	31	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	34	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	34	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	34	0.95
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	3	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	3	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	3	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	6	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	6	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	6	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	8	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	8	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	8	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	23	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	23	0.94
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	23	0.94
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	8	0.94
(1,2106)	1:42:A:ASP:HB2	1:43:A:GLN:HE21	6	0.93
(1,2106)	1:42:A:ASP:HB3	1:43:A:GLN:HE21	6	0.93
(1,2106)	1:42:A:ASP:HB2	1:43:A:GLN:HE21	14	0.93
(1,2106)	1:42:A:ASP:HB3	1:43:A:GLN:HE21	14	0.93
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	37	0.93
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	37	0.93
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	37	0.93
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	24	0.93
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	4	0.92
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	4	0.92
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	4	0.92
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	36	0.92
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	36	0.92
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	36	0.92
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	40	0.92
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	7	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	7	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	12	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	12	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	12	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	19	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	19	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	19	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	40	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	40	0.91
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	40	0.91
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	1	0.91
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	39	0.91
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	24	0.9
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	25	0.9
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	15	0.9
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	5	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	5	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	5	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	21	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	21	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	21	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	32	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	32	0.89
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	32	0.89
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	12	0.89
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	14	0.89
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	6	0.88
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	9	0.88
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	25	0.87
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	25	0.87
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	25	0.87
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	28	0.87
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	15	0.87
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	35	0.87
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	8	0.87
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	11	0.87
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	38	0.86
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	38	0.86
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	38	0.86
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	35	0.86
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	20	0.86
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	3	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	4	0.85
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	6	0.85
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	19	0.85
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	27	0.85
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	32	0.85
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	40	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	3	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	16	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	21	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	22	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	23	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	26	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	34	0.84
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	37	0.84
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	3	0.84
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	21	0.83
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	25	0.83
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	40	0.83
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	11	0.83
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	40	0.83
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	21	0.83
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	29	0.83
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	6	0.82
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	38	0.82
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	30	0.82
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	33	0.82
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	36	0.82
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	6	0.82
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	12	0.81
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	15	0.81
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	4	0.81
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	13	0.81
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	17	0.81
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	31	0.81
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	10	0.81
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	18	0.81
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	39	0.81
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	3	0.8
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	7	0.8
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	27	0.8
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	31	0.8
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	34	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	14	0.8
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	8	0.8
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	20	0.8
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	28	0.8
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	34	0.8
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD11	22	0.79
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD12	22	0.79
(1,1626)	1:30:A:GLN:HE21	1:121:A:LEU:HD13	22	0.79
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	18	0.79
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	23	0.79
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	26	0.79
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	30	0.79
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	37	0.79
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	29	0.79
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	34	0.79
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	37	0.79
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	29	0.79
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	16	0.79
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	27	0.79
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	8	0.78
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	32	0.78
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	36	0.78
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	6	0.78
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	32	0.78
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	36	0.78
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	10	0.78
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	30	0.78
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	35	0.78
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	37	0.78
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	9	0.77
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	5	0.77
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	7	0.77
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	18	0.77
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	7	0.77
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	39	0.76
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	2	0.76
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	39	0.76
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	24	0.75
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	35	0.75
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	38	0.75
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	19	0.74
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	18	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	38	0.73
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	5	0.72
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	12	0.72
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	23	0.72
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	12	0.72
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	17	0.72
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	26	0.72
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	14	0.71
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	22	0.71
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	2	0.71
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	10	0.71
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	15	0.71
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	3	0.71
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	7	0.71
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	18	0.71
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	3	0.71
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	13	0.71
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	7	0.7
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	30	0.7
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	35	0.7
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	1	0.7
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	19	0.7
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	22	0.7
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	25	0.7
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	33	0.7
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	36	0.7
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	34	0.7
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	17	0.69
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	19	0.69
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	27	0.69
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	40	0.69
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	4	0.68
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	8	0.68
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	8	0.68
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	15	0.68
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	28	0.68
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	39	0.68
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	20	0.67
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	1	0.67
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	5	0.67
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	11	0.67
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	21	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	37	0.67
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	2	0.67
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	21	0.67
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	29	0.67
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	32	0.67
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	9	0.67
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	25	0.67
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	9	0.66
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	16	0.66
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	12	0.66
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	36	0.65
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	10	0.65
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	14	0.65
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	1	0.65
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	22	0.64
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	33	0.64
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	4	0.64
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	5	0.64
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	30	0.64
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	10	0.63
(1,667)	1:38:A:SER:HG	1:43:A:GLN:HE22	38	0.62
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	20	0.62
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	23	0.62
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	27	0.62
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	31	0.62
(1,521)	1:114:A:ASN:H	1:114:A:ASN:HD21	24	0.62
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	39	0.61
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	11	0.6
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	14	0.6
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	23	0.6
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	33	0.6
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	6	0.59
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	16	0.59
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	25	0.59
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	33	0.58
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	33	0.58
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	33	0.58
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	26	0.58
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	32	0.57
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	32	0.57
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	32	0.57
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	31	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	22	0.56
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	22	0.56
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	22	0.56
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	34	0.56
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	24	0.56
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	32	0.56
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	37	0.55
(1,662)	1:113:A:ASN:HD21	1:114:A:ASN:H	13	0.55
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	33	0.54
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	10	0.54
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	26	0.54
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	6	0.53
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	32	0.53
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	40	0.53
(1,802)	1:13:A:PHE:HE1	1:37:A:ASN:HD22	9	0.53
(1,802)	1:13:A:PHE:HE2	1:37:A:ASN:HD22	9	0.53
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	13	0.53
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	30	0.53
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	21	0.52
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	21	0.52
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	21	0.52
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	4	0.52
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	10	0.52
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	21	0.52
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	36	0.52
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	38	0.52
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	32	0.52
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	4	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	4	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	4	0.52
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	6	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	6	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	6	0.52
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	10	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	10	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	10	0.52
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	11	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	11	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	11	0.52
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	12	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	12	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	12	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	18	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	18	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	18	0.52
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	24	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	24	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	24	0.52
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	30	0.52
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	30	0.52
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	30	0.52
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	9	0.52
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	28	0.52
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	10	0.52
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	11	0.52
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	18	0.52
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	23	0.52
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	35	0.52
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	28	0.52
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	10	0.51
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	10	0.51
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	10	0.51
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	1	0.51
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	5	0.51
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	7	0.51
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	11	0.51
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	22	0.51
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	34	0.51
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	8	0.51
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	31	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	1	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	1	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	1	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	2	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	2	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	2	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	5	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	5	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	5	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	7	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	7	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	7	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	21	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	21	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	21	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	22	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	22	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	22	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	23	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	23	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	23	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	29	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	29	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	29	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	32	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	32	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	32	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	33	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	33	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	33	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	34	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	34	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	34	0.51
