



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:54 PM UTC

PDB ID : 2MSX / pdb_00002msx
BMRB ID : 25139
Title : The solution structure of the MANEC-type domain from Hepatocyte Growth Factor Inhibitor 1 reveals an unexpected PAN/apple domain-type fold
Authors : Hong, Z.; Nowakowski, M.E.; Spronk, C.; Petersen, S.V.; Petersen, J.S.; Kozminski, W.; Mulder, F.; Jensen, J.K.
Deposited on : 2014-08-09

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

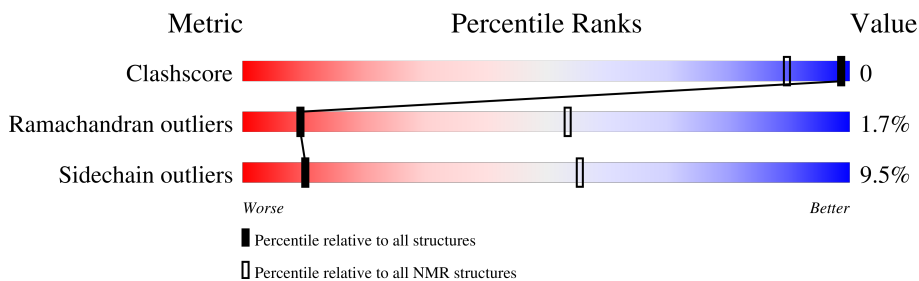
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	114	

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:54-A:153 (100)	0.46	9

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1741 atoms, of which 841 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kunitz-type protease inhibitor 1.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	114	1741	561	841	164	167	8	0

There are 9 discrepancies between the modelled and reference sequences:

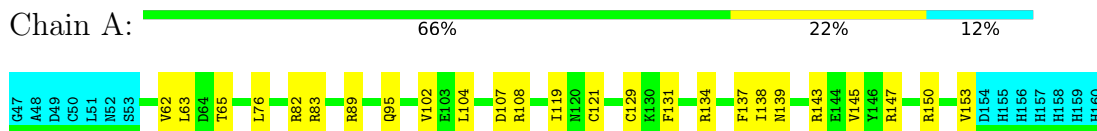
Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLN	ASN	conflict	UNP O43278
A	153	VAL	-	expression tag	UNP O43278
A	154	ASP	-	expression tag	UNP O43278
A	155	HIS	-	expression tag	UNP O43278
A	156	HIS	-	expression tag	UNP O43278
A	157	HIS	-	expression tag	UNP O43278
A	158	HIS	-	expression tag	UNP O43278
A	159	HIS	-	expression tag	UNP O43278
A	160	HIS	-	expression tag	UNP O43278

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: Kunitz-type protease inhibitor 1

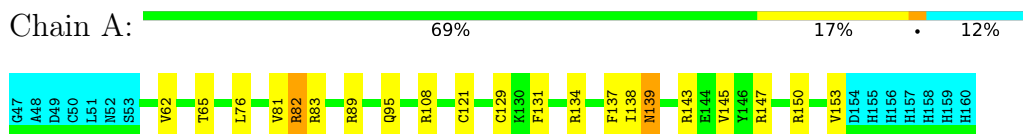


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

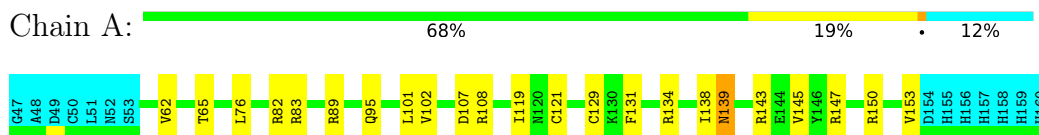
4.2.1 Score per residue for model 1

- Molecule 1: Kunitz-type protease inhibitor 1



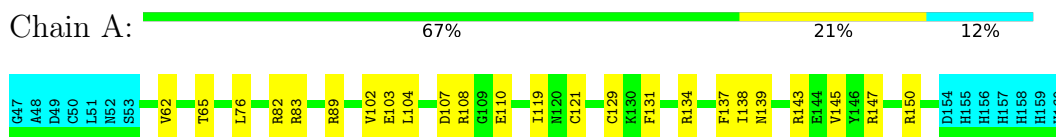
4.2.2 Score per residue for model 2

- Molecule 1: Kunitz-type protease inhibitor 1



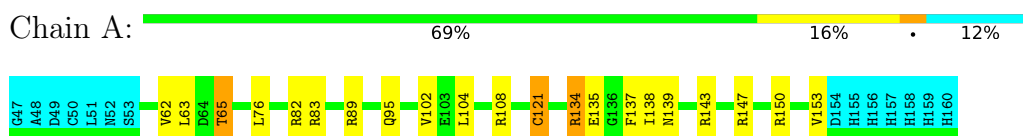
4.2.3 Score per residue for model 3

- Molecule 1: Kunitz-type protease inhibitor 1



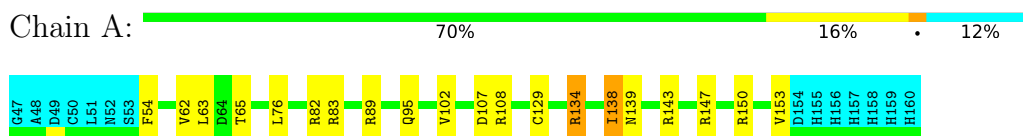
4.2.4 Score per residue for model 4

- Molecule 1: Kunitz-type protease inhibitor 1



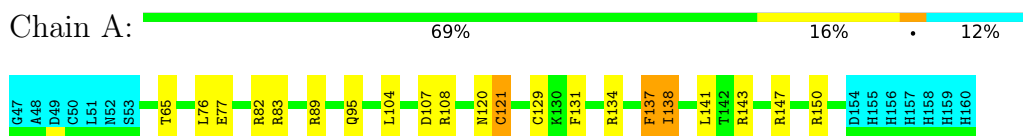
4.2.5 Score per residue for model 5

- Molecule 1: Kunitz-type protease inhibitor 1



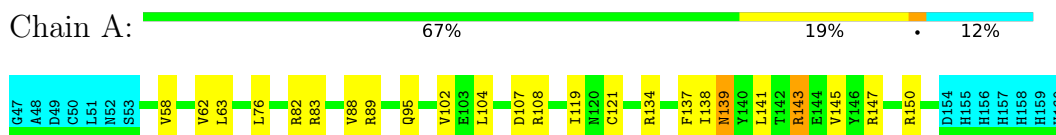
4.2.6 Score per residue for model 6

- Molecule 1: Kunitz-type protease inhibitor 1



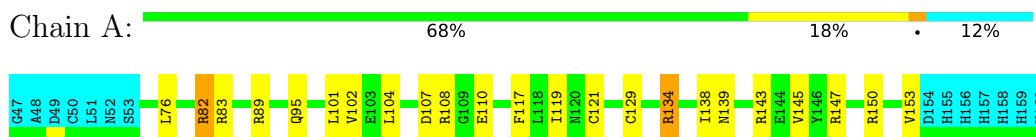
4.2.7 Score per residue for model 7

- Molecule 1: Kunitz-type protease inhibitor 1



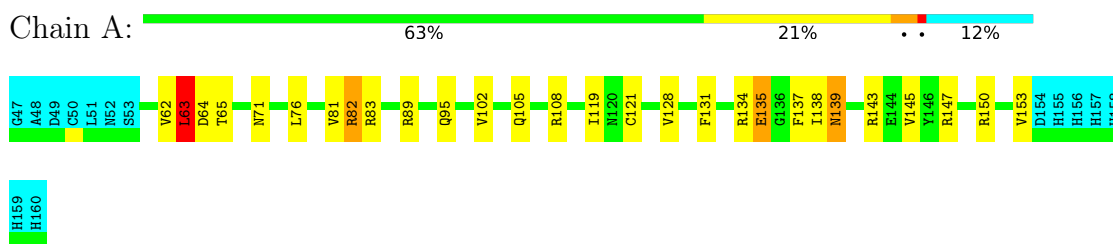
4.2.8 Score per residue for model 8

- Molecule 1: Kunitz-type protease inhibitor 1



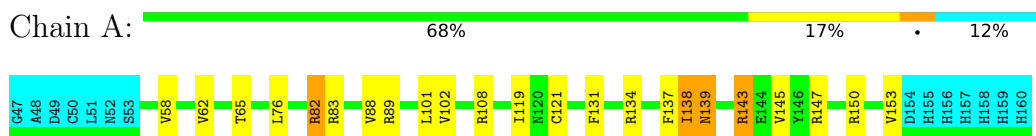
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Kunitz-type protease inhibitor 1