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	38	0.51
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	38	0.51
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	38	0.51
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	2	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	2	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	4	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	5	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	6	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	8	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	12	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	13	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	14	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	15	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	17	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	20	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	21	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	27	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	29	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	30	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	37	0.51
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	40	0.51
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	27	0.51
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	30	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	15	0.5
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	18	0.5
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	29	0.5
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	2	0.5
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	15	0.5
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	18	0.5
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	25	0.5
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	33	0.5
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	36	0.5
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	40	0.5
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	16	0.5
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	16	0.5
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	16	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	1	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	7	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	9	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	16	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	19	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	22	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	24	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	26	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	28	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	31	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	32	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	33	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	34	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	36	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	38	0.5
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	39	0.5
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	13	0.49
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	23	0.49
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	27	0.49
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	11	0.49
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	21	0.49
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	36	0.49
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	36	0.49
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	36	0.49
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	13	0.49
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	17	0.49
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	10	0.48
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	10	0.48
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	38	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	4	0.48
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	4	0.48
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	4	0.48
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	34	0.48
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	34	0.48
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	34	0.48
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	20	0.48
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	20	0.48
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	20	0.48
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	31	0.48
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	16	0.48
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	20	0.48
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	23	0.48
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	35	0.48
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	22	0.48
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	13	0.48
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	5	0.48
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	8	0.48
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	20	0.48
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	35	0.48
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	20	0.47
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	20	0.47
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	2	0.47
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	13	0.47
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	17	0.47
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	28	0.47
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	29	0.47
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	39	0.47
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	9	0.47
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	9	0.47
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	28	0.47
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	29	0.47
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	1	0.47
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	29	0.47
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	2	0.47
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	24	0.47
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	5	0.46
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	5	0.46
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	14	0.46
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	14	0.46
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	15	0.46
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	15	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	35	0.46
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	35	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	3	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	4	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	8	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	16	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	20	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	21	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	26	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	33	0.46
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	36	0.46
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	14	0.46
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	14	0.46
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	14	0.46
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	37	0.46
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	12	0.46
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	22	0.46
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	27	0.46
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	39	0.46
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	17	0.46
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	3	0.46
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	9	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	9	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	16	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	16	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	18	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	18	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	22	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	22	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	24	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	24	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	27	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	27	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	29	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	29	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	30	0.45
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	30	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	6	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	11	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	15	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	23	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	25	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	27	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	30	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	32	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	35	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	37	0.45
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	40	0.45
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	2	0.45
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	2	0.45
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	2	0.45
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	26	0.45
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	26	0.45
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	26	0.45
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	20	0.45
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	28	0.45
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	14	0.45
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	7	0.45
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	19	0.45
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	33	0.45
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	12	0.45
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	17	0.45
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	19	0.45
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	23	0.45
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	37	0.45
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	3	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	3	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	6	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	6	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	7	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	7	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	8	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	8	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	17	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	17	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	21	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	21	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	23	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	23	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	26	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	26	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	31	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	31	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	33	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	33	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	34	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	34	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	36	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	36	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	37	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	37	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	38	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	38	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	39	0.44
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	39	0.44
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	12	0.44
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	14	0.44
(1,1851)	1:114:A:ASN:HB2	1:114:A:ASN:HD21	34	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	11	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	11	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	11	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	23	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	23	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	23	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	35	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	35	0.44
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	35	0.44
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	2	0.44
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	12	0.44
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	24	0.44
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	25	0.44
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	26	0.44
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	3	0.44
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	5	0.44
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	38	0.44
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	15	0.44
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	15	0.44
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	15	0.44
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	36	0.44
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	4	0.43
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	4	0.43
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	12	0.43
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	12	0.43
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	36	0.43
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	36	0.43
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	36	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	16	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	16	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	16	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	33	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	33	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	33	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	40	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	40	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	40	0.43
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	4	0.43
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	14	0.43
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	27	0.43
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	27	0.43
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	27	0.43
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	37	0.43
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	37	0.43
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	37	0.43
(1,177)	1:43:A:GLN:H	1:43:A:GLN:HE21	25	0.43
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	4	0.43
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	22	0.43
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	40	0.43
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	2	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	2	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	2	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	12	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	12	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	12	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	25	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	25	0.42
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	25	0.42
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	30	0.42
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	19	0.42
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	35	0.42
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	17	0.42
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	9	0.42
(1,504)	1:110:A:ASN:H	1:113:A:ASN:HD21	4	0.42
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	9	0.42
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	15	0.42
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	18	0.42
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	32	0.41
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	32	0.41
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	11	0.41
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	11	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	15	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	15	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	15	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	21	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	21	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	21	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	30	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	30	0.41
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	30	0.41
(1,1022)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	16	0.41
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	3	0.41
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	8	0.41
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	17	0.41
(1,1021)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	39	0.41
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	33	0.41
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	24	0.41
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	40	0.41
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	40	0.41
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	40	0.41
(1,671)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	11	0.41
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	21	0.41
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	40	0.4
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	40	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	6	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	6	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	6	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	38	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	38	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	38	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	27	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	27	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	27	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	28	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	28	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	28	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	32	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	32	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	32	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	39	0.4
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	39	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	39	0.4
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	17	0.4
(1,802)	1:13:A:PHE:HE1	1:37:A:ASN:HD22	28	0.4
(1,802)	1:13:A:PHE:HE2	1:37:A:ASN:HD22	28	0.4
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	7	0.4
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	5	0.39
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	5	0.39
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	5	0.39
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	8	0.39
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	8	0.39