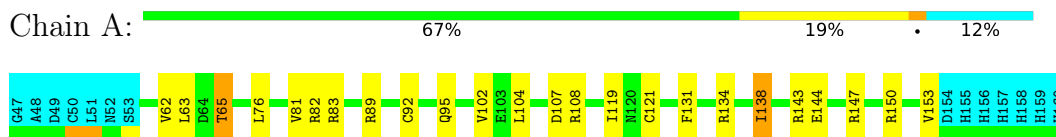
4.2.10 Score per residue for model 10

- Molecule 1: Kunitz-type protease inhibitor 1



4.2.11 Score per residue for model 11

- Molecule 1: Kunitz-type protease inhibitor 1



4.2.12 Score per residue for model 12

- Molecule 1: Kunitz-type protease inhibitor 1





4.2.13 Score per residue for model 13

- Molecule 1: Kunitz-type protease inhibitor 1

Chain A: 62% 25% 12%



4.2.14 Score per residue for model 14

- Molecule 1: Kunitz-type protease inhibitor 1

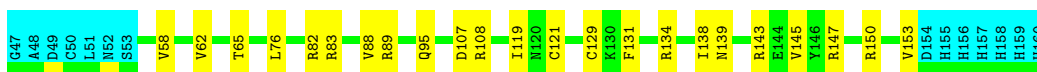
Chain A: 70% 18% 12%



4.2.15 Score per residue for model 15

- Molecule 1: Kunitz-type protease inhibitor 1

Chain A: 68% 20% 12%



4.2.16 Score per residue for model 16

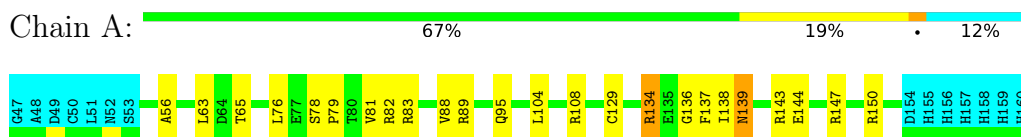
- Molecule 1: Kunitz-type protease inhibitor 1

Chain A: 68% 17% 12%



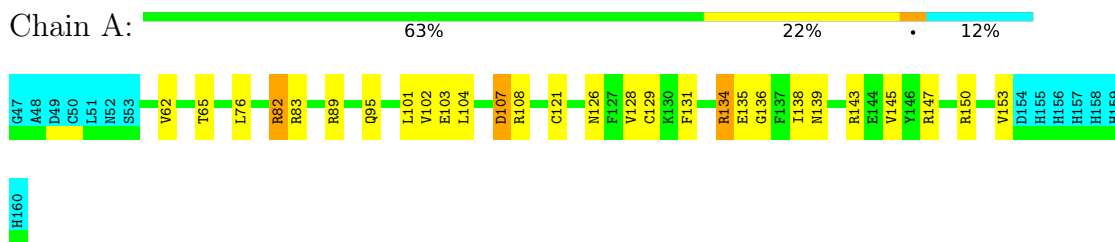
4.2.17 Score per residue for model 17

- Molecule 1: Kunitz-type protease inhibitor 1



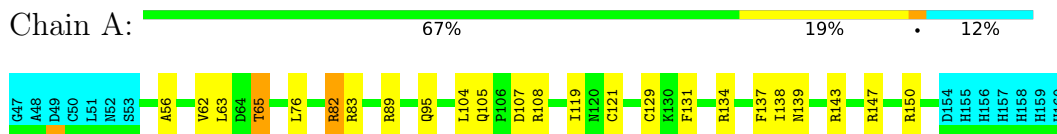
4.2.18 Score per residue for model 18

- Molecule 1: Kunitz-type protease inhibitor 1



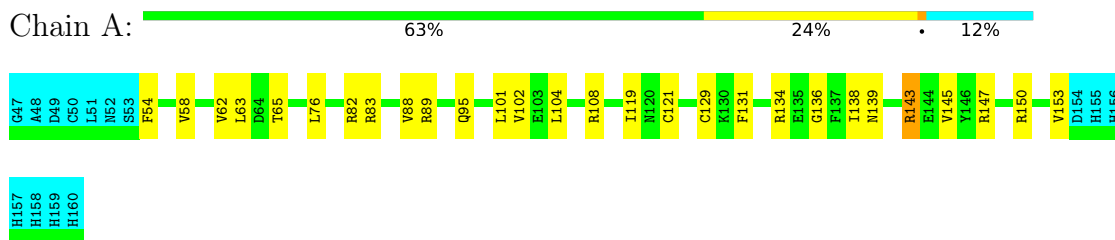
4.2.19 Score per residue for model 19

- Molecule 1: Kunitz-type protease inhibitor 1



4.2.20 Score per residue for model 20

- Molecule 1: Kunitz-type protease inhibitor 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA	structure solution	
YASARA2	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	2133
Number of shifts mapped to atoms	2133
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	1.55±0.03	8±0/803 (1.0± 0.0%)	1.33±0.03	8±2/1093 (0.8± 0.2%)
All	All	1.55	164/16060 (1.0%)	1.33	169/21860 (0.8%)

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	150	ARG	CZ-NH2	-7.53	1.23	1.33	16	20
1	A	108	ARG	CZ-NH2	-7.28	1.24	1.33	16	20
1	A	83	ARG	CZ-NH2	-6.62	1.24	1.33	13	20
1	A	147	ARG	CZ-NH2	-6.50	1.25	1.33	16	20
1	A	134	ARG	CZ-NH2	-6.32	1.25	1.33	4	20
1	A	82	ARG	CZ-NH2	-6.07	1.25	1.33	16	20
1	A	143	ARG	CZ-NH2	-5.98	1.25	1.33	20	20
1	A	89	ARG	CZ-NH2	-5.94	1.25	1.33	8	20
1	A	105	GLN	CA-C	5.79	1.60	1.52	13	1
1	A	150	ARG	CZ-NH1	-5.35	1.25	1.32	6	1
1	A	83	ARG	CZ-NH1	-5.34	1.25	1.32	17	1
1	A	153	VAL	N-CA	5.05	1.50	1.46	4	1

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	134	ARG	N-CA-C	9.26	121.92	108.86	17	17
1	A	95	GLN	N-CA-C	8.87	122.06	111.33	20	18
1	A	102	VAL	N-CA-C	7.78	119.97	108.45	10	15
1	A	104	LEU	N-CA-C	7.45	121.42	110.17	13	7
1	A	153	VAL	CB-CA-C	-7.12	102.93	110.62	5	15
1	A	126	ASN	N-CA-C	6.97	121.63	113.20	18	1
1	A	131	PHE	N-CA-C	6.75	119.43	109.24	11	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	62	VAL	N-CA-C	6.65	118.29	108.65	11	16
1	A	65	THR	N-CA-C	6.58	118.11	111.07	9	8
1	A	139	ASN	N-CA-C	6.25	119.69	109.06	9	7
1	A	78	SER	CA-C-N	6.14	125.84	119.82	17	1
1	A	78	SER	C-N-CA	6.14	125.84	119.82	17	1
1	A	137	PHE	N-CA-C	6.07	118.40	109.24	10	11
1	A	108	ARG	N-CA-C	6.03	120.92	113.50	8	2
1	A	63	LEU	N-CA-C	5.97	118.92	109.96	17	6
1	A	135	GLU	N-CA-C	5.89	119.65	112.23	4	1
1	A	81	VAL	CB-CA-C	-5.82	103.74	111.13	13	6
1	A	138	ILE	N-CA-C	5.81	117.08	108.65	16	2
1	A	121	CYS	N-CA-C	5.73	119.57	112.47	4	1
1	A	88	VAL	CB-CA-C	-5.68	104.38	112.22	13	2
1	A	138	ILE	CB-CA-C	-5.59	102.55	110.82	11	3
1	A	129	CYS	N-CA-C	5.52	117.85	110.35	5	2
1	A	136	GLY	N-CA-C	5.40	122.55	115.47	17	1
1	A	54	PHE	N-CA-C	5.32	118.23	109.72	5	1
1	A	102	VAL	CB-CA-C	-5.28	101.57	110.71	10	3
1	A	58	VAL	N-CA-C	5.27	113.92	109.02	10	1
1	A	62	VAL	CB-CA-C	-5.22	103.10	110.82	1	1
1	A	79	PRO	N-CA-C	5.21	120.70	113.98	17	1
1	A	145	VAL	CB-CA-C	-5.12	105.31	110.88	2	3
1	A	82	ARG	N-CA-C	5.08	119.46	113.16	19	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	786	755	755	0±1
All	All	15720	15100	15100	7