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	8	0.39
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	1	0.39
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	29	0.39
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	7	0.39
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	18	0.39
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	35	0.39
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	10	0.39
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	29	0.39
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	38	0.39
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	18	0.38
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	18	0.38
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	18	0.38
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	3	0.38
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	3	0.38
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	3	0.38
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	4	0.38
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	4	0.38
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	4	0.38
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	10	0.38
(1,802)	1:13:A:PHE:HE1	1:37:A:ASN:HD22	20	0.38
(1,802)	1:13:A:PHE:HE2	1:37:A:ASN:HD22	20	0.38
(1,768)	1:110:A:ASN:HB3	1:113:A:ASN:HD21	1	0.38
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	9	0.38
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	9	0.38
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	9	0.38
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	1	0.38
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	11	0.38
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	11	0.37
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	11	0.37
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	19	0.37
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	19	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	13	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	13	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	13	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	17	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	17	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	17	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	37	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	37	0.37
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	37	0.37
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	24	0.37
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	12	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	12	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	12	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	15	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	15	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	15	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	23	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	23	0.36
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	23	0.36
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	29	0.36
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	29	0.36
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	29	0.36
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	38	0.36
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	38	0.36
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	38	0.36
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	9	0.36
(1,802)	1:13:A:PHE:HE1	1:37:A:ASN:HD22	16	0.36
(1,802)	1:13:A:PHE:HE2	1:37:A:ASN:HD22	16	0.36
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	5	0.36
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	25	0.35
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	25	0.35
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	6	0.35
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	6	0.35
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	6	0.35
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	34	0.35
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	34	0.35
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	34	0.35
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	9	0.35
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	1	0.35
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	12	0.35
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB1	36	0.34
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB2	36	0.34
(1,1514)	1:114:A:ASN:HD22	1:115:A:ALA:HB3	36	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	10	0.34
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	24	0.34
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	4	0.34
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	13	0.34
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	17	0.34
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	13	0.34
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	23	0.34
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	25	0.34
(1,2106)	1:42:A:ASP:HB2	1:43:A:GLN:HE21	33	0.33
(1,2106)	1:42:A:ASP:HB3	1:43:A:GLN:HE21	33	0.33
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	28	0.33
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	28	0.33
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	7	0.33
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	7	0.33
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	7	0.33
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	18	0.33
(1,674)	1:36:A:THR:HG21	1:37:A:ASN:HD21	13	0.33
(1,674)	1:36:A:THR:HG22	1:37:A:ASN:HD21	13	0.33
(1,674)	1:36:A:THR:HG23	1:37:A:ASN:HD21	13	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	2	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	8	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	14	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	30	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	34	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	36	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	37	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	38	0.33
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	39	0.33
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	16	0.33
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	37	0.32
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	37	0.32
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	37	0.32
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	24	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	6	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	11	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	12	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	20	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	21	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	23	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	28	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	29	0.32
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	35	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	40	0.32
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	2	0.32
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	16	0.32
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	26	0.32
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	29	0.32
(1,154)	1:39:A:SER:H	1:43:A:GLN:HE21	16	0.32
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	2	0.32
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	37	0.32
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	16	0.31
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	16	0.31
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	25	0.31
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	27	0.31
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	33	0.31
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	20	0.31
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	28	0.31
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	20	0.31
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	30	0.31
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	2	0.3
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	2	0.3
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	13	0.3
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	13	0.3
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	7	0.3
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	3	0.3
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	15	0.3
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	26	0.3
(1,673)	1:114:A:ASN:HA	1:114:A:ASN:HD21	32	0.3
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	6	0.3
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	37	0.3
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	37	0.3
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	37	0.3
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	3	0.3
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	15	0.3
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	27	0.3
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	28	0.3
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	30	0.29
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	30	0.29
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	30	0.29
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	11	0.29
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	20	0.29
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	14	0.29
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	14	0.29
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	14	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	14	0.29
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	14	0.29
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	14	0.29
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	14	0.29
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	14	0.29
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	14	0.29
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	8	0.29
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	11	0.29
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	21	0.29
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	30	0.29
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	27	0.28
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	27	0.28
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	27	0.28
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	23	0.28
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	23	0.28
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	23	0.28
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	23	0.28
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	23	0.28
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	23	0.28
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	23	0.28
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	23	0.28
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	23	0.28
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	34	0.28
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	34	0.28
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	34	0.28
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	38	0.28
(1,2021)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	1	0.27
(1,2021)	1:27:A:PRO:HB3	1:30:A:GLN:HE22	1	0.27
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	31	0.27
(1,1119)	1:54:A:ILE:HD11	1:62:A:LYS:HE2	35	0.27
(1,1119)	1:54:A:ILE:HD11	1:62:A:LYS:HE3	35	0.27
(1,1119)	1:54:A:ILE:HD12	1:62:A:LYS:HE2	35	0.27
(1,1119)	1:54:A:ILE:HD12	1:62:A:LYS:HE3	35	0.27
(1,1119)	1:54:A:ILE:HD13	1:62:A:LYS:HE2	35	0.27
(1,1119)	1:54:A:ILE:HD13	1:62:A:LYS:HE3	35	0.27
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	19	0.27
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	24	0.27
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	14	0.27
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	17	0.27
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	33	0.27
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	9	0.27
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	32	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	32	0.26
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	33	0.26
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	33	0.26
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	14	0.26
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	31	0.26
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	5	0.26
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	5	0.26
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	5	0.26
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	6	0.26
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	25	0.26
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	18	0.25
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	18	0.25
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	18	0.25
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	18	0.25
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	18	0.25
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	18	0.25
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	5	0.25
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	33	0.25
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	33	0.25
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	33	0.25
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	33	0.25
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	33	0.25
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	33	0.25
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	33	0.25
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	33	0.25
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	33	0.25
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	18	0.25
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	3	0.25
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	3	0.25
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	3	0.25
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	17	0.25
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	17	0.25
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	17	0.25
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	4	0.25
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	39	0.25
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	40	0.25
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	6	0.24
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	6	0.24
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	40	0.24
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	40	0.24
(1,1480)	1:109:A:ARG:HG2	1:114:A:ASN:HD22	5	0.24
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	4	0.24
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	4	0.24
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	38	0.24
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	38	0.24
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	38	0.24
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	12	0.24
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	37	0.24
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	21	0.23
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	21	0.23
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	36	0.23
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	36	0.23
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	22	0.23
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	7	0.23
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	7	0.23
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	7	0.23
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	33	0.23
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	33	0.23
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	33	0.23
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	35	0.23
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	35	0.23
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	35	0.23
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	36	0.23
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	36	0.23
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	36	0.23
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	26	0.23
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	1	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	1	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	4	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	4	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	5	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	5	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	10	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	10	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	11	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	11	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	22	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	22	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	34	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	34	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	38	0.22
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	38	0.22
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	24	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	24	0.22
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	24	0.22
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	16	0.22
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	16	0.22
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	16	0.22
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	16	0.22
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	16	0.22
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	16	0.22
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	11	0.22
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	11	0.22
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	11	0.22
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	11	0.22
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	11	0.22
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	11	0.22
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	11	0.22
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	11	0.22
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	11	0.22
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	18	0.22
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	18	0.22
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	18	0.22
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	18	0.22
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	18	0.22
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	18	0.22
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	18	0.22
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	18	0.22
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	18	0.22
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	22	0.22
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	25	0.22
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	32	0.22
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	36	0.22
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	7	0.21
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	7	0.21
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	15	0.21
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	15	0.21
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	18	0.21
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	18	0.21
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD11	35	0.21
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD12	35	0.21
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD13	35	0.21
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD21	35	0.21
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD22	35	0.21
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD23	35	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD11	35	0.21
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD12	35	0.21
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD13	35	0.21
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD21	35	0.21
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD22	35	0.21
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD23	35	0.21
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	1	0.21
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	1	0.21
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	1	0.21
(1,1388)	1:108:A:THR:HG21	1:109:A:ARG:H	30	0.21
(1,1388)	1:108:A:THR:HG22	1:109:A:ARG:H	30	0.21
(1,1388)	1:108:A:THR:HG23	1:109:A:ARG:H	30	0.21
(1,802)	1:13:A:PHE:HE1	1:37:A:ASN:HD22	25	0.21
(1,802)	1:13:A:PHE:HE2	1:37:A:ASN:HD22	25	0.21
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	11	0.21
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	15	0.21
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	19	0.21
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	21	0.21
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	26	0.21
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	35	0.21
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	36	0.21
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	13	0.2
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	13	0.2
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	23	0.2
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	23	0.2
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	27	0.2
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	27	0.2
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	29	0.2
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	29	0.2
(1,1092)	1:49:A:ARG:H	1:50:A:ALA:HB1	28	0.2
(1,1092)	1:49:A:ARG:H	1:50:A:ALA:HB2	28	0.2
(1,1092)	1:49:A:ARG:H	1:50:A:ALA:HB3	28	0.2
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	14	0.2
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	14	0.2
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	14	0.2
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	14	0.2
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	14	0.2
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	14	0.2
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	18	0.2
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	18	0.2
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	18	0.2
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	18	0.2
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	18	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	10	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	10	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	10	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	10	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	10	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	10	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	10	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	10	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	10	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	18	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	18	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	18	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	18	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	18	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	18	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	18	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	18	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	18	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	25	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	25	0.2
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	25	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	25	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	25	0.2
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	25	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	25	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	25	0.2
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	25	0.2
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	12	0.2
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	12	0.2
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	12	0.2
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	12	0.2
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	12	0.2
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	12	0.2
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	12	0.2
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	12	0.2
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	12	0.2
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	5	0.2
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	20	0.2
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	34	0.2
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	9	0.19
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	14	0.19
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	14	0.19
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG21	28	0.19
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG22	28	0.19
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG23	28	0.19
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG21	28	0.19
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG22	28	0.19
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG23	28	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	15	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	15	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	15	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	15	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	15	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	15	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	20	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	20	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	20	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	20	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	20	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	20	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	25	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	25	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	25	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	25	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	25	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	25	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	28	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	28	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	28	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	28	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	28	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	28	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	35	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	35	0.19
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	35	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	35	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	35	0.19
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	35	0.19
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	15	0.19
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	18	0.19
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	30	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	39	0.19
(1,709)	1:12:A:TRP:HZ3	1:114:A:ASN:HD22	22	0.19
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	16	0.19
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	34	0.19
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	32	0.19
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	18	0.19
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	37	0.18
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	37	0.18
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD11	28	0.18
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD12	28	0.18
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD13	28	0.18
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	11	0.18
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	11	0.18
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	11	0.18
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	11	0.18
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	11	0.18
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	11	0.18
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	16	0.18
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	16	0.18
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	16	0.18
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	16	0.18
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	16	0.18
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	16	0.18
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	8	0.18
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	23	0.18
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	27	0.18
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	36	0.18
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	37	0.18
(1,802)	1:13:A:PHE:HE1	1:37:A:ASN:HD22	26	0.18
(1,802)	1:13:A:PHE:HE2	1:37:A:ASN:HD22	26	0.18
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	2	0.18
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	24	0.18
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	28	0.18
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	33	0.18
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	37	0.18
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	40	0.18
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	23	0.18
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB1	18	0.18
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB2	18	0.18
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB3	18	0.18
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	2	0.17
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	12	0.17
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	12	0.17
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	24	0.17
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	24	0.17
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	31	0.17
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	31	0.17
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	35	0.17
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	35	0.17
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	30	0.17
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	30	0.17
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	30	0.17
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	30	0.17
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	30	0.17
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	30	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	3	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	3	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	3	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	3	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	3	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	3	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	5	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	5	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	5	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	5	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	5	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	5	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	10	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	10	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	10	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	10	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	10	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	10	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	21	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	21	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	21	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	21	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	21	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	21	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	31	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	31	0.17
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	31	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	31	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	31	0.17
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	31	0.17
(1,1056)	1:44:A:ILE:HD11	1:73:A:LEU:HG	31	0.17
(1,1056)	1:44:A:ILE:HD12	1:73:A:LEU:HG	31	0.17
(1,1056)	1:44:A:ILE:HD13	1:73:A:LEU:HG	31	0.17
(1,1056)	1:44:A:ILE:HD11	1:73:A:LEU:HG	35	0.17
(1,1056)	1:44:A:ILE:HD12	1:73:A:LEU:HG	35	0.17
(1,1056)	1:44:A:ILE:HD13	1:73:A:LEU:HG	35	0.17
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	3	0.17
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	6	0.17
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	7	0.17
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	26	0.17
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	31	0.17
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	34	0.17
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	35	0.17
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	8	0.17
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	10	0.17
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	12	0.17
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	26	0.17
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	26	0.17
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	26	0.17
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	13	0.17
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	3	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	3	0.16
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	8	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	8	0.16
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	17	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	17	0.16
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	19	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	19	0.16
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	20	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	20	0.16
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	25	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	25	0.16
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	28	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	28	0.16
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	30	0.16
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	30	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD11	18	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD12	18	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD13	18	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD21	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD22	18	0.16
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD23	18	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD11	18	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD12	18	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD13	18	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD21	18	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD22	18	0.16
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD23	18	0.16
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD11	10	0.16
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD12	10	0.16
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD13	10	0.16
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD11	16	0.16
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD12	16	0.16
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD13	16	0.16
(1,1110)	1:54:A:ILE:HG21	1:55:A:ARG:H	18	0.16
(1,1110)	1:54:A:ILE:HG22	1:55:A:ARG:H	18	0.16
(1,1110)	1:54:A:ILE:HG23	1:55:A:ARG:H	18	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	8	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	8	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	8	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	8	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	8	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	8	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	12	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	12	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	12	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	12	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	12	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	12	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	26	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	26	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	26	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	26	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	26	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	26	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	33	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	33	0.16
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	33	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	33	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	33	0.16
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	33	0.16
(1,1056)	1:44:A:ILE:HD11	1:73:A:LEU:HG	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:44:A:ILE:HD12	1:73:A:LEU:HG	16	0.16
(1,1056)	1:44:A:ILE:HD13	1:73:A:LEU:HG	16	0.16
(1,1056)	1:44:A:ILE:HD11	1:73:A:LEU:HG	21	0.16
(1,1056)	1:44:A:ILE:HD12	1:73:A:LEU:HG	21	0.16
(1,1056)	1:44:A:ILE:HD13	1:73:A:LEU:HG	21	0.16
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	21	0.16
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	38	0.16
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	26	0.16
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	26	0.16
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	26	0.16
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	26	0.16
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	26	0.16
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	26	0.16
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	26	0.16
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	26	0.16
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	26	0.16
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	30	0.16
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	30	0.16
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	30	0.16
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	30	0.16
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	30	0.16
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	30	0.16
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	30	0.16
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	30	0.16
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	30	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	4	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	7	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	14	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	17	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	23	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	27	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	29	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	30	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	38	0.16
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	39	0.16
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	28	0.16
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	28	0.16
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	28	0.16
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	1	0.16
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	31	0.16
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	36	0.16
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG2	30	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG3	30	0.15
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG2	30	0.15
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG3	30	0.15
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG2	30	0.15
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG3	30	0.15
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	10	0.15
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	10	0.15
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	10	0.15
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	10	0.15
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	10	0.15
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	10	0.15
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	28	0.15
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	28	0.15