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:135:GLU:CD	1:A:135:GLU:H	0.52	2.13	9	1
1:A:63:LEU:HG	1:A:65:THR:H	0.46	1.69	4	3
1:A:71:ASN:HD22	1:A:128:VAL:HB	0.42	1.73	13	2
1:A:63:LEU:HD22	1:A:64:ASP:N	0.41	2.30	9	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	100/114 (88%)	93±2 (93±2%)	5±1 (5±1%)	2±1 (2±1%)	9	53
All	All	2000/2280 (88%)	1861 (93%)	105 (5%)	34 (2%)	9	53

All 9 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	107	ASP	11
1	A	65	THR	10
1	A	58	VAL	4
1	A	105	GLN	2
1	A	56	ALA	2
1	A	136	GLY	2
1	A	121	CYS	1
1	A	137	PHE	1
1	A	128	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/97 (88%)	77±2 (91±2%)	8±2 (9±2%)	10	55
All	All	1700/1940 (88%)	1539 (91%)	161 (9%)	10	55

All 25 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	76	LEU	20
1	A	138	ILE	20
1	A	121	CYS	18
1	A	139	ASN	18
1	A	119	ILE	12
1	A	129	CYS	10
1	A	145	VAL	9
1	A	101	LEU	7
1	A	134	ARG	7
1	A	82	ARG	6
1	A	104	LEU	6
1	A	88	VAL	5
1	A	110	GLU	3
1	A	143	ARG	3
1	A	135	GLU	3
1	A	103	GLU	2
1	A	141	LEU	2
1	A	117	PHE	2
1	A	144	GLU	2
1	A	77	GLU	1
1	A	120	ASN	1
1	A	63	LEU	1
1	A	92	CYS	1
1	A	107	ASP	1
1	A	54	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	1026
Number of shifts mapped to atoms	1026
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	106	-0.15 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	99	-0.02 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	100	0.28 ± 0.09	None needed (< 0.5 ppm)
^{15}N	99	0.21 ± 0.48	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 73%, i.e. 981 atoms were assigned a chemical shift out of a possible 1352. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	470/498 (94%)	182/202 (90%)	195/200 (98%)	93/96 (97%)
Sidechain	487/736 (66%)	322/478 (67%)	165/222 (74%)	0/36 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	24/118 (20%)	23/57 (40%)	0/60 (0%)	1/1 (100%)
Overall	981/1352 (73%)	527/737 (72%)	360/482 (75%)	94/133 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 1026 atoms were assigned a chemical shift out of a possible 1521. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	495/569 (87%)	190/231 (82%)	206/228 (90%)	99/110 (90%)
Sidechain	507/792 (64%)	332/514 (65%)	175/241 (73%)	0/37 (0%)
Aromatic	24/160 (15%)	23/81 (28%)	0/72 (0%)	1/7 (14%)
Overall	1026/1521 (67%)	545/826 (66%)	381/541 (70%)	100/154 (65%)