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	28	0.15
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	28	0.15
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	28	0.15
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	28	0.15
(1,2152)	1:53:A:ARG:HD2	1:54:A:ILE:H	23	0.15
(1,2152)	1:53:A:ARG:HD3	1:54:A:ILE:H	23	0.15
(1,2106)	1:42:A:ASP:HB2	1:43:A:GLN:HE21	25	0.15
(1,2106)	1:42:A:ASP:HB3	1:43:A:GLN:HE21	25	0.15
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	16	0.15
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	16	0.15
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	26	0.15
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	26	0.15
(1,2085)	1:37:A:ASN:HB2	1:37:A:ASN:HD21	39	0.15
(1,2085)	1:37:A:ASN:HB3	1:37:A:ASN:HD21	39	0.15
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD2	35	0.15
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD3	35	0.15
(1,1119)	1:54:A:ILE:HD11	1:62:A:LYS:HE2	18	0.15
(1,1119)	1:54:A:ILE:HD11	1:62:A:LYS:HE3	18	0.15
(1,1119)	1:54:A:ILE:HD12	1:62:A:LYS:HE2	18	0.15
(1,1119)	1:54:A:ILE:HD12	1:62:A:LYS:HE3	18	0.15
(1,1119)	1:54:A:ILE:HD13	1:62:A:LYS:HE2	18	0.15
(1,1119)	1:54:A:ILE:HD13	1:62:A:LYS:HE3	18	0.15
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	20	0.15
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	20	0.15
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	20	0.15
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	20	0.15
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	20	0.15
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	20	0.15
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	23	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	23	0.15
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	23	0.15
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	23	0.15
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	23	0.15
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	23	0.15
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	27	0.15
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	27	0.15
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	27	0.15
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	27	0.15
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	27	0.15
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	27	0.15
(1,1056)	1:44:A:ILE:HD11	1:73:A:LEU:HG	2	0.15
(1,1056)	1:44:A:ILE:HD12	1:73:A:LEU:HG	2	0.15
(1,1056)	1:44:A:ILE:HD13	1:73:A:LEU:HG	2	0.15
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	12	0.15
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	18	0.15
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	18	0.15
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	18	0.15
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	24	0.15
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	24	0.15
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	24	0.15
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	25	0.15
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	25	0.15
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	25	0.15
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	29	0.15
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG2	3	0.14
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG3	3	0.14
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG2	3	0.14
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG3	3	0.14
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG2	3	0.14
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG3	3	0.14
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	11	0.14
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	11	0.14
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	11	0.14
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	11	0.14
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	11	0.14
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	11	0.14
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	25	0.14
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	25	0.14
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	25	0.14
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	25	0.14
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	25	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	25	0.14
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD11	28	0.14
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD12	28	0.14
(1,1814)	1:72:A:TYR:HA	1:106:A:ILE:HD13	28	0.14
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG21	1	0.14
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG22	1	0.14
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG23	1	0.14
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG21	1	0.14
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG22	1	0.14
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG23	1	0.14
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD11	20	0.14
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD12	20	0.14
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD13	20	0.14
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD11	20	0.14
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD12	20	0.14
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD13	20	0.14
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	6	0.14
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	6	0.14
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	6	0.14
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	6	0.14
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	6	0.14
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	6	0.14
(1,1053)	1:44:A:ILE:HD11	1:94:A:ALA:HB1	31	0.14
(1,1053)	1:44:A:ILE:HD11	1:94:A:ALA:HB2	31	0.14
(1,1053)	1:44:A:ILE:HD11	1:94:A:ALA:HB3	31	0.14
(1,1053)	1:44:A:ILE:HD12	1:94:A:ALA:HB1	31	0.14
(1,1053)	1:44:A:ILE:HD12	1:94:A:ALA:HB2	31	0.14
(1,1053)	1:44:A:ILE:HD12	1:94:A:ALA:HB3	31	0.14
(1,1053)	1:44:A:ILE:HD13	1:94:A:ALA:HB1	31	0.14
(1,1053)	1:44:A:ILE:HD13	1:94:A:ALA:HB2	31	0.14
(1,1053)	1:44:A:ILE:HD13	1:94:A:ALA:HB3	31	0.14
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	28	0.14
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	14	0.14
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	14	0.14
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	14	0.14
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	14	0.14
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	14	0.14
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	14	0.14
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	14	0.14
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	14	0.14
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	14	0.14
(1,704)	1:12:A:TRP:HE3	1:114:A:ASN:HD22	31	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	29	0.14
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	29	0.14
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	29	0.14
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	29	0.14
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	29	0.14
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	29	0.14
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	29	0.14
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	29	0.14
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	29	0.14
(1,525)	1:114:A:ASN:HD22	1:116:A:ALA:H	34	0.14
(1,272)	1:59:A:GLY:H	1:60:A:LYS:HB2	25	0.14
(1,272)	1:59:A:GLY:H	1:60:A:LYS:HB3	25	0.14
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	7	0.14
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	22	0.14
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	32	0.14
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	38	0.14
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	18	0.13
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	18	0.13
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	18	0.13
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	18	0.13
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	18	0.13
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	18	0.13
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	26	0.13
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	26	0.13
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	26	0.13
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	26	0.13
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	26	0.13
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	26	0.13
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	27	0.13
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	27	0.13
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	27	0.13
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	27	0.13
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	27	0.13
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	27	0.13
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	35	0.13
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	35	0.13
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	35	0.13
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	35	0.13
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	35	0.13
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	35	0.13
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	40	0.13
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	40	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	40	0.13
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	40	0.13
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	40	0.13
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	40	0.13
(1,1957)	1:15:A:ALA:HB1	1:67:A:ARG:HD2	20	0.13
(1,1957)	1:15:A:ALA:HB1	1:67:A:ARG:HD3	20	0.13
(1,1957)	1:15:A:ALA:HB2	1:67:A:ARG:HD2	20	0.13
(1,1957)	1:15:A:ALA:HB2	1:67:A:ARG:HD3	20	0.13
(1,1957)	1:15:A:ALA:HB3	1:67:A:ARG:HD2	20	0.13
(1,1957)	1:15:A:ALA:HB3	1:67:A:ARG:HD3	20	0.13
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG21	2	0.13
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG22	2	0.13
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG23	2	0.13
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG21	2	0.13
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG22	2	0.13
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG23	2	0.13
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD11	31	0.13
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD12	31	0.13
(1,1460)	1:72:A:TYR:HE1	1:106:A:ILE:HD13	31	0.13
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD11	31	0.13
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD12	31	0.13
(1,1460)	1:72:A:TYR:HE2	1:106:A:ILE:HD13	31	0.13
(1,1142)	1:62:A:LYS:HA	1:62:A:LYS:HD2	15	0.13
(1,1142)	1:62:A:LYS:HA	1:62:A:LYS:HD3	15	0.13
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	13	0.13
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	13	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	13	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	13	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	13	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	13	0.13
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	25	0.13
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	25	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	25	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	25	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	25	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	25	0.13
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	26	0.13
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	26	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	26	0.13
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	26	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	26	0.13
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	26	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	1	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	1	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	1	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	1	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	1	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	1	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	29	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	29	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	29	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	29	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	29	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	29	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	30	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	30	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	30	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	30	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	30	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	30	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	40	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	40	0.13
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	40	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	40	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	40	0.13
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	40	0.13
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	4	0.13
(1,917)	1:27:A:PRO:HB2	1:30:A:GLN:HE22	32	0.13
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	40	0.13
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	40	0.13
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	40	0.13
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	40	0.13
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	40	0.13
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	40	0.13
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	40	0.13
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	40	0.13
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	40	0.13
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	25	0.13
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	25	0.13
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	25	0.13
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	25	0.13
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	25	0.13
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	25	0.13
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	25	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	25	0.13
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	25	0.13
(1,690)	1:8:A:ASN:H	1:9:A:THR:HG21	27	0.13
(1,690)	1:8:A:ASN:H	1:9:A:THR:HG22	27	0.13
(1,690)	1:8:A:ASN:H	1:9:A:THR:HG23	27	0.13
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	3	0.13
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	15	0.13
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	15	0.13
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	15	0.13
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	15	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB1	10	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB2	10	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB3	10	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB1	14	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB2	14	0.13
(1,13)	1:9:A:THR:H	1:10:A:ALA:HB3	14	0.13
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG2	8	0.12
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG3	8	0.12
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG2	8	0.12
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG3	8	0.12
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG2	8	0.12
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG3	8	0.12
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG2	29	0.12
(1,2294)	1:101:A:THR:HG21	1:102:A:PRO:HG3	29	0.12
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG2	29	0.12
(1,2294)	1:101:A:THR:HG22	1:102:A:PRO:HG3	29	0.12
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG2	29	0.12
(1,2294)	1:101:A:THR:HG23	1:102:A:PRO:HG3	29	0.12
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	3	0.12
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	3	0.12
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	3	0.12
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	3	0.12
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	3	0.12
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	3	0.12
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	5	0.12
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	5	0.12
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	5	0.12
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	5	0.12
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	5	0.12
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	5	0.12
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	12	0.12
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	12	0.12
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	12	0.12
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	12	0.12
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	12	0.12
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	14	0.12
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	14	0.12
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	14	0.12
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	14	0.12
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	14	0.12
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	14	0.12
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	23	0.12
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	23	0.12
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	23	0.12
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	23	0.12
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	23	0.12
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	23	0.12
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	31	0.12
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	31	0.12
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	31	0.12
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	31	0.12
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	31	0.12
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	31	0.12
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD2	14	0.12
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD3	14	0.12
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD2	28	0.12
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD3	28	0.12
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD2	33	0.12
(1,1752)	1:60:A:LYS:HA	1:60:A:LYS:HD3	33	0.12
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG21	13	0.12
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG22	13	0.12
(1,1659)	1:27:A:PRO:HG2	1:125:A:THR:HG23	13	0.12
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG21	13	0.12
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG22	13	0.12
(1,1659)	1:27:A:PRO:HG3	1:125:A:THR:HG23	13	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD11	26	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD12	26	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD13	26	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD11	40	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD12	40	0.12
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD13	40	0.12
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	14	0.12
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	14	0.12
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	15	0.12
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	15	0.12
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	15	0.12
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	25	0.12
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	25	0.12
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	25	0.12
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	27	0.12
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	27	0.12
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	27	0.12
(1,1293)	1:87:A:LYS:HG2	1:90:A:ILE:HD11	14	0.12
(1,1293)	1:87:A:LYS:HG2	1:90:A:ILE:HD12	14	0.12
(1,1293)	1:87:A:LYS:HG2	1:90:A:ILE:HD13	14	0.12
(1,1126)	1:60:A:LYS:H	1:60:A:LYS:HB2	25	0.12
(1,1126)	1:60:A:LYS:H	1:60:A:LYS:HB3	25	0.12
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	14	0.12
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	14	0.12
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	14	0.12