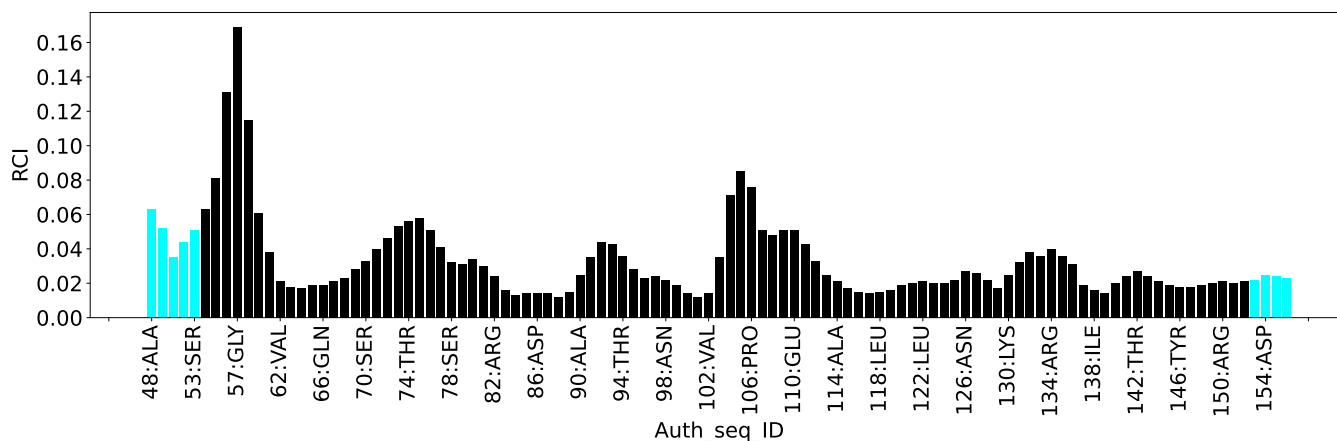
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *Assigned_chemical_shift_list_2*

7.2.1 Bookkeeping [i](#)

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

Total number of shifts	1107
Number of shifts mapped to atoms	1107
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	99	-0.24 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	95	0.00 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	99	0.35 ± 0.46	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1051 atoms were assigned a chemical shift out of a possible 1352. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	376/498 (76%)	190/202 (94%)	93/200 (46%)	93/96 (97%)
Sidechain	593/736 (81%)	405/478 (85%)	184/222 (83%)	4/36 (11%)
Aromatic	82/118 (69%)	41/57 (72%)	40/60 (67%)	1/1 (100%)
Overall	1051/1352 (78%)	636/737 (86%)	317/482 (66%)	98/133 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1107 atoms were assigned a chemical shift out of a possible 1521. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	400/569 (70%)	202/231 (87%)	99/228 (43%)	99/110 (90%)
Sidechain	625/792 (79%)	427/514 (83%)	193/241 (80%)	5/37 (14%)
Aromatic	82/160 (51%)	41/81 (51%)	40/72 (56%)	1/7 (14%)
Overall	1107/1521 (73%)	670/826 (81%)	332/541 (61%)	105/154 (68%)

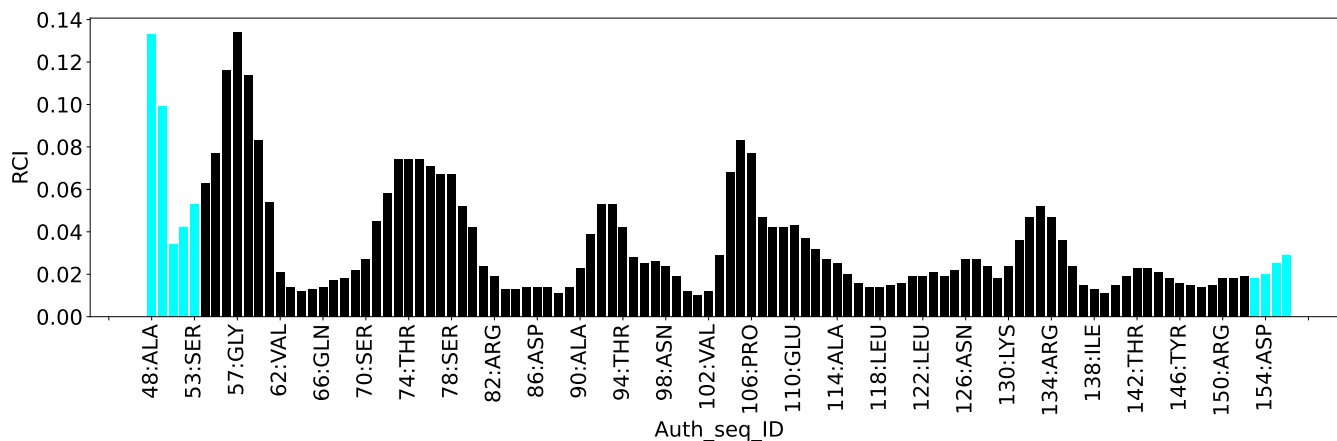
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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	533
Intra-residue ($ i-j =0$)	175
Sequential ($ i-j =1$)	215
Medium range ($ i-j >1$ and $ i-j <5$)	92
Long range ($ i-j \geq 5$)	51
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	4.7
Number of long range restraints per residue ¹	0.4