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	14	0.12
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	14	0.12
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	14	0.12
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	31	0.12
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	31	0.12
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	31	0.12
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	31	0.12
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	31	0.12
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	31	0.12
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE2	40	0.12
(1,1108)	1:54:A:ILE:HG21	1:62:A:LYS:HE3	40	0.12
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE2	40	0.12
(1,1108)	1:54:A:ILE:HG22	1:62:A:LYS:HE3	40	0.12
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE2	40	0.12
(1,1108)	1:54:A:ILE:HG23	1:62:A:LYS:HE3	40	0.12
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	13	0.12
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	13	0.12
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	13	0.12
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	13	0.12
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	13	0.12
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	13	0.12
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	24	0.12
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	24	0.12
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	24	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	24	0.12
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	24	0.12
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	24	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	6	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	6	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	6	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	6	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	6	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	6	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	6	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	6	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	6	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	20	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	20	0.12
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	20	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	20	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	20	0.12
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	20	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	20	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	20	0.12
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	20	0.12
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	2	0.12
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	2	0.12
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	2	0.12
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	16	0.12
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	16	0.12
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	16	0.12
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	31	0.12
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	31	0.12
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	31	0.12
(1,272)	1:59:A:GLY:H	1:60:A:LYS:HB2	28	0.12
(1,272)	1:59:A:GLY:H	1:60:A:LYS:HB3	28	0.12
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	10	0.12
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	27	0.12
(1,2252)	1:81:A:LEU:HD11	1:85:A:ALA:HA	14	0.11
(1,2252)	1:81:A:LEU:HD12	1:85:A:ALA:HA	14	0.11
(1,2252)	1:81:A:LEU:HD13	1:85:A:ALA:HA	14	0.11
(1,2252)	1:81:A:LEU:HD21	1:85:A:ALA:HA	14	0.11
(1,2252)	1:81:A:LEU:HD22	1:85:A:ALA:HA	14	0.11
(1,2252)	1:81:A:LEU:HD23	1:85:A:ALA:HA	14	0.11
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	6	0.11
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	6	0.11
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	6	0.11
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	6	0.11
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	6	0.11
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	20	0.11
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	20	0.11
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	20	0.11
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	20	0.11
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	20	0.11
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	20	0.11
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	30	0.11
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	30	0.11
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	30	0.11
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	30	0.11
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	30	0.11
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	30	0.11
(1,2210)	1:73:A:LEU:HD11	1:92:A:TRP:HE3	3	0.11
(1,2210)	1:73:A:LEU:HD12	1:92:A:TRP:HE3	3	0.11
(1,2210)	1:73:A:LEU:HD13	1:92:A:TRP:HE3	3	0.11
(1,2210)	1:73:A:LEU:HD21	1:92:A:TRP:HE3	3	0.11
(1,2210)	1:73:A:LEU:HD22	1:92:A:TRP:HE3	3	0.11
(1,2210)	1:73:A:LEU:HD23	1:92:A:TRP:HE3	3	0.11
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD1	11	0.11
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD2	11	0.11
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD1	11	0.11
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD2	11	0.11
(1,2175)	1:64:A:LEU:H	1:64:A:LEU:HD11	29	0.11
(1,2175)	1:64:A:LEU:H	1:64:A:LEU:HD12	29	0.11
(1,2175)	1:64:A:LEU:H	1:64:A:LEU:HD13	29	0.11
(1,2175)	1:64:A:LEU:H	1:64:A:LEU:HD21	29	0.11
(1,2175)	1:64:A:LEU:H	1:64:A:LEU:HD22	29	0.11
(1,2175)	1:64:A:LEU:H	1:64:A:LEU:HD23	29	0.11
(1,1979)	1:16:A:LEU:HD11	1:134:A:GLU:H	3	0.11
(1,1979)	1:16:A:LEU:HD12	1:134:A:GLU:H	3	0.11
(1,1979)	1:16:A:LEU:HD13	1:134:A:GLU:H	3	0.11
(1,1979)	1:16:A:LEU:HD21	1:134:A:GLU:H	3	0.11
(1,1979)	1:16:A:LEU:HD22	1:134:A:GLU:H	3	0.11
(1,1979)	1:16:A:LEU:HD23	1:134:A:GLU:H	3	0.11
(1,1979)	1:16:A:LEU:HD11	1:134:A:GLU:H	27	0.11
(1,1979)	1:16:A:LEU:HD12	1:134:A:GLU:H	27	0.11
(1,1979)	1:16:A:LEU:HD13	1:134:A:GLU:H	27	0.11
(1,1979)	1:16:A:LEU:HD21	1:134:A:GLU:H	27	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1979)	1:16:A:LEU:HD22	1:134:A:GLU:H	27	0.11
(1,1979)	1:16:A:LEU:HD23	1:134:A:GLU:H	27	0.11
(1,1979)	1:16:A:LEU:HD11	1:134:A:GLU:H	35	0.11
(1,1979)	1:16:A:LEU:HD12	1:134:A:GLU:H	35	0.11
(1,1979)	1:16:A:LEU:HD13	1:134:A:GLU:H	35	0.11
(1,1979)	1:16:A:LEU:HD21	1:134:A:GLU:H	35	0.11
(1,1979)	1:16:A:LEU:HD22	1:134:A:GLU:H	35	0.11
(1,1979)	1:16:A:LEU:HD23	1:134:A:GLU:H	35	0.11
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD11	20	0.11
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD12	20	0.11
(1,1881)	1:16:A:LEU:HG	1:119:A:LEU:HD13	20	0.11
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG21	29	0.11
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG22	29	0.11
(1,1546)	1:37:A:ASN:HD21	1:117:A:ILE:HG23	29	0.11
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD11	28	0.11
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD12	28	0.11
(1,1453)	1:42:A:ASP:HB3	1:106:A:ILE:HD13	28	0.11
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	18	0.11
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	18	0.11
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	18	0.11
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	26	0.11
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	26	0.11
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	26	0.11
(1,1425)	1:101:A:THR:HG21	1:102:A:PRO:HB2	35	0.11
(1,1425)	1:101:A:THR:HG22	1:102:A:PRO:HB2	35	0.11
(1,1425)	1:101:A:THR:HG23	1:102:A:PRO:HB2	35	0.11
(1,1110)	1:54:A:ILE:HG21	1:55:A:ARG:H	16	0.11
(1,1110)	1:54:A:ILE:HG22	1:55:A:ARG:H	16	0.11
(1,1110)	1:54:A:ILE:HG23	1:55:A:ARG:H	16	0.11
(1,1104)	1:54:A:ILE:HG21	1:62:A:LYS:HG2	35	0.11
(1,1104)	1:54:A:ILE:HG21	1:62:A:LYS:HG3	35	0.11
(1,1104)	1:54:A:ILE:HG22	1:62:A:LYS:HG2	35	0.11
(1,1104)	1:54:A:ILE:HG22	1:62:A:LYS:HG3	35	0.11
(1,1104)	1:54:A:ILE:HG23	1:62:A:LYS:HG2	35	0.11
(1,1104)	1:54:A:ILE:HG23	1:62:A:LYS:HG3	35	0.11
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	2	0.11
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	2	0.11
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	2	0.11
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	2	0.11
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	2	0.11
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	2	0.11
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	7	0.11
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	7	0.11
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	7	0.11
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	7	0.11
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	7	0.11
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	10	0.11
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	10	0.11
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	10	0.11
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	11	0.11
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	11	0.11
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	11	0.11
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	15	0.11
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	15	0.11
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	15	0.11
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	18	0.11
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	18	0.11
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	18	0.11
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	8	0.11
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	8	0.11
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	8	0.11
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	8	0.11
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	8	0.11
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	8	0.11
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	8	0.11
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	8	0.11
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	8	0.11
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	17	0.11
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	17	0.11
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	17	0.11
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	17	0.11
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	17	0.11
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	17	0.11
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	17	0.11
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	17	0.11
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	17	0.11
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	7	0.11
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	7	0.11
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	7	0.11
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	7	0.11
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	7	0.11
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	7	0.11
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	7	0.11
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	7	0.11
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	16	0.11
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	16	0.11
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	16	0.11
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	16	0.11
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	16	0.11
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	16	0.11
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	16	0.11
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	16	0.11
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	16	0.11
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	1	0.11
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	1	0.11
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	1	0.11
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	6	0.11
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	6	0.11
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	6	0.11
(1,657)	1:112:A:ALA:HB1	1:113:A:ASN:HD22	12	0.11
(1,657)	1:112:A:ALA:HB2	1:113:A:ASN:HD22	12	0.11
(1,657)	1:112:A:ALA:HB3	1:113:A:ASN:HD22	12	0.11
(1,228)	1:50:A:ALA:H	1:51:A:THR:HG21	28	0.11
(1,228)	1:50:A:ALA:H	1:51:A:THR:HG22	28	0.11
(1,228)	1:50:A:ALA:H	1:51:A:THR:HG23	28	0.11
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	4	0.11
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	11	0.11
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	1	0.1
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	1	0.1
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	1	0.1
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	1	0.1
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	1	0.1
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	1	0.1
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	2	0.1
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	2	0.1
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	2	0.1
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	2	0.1
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	2	0.1
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	2	0.1
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	8	0.1
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	8	0.1
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	8	0.1
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	8	0.1
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	8	0.1
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	15	0.1
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	15	0.1
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	15	0.1
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	15	0.1
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	15	0.1
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	15	0.1
(1,2250)	1:81:A:LEU:HD11	1:82:A:PRO:HD3	33	0.1
(1,2250)	1:81:A:LEU:HD12	1:82:A:PRO:HD3	33	0.1
(1,2250)	1:81:A:LEU:HD13	1:82:A:PRO:HD3	33	0.1
(1,2250)	1:81:A:LEU:HD21	1:82:A:PRO:HD3	33	0.1
(1,2250)	1:81:A:LEU:HD22	1:82:A:PRO:HD3	33	0.1
(1,2250)	1:81:A:LEU:HD23	1:82:A:PRO:HD3	33	0.1
(1,2210)	1:73:A:LEU:HD11	1:92:A:TRP:HE3	10	0.1
(1,2210)	1:73:A:LEU:HD12	1:92:A:TRP:HE3	10	0.1
(1,2210)	1:73:A:LEU:HD13	1:92:A:TRP:HE3	10	0.1
(1,2210)	1:73:A:LEU:HD21	1:92:A:TRP:HE3	10	0.1
(1,2210)	1:73:A:LEU:HD22	1:92:A:TRP:HE3	10	0.1
(1,2210)	1:73:A:LEU:HD23	1:92:A:TRP:HE3	10	0.1
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD1	28	0.1
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD2	28	0.1
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD1	28	0.1
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD2	28	0.1
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD1	40	0.1
(1,2186)	1:67:A:ARG:HG2	1:69:A:TYR:HD2	40	0.1
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD1	40	0.1
(1,2186)	1:67:A:ARG:HG3	1:69:A:TYR:HD2	40	0.1
(1,2136)	1:48:A:ARG:HD2	1:90:A:ILE:HD11	14	0.1
(1,2136)	1:48:A:ARG:HD2	1:90:A:ILE:HD12	14	0.1
(1,2136)	1:48:A:ARG:HD2	1:90:A:ILE:HD13	14	0.1
(1,2136)	1:48:A:ARG:HD3	1:90:A:ILE:HD11	14	0.1
(1,2136)	1:48:A:ARG:HD3	1:90:A:ILE:HD12	14	0.1
(1,2136)	1:48:A:ARG:HD3	1:90:A:ILE:HD13	14	0.1
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD11	15	0.1
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD12	15	0.1
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD13	15	0.1
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD21	15	0.1
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD22	15	0.1
(1,2035)	1:30:A:GLN:HG2	1:121:A:LEU:HD23	15	0.1
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD11	15	0.1
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD12	15	0.1
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD13	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD21	15	0.1
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD22	15	0.1
(1,2035)	1:30:A:GLN:HG3	1:121:A:LEU:HD23	15	0.1
(1,1866)	1:53:A:ARG:HA	1:61:A:MET:HE1	35	0.1
(1,1866)	1:53:A:ARG:HA	1:61:A:MET:HE2	35	0.1
(1,1866)	1:53:A:ARG:HA	1:61:A:MET:HE3	35	0.1
(1,1301)	1:90:A:ILE:HD11	1:91:A:ILE:H	35	0.1
(1,1301)	1:90:A:ILE:HD12	1:91:A:ILE:H	35	0.1
(1,1301)	1:90:A:ILE:HD13	1:91:A:ILE:H	35	0.1
(1,1104)	1:54:A:ILE:HG21	1:62:A:LYS:HG2	6	0.1
(1,1104)	1:54:A:ILE:HG21	1:62:A:LYS:HG3	6	0.1
(1,1104)	1:54:A:ILE:HG22	1:62:A:LYS:HG2	6	0.1
(1,1104)	1:54:A:ILE:HG22	1:62:A:LYS:HG3	6	0.1
(1,1104)	1:54:A:ILE:HG23	1:62:A:LYS:HG2	6	0.1
(1,1104)	1:54:A:ILE:HG23	1:62:A:LYS:HG3	6	0.1
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD11	17	0.1
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD12	17	0.1
(1,1081)	1:46:A:TYR:HD1	1:91:A:ILE:HD13	17	0.1
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD11	17	0.1
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD12	17	0.1
(1,1081)	1:46:A:TYR:HD2	1:91:A:ILE:HD13	17	0.1
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	12	0.1
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	12	0.1
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	12	0.1
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	23	0.1
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	23	0.1
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	23	0.1
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	25	0.1
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	25	0.1
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	25	0.1
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	27	0.1
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	27	0.1
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	27	0.1
(1,1008)	1:34:A:ILE:HD11	1:35:A:ASN:H	35	0.1
(1,1008)	1:34:A:ILE:HD12	1:35:A:ASN:H	35	0.1
(1,1008)	1:34:A:ILE:HD13	1:35:A:ASN:H	35	0.1
(1,943)	1:32:A:VAL:HG21	1:70:A:PHE:HE1	11	0.1
(1,943)	1:32:A:VAL:HG21	1:70:A:PHE:HE2	11	0.1
(1,943)	1:32:A:VAL:HG22	1:70:A:PHE:HE1	11	0.1
(1,943)	1:32:A:VAL:HG22	1:70:A:PHE:HE2	11	0.1
(1,943)	1:32:A:VAL:HG23	1:70:A:PHE:HE1	11	0.1
(1,943)	1:32:A:VAL:HG23	1:70:A:PHE:HE2	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	3	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	3	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	3	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	3	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	3	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	3	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	3	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	3	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	3	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	16	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	16	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	16	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	16	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	16	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	16	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	16	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	16	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	16	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB1	27	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB2	27	0.1
(1,828)	1:15:A:ALA:HB1	1:50:A:ALA:HB3	27	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB1	27	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB2	27	0.1
(1,828)	1:15:A:ALA:HB2	1:50:A:ALA:HB3	27	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB1	27	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB2	27	0.1
(1,828)	1:15:A:ALA:HB3	1:50:A:ALA:HB3	27	0.1
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE1	20	0.1
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE2	20	0.1
(1,700)	1:54:A:ILE:HD11	1:61:A:MET:HE3	20	0.1
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE1	20	0.1
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE2	20	0.1
(1,700)	1:54:A:ILE:HD12	1:61:A:MET:HE3	20	0.1
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE1	20	0.1
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE2	20	0.1
(1,700)	1:54:A:ILE:HD13	1:61:A:MET:HE3	20	0.1
(1,661)	1:112:A:ALA:H	1:113:A:ASN:HD21	1	0.1
(1,300)	1:64:A:LEU:H	1:64:A:LEU:HB2	18	0.1
(1,300)	1:64:A:LEU:H	1:64:A:LEU:HB3	18	0.1
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	21	0.1
(1,136)	1:37:A:ASN:H	1:37:A:ASN:HD21	33	0.1

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

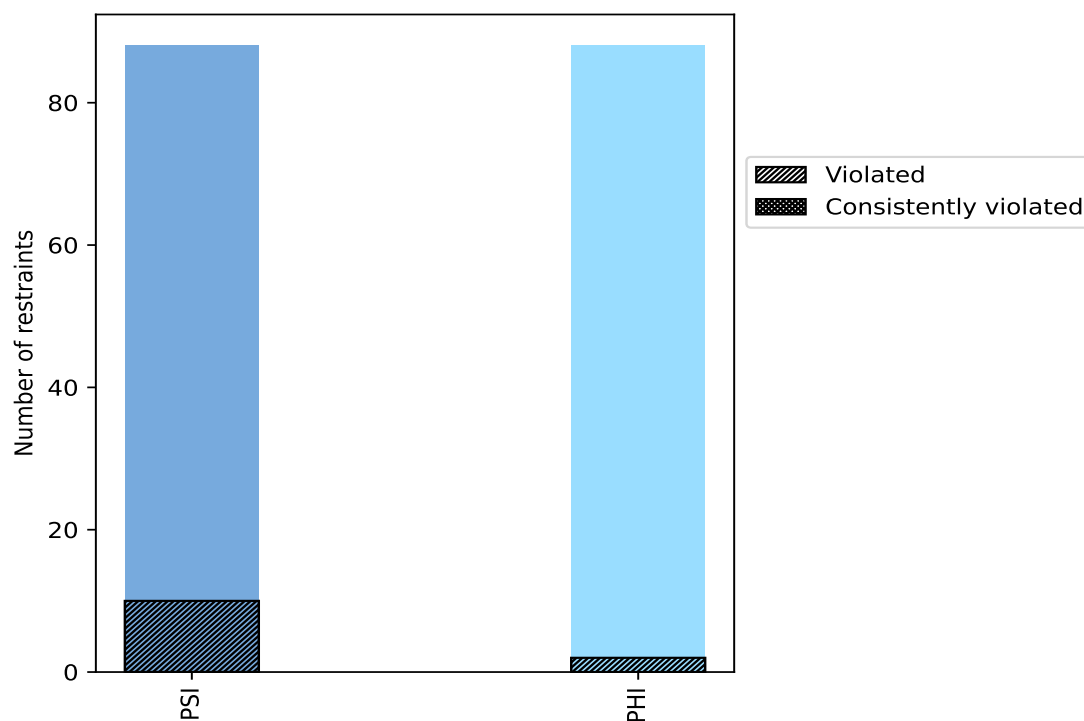
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	88	50.0	10	11.4	5.7	0	0.0	0.0
PHI	88	50.0	2	2.3	1.1	0	0.0	0.0
Total	176	100.0	12	6.8	6.8	0	0.0	0.0

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

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



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

10.2 Dihedral-angle violation statistics for each model

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

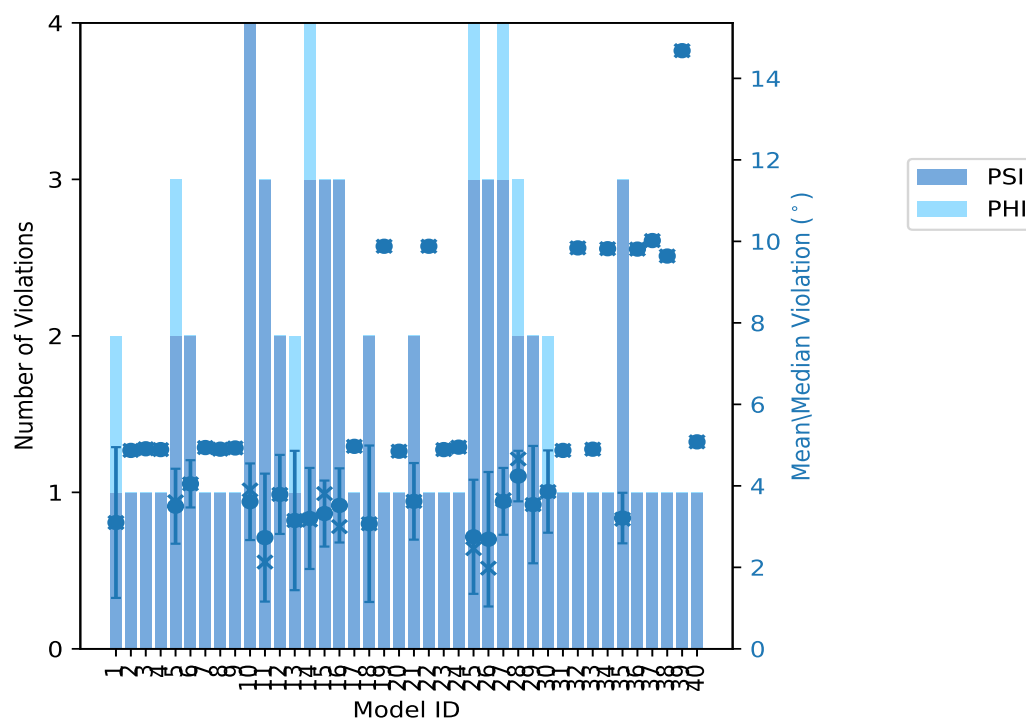
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	1	2	3.1	4.94	1.85	3.1
2	1	0	1	4.87	4.87	0.0	4.87
3	1	0	1	4.91	4.91	0.0	4.91
4	1	0	1	4.89	4.89	0.0	4.89
5	2	1	3	3.5	4.57	0.92	3.61
6	2	0	2	4.05	4.63	0.58	4.05
7	1	0	1	4.94	4.94	0.0	4.94
8	1	0	1	4.9	4.9	0.0	4.9
9	1	0	1	4.93	4.93	0.0	4.93
10	4	0	4	3.61	4.53	0.94	3.9
11	3	0	3	2.73	4.88	1.57	2.13
12	2	0	2	3.79	4.76	0.97	3.79
13	1	1	2	3.15	4.86	1.71	3.15
14	3	1	4	3.2	4.82	1.24	3.16
15	3	0	3	3.32	3.97	0.81	3.81
16	3	0	3	3.52	4.8	0.91	3.0
17	1	0	1	4.97	4.97	0.0	4.97
18	2	0	2	3.07	4.99	1.92	3.07
19	1	0	1	9.88	9.88	0.0	9.88
20	1	0	1	4.85	4.85	0.0	4.85
21	2	0	2	3.62	4.56	0.94	3.62
22	1	0	1	9.88	9.88	0.0	9.88
23	1	0	1	4.89	4.89	0.0	4.89
24	1	0	1	4.95	4.95	0.0	4.95
25	3	1	4	2.75	4.84	1.4	2.46
26	3	0	3	2.69	4.97	1.65	1.98
27	3	1	4	3.62	4.73	0.82	3.66
28	2	1	3	4.24	4.69	0.62	4.66
29	2	0	2	3.54	4.98	1.44	3.54
30	1	1	2	3.86	4.87	1.01	3.86
31	1	0	1	4.87	4.87	0.0	4.87
32	1	0	1	9.84	9.84	0.0	9.84
33	1	0	1	4.9	4.9	0.0	4.9
34	1	0	1	9.82	9.82	0.0	9.82
35	3	0	3	3.21	3.98	0.62	3.18
36	1	0	1	9.81	9.81	0.0	9.81
37	1	0	1	10.02	10.02	0.0	10.02
38	1	0	1	9.64	9.64	0.0	9.64

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
39	1	0	1	14.68	14.68	0.0	14.68
40	1	0	1	5.08	5.08	0.0	5.08

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
5	1	6	1	2.5
0	0	0	2	5.0
1	0	1	3	7.5
0	0	0	4	10.0

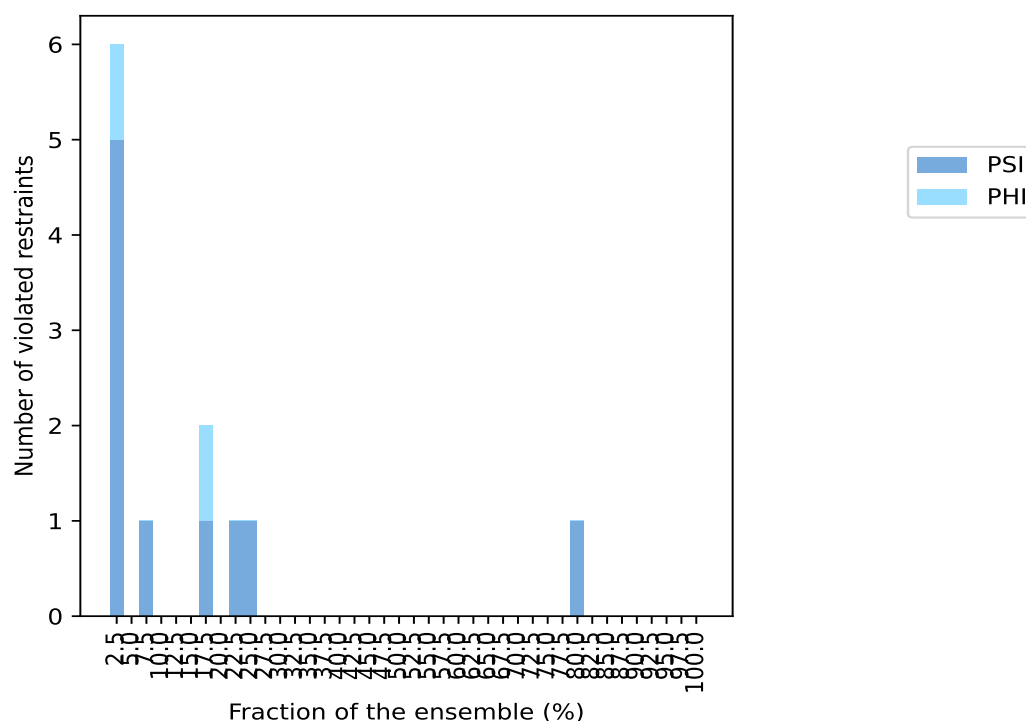
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	5	12.5
0	0	0	6	15.0
1	1	2	7	17.5
0	0	0	8	20.0
1	0	1	9	22.5
1	0	1	10	25.0
0	0	0	11	27.5
0	0	0	12	30.0
0	0	0	13	32.5
0	0	0	14	35.0
0	0	0	15	37.5
0	0	0	16	40.0
0	0	0	17	42.5
0	0	0	18	45.0
0	0	0	19	47.5
0	0	0	20	50.0
0	0	0	21	52.5
0	0	0	22	55.0
0	0	0	23	57.5
0	0	0	24	60.0
0	0	0	25	62.5
0	0	0	26	65.0
0	0	0	27	67.5
0	0	0	28	70.0
0	0	0	29	72.5
0	0	0	30	75.0
0	0	0	31	77.5
1	0	1	32	80.0
0	0	0	33	82.5
0	0	0	34	85.0
0	0	0	35	87.5
0	0	0	36	90.0
0	0	0	37	92.5
0	0	0	38	95.0
0	0	0	39	97.5
0	0	0	40	100.0

¹ Number of models with violations

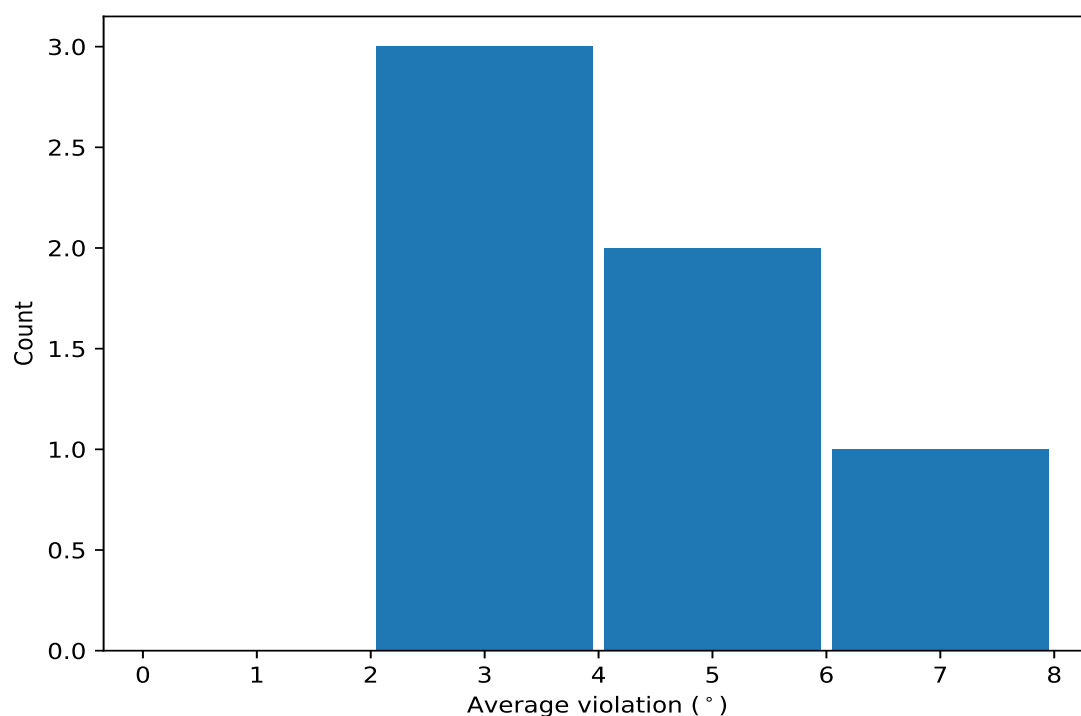
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

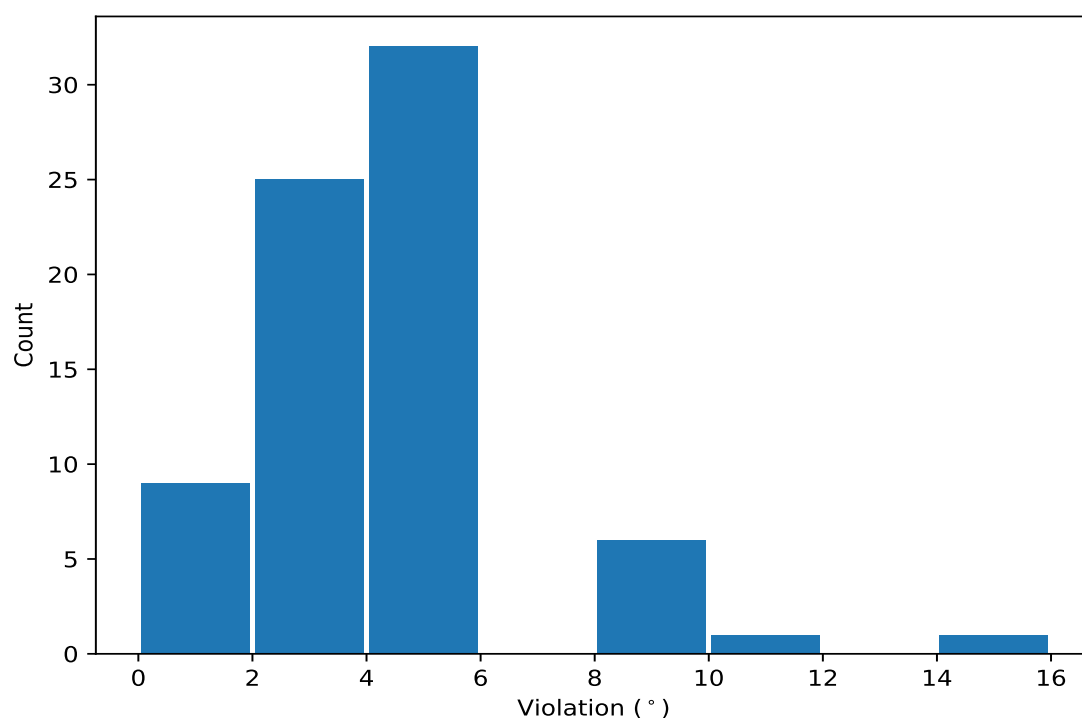
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	32	4.34	0.86	4.87
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	10	7.35	3.82	9.82
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	9	4.18	0.94	4.57
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	7	3.42	0.9	3.81
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	7	2.1	0.75	1.75
(1,60)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:ARG:N	3	2.71	1.55	2.11

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 (°)
(1,62)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:ILE:N	39	14.68
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	37	10.02
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	19	9.88
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	22	9.88
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	32	9.84
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	34	9.82
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	36	9.81
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	38	9.64
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	40	5.08
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	18	4.99
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	29	4.98
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	17	4.97
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	26	4.97
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	24	4.95
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	1	4.94
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	7	4.94
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	9	4.93
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	3	4.91
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	8	4.9
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	33	4.9
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	4	4.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	23	4.89
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	11	4.88
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	2	4.87
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	30	4.87
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	31	4.87
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	13	4.86
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	20	4.85
(1,60)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:ARG:N	25	4.84
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	14	4.82
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	16	4.8
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	12	4.76
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	27	4.73
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	28	4.69
(1,5)	1:12:A:TRP:C	1:13:A:PHE:N	1:13:A:PHE:CA	1:13:A:PHE:C	28	4.66
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	6	4.63
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	5	4.57
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	21	4.56
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	10	4.53
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	10	4.22
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	35	3.98
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	15	3.97
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	14	3.89
(1,88)	1:75:A:THR:N	1:75:A:THR:CA	1:75:A:THR:C	1:76:A:GLY:N	27	3.86
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	15	3.81
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	5	3.61
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	10	3.59
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	6	3.47
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	27	3.46
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	28	3.36
(1,20)	1:23:A:ASP:N	1:23:A:ASP:CA	1:23:A:ASP:C	1:24:A:LEU:N	35	3.18
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	25	3.16
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	16	3.0
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	30	2.86
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	12	2.82
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	16	2.75
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	21	2.67
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	35	2.47
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	27	2.45
(1,4)	1:12:A:TRP:N	1:12:A:TRP:CA	1:12:A:TRP:C	1:13:A:PHE:N	14	2.44
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	5	2.33
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	15	2.18
(1,164)	1:126:A:THR:N	1:126:A:THR:CA	1:126:A:THR:C	1:127:A:LEU:N	11	2.13
(1,60)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:ARG:N	29	2.11
(1,84)	1:72:A:TYR:N	1:72:A:TYR:CA	1:72:A:TYR:C	1:73:A:LEU:N	10	2.09
(1,18)	1:19:A:HIS:N	1:19:A:HIS:CA	1:19:A:HIS:C	1:20:A:GLY:N	26	1.98
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	25	1.75
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	14	1.64
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	13	1.44
(1,43)	1:40:A:PRO:C	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1	1.25
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	25	1.24
(1,60)	1:52:A:ARG:N	1:52:A:ARG:CA	1:52:A:ARG:C	1:53:A:ARG:N	11	1.19

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:30:A:GLN:N	1:30:A:GLN:CA	1:30:A:GLN:C	1:31:A:GLY:N	18	1.15
(1,46)	1:42:A:ASP:N	1:42:A:ASP:CA	1:42:A:ASP:C	1:43:A:GLN:N	26	1.11