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	8.8	0.2
0.2-0.5 (Medium)	15.2	0.5
>0.5 (Large)	14.9	7.87

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis i

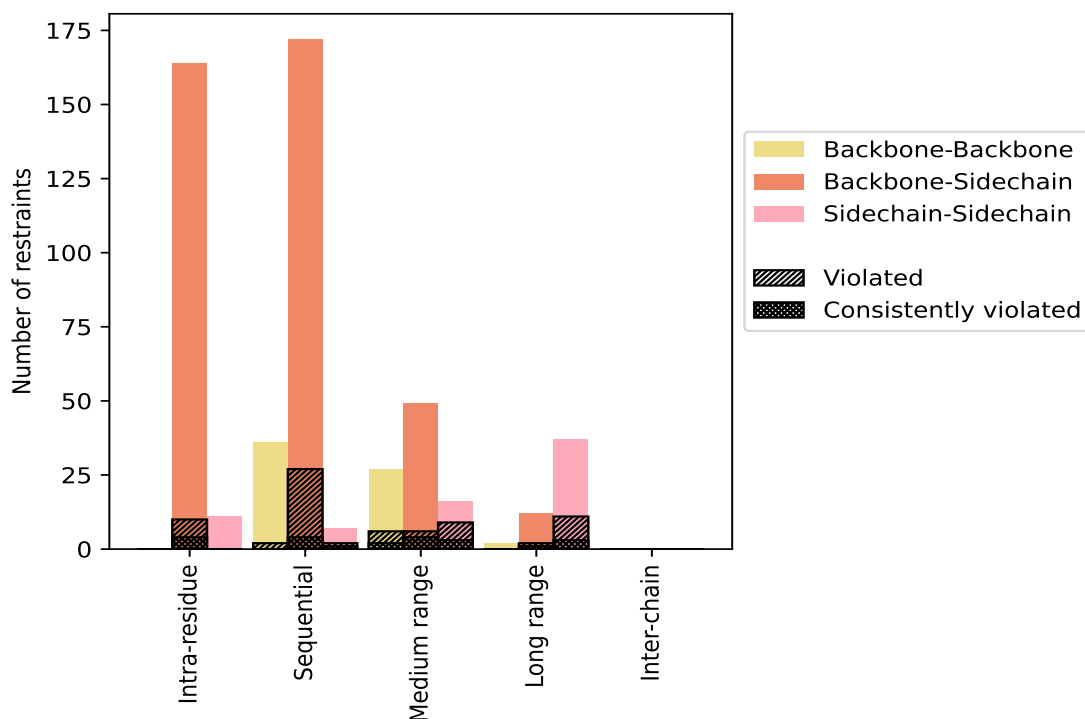
9.1 Summary of distance violations i

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 ($i-j =0$)	175	32.8	10	5.7	1.9	4	2.3	0.8
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	164	30.8	10	6.1	1.9	4	2.4	0.8
Sidechain-Sidechain	11	2.1	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	215	40.3	31	14.4	5.8	5	2.3	0.9
Backbone-Backbone	36	6.8	2	5.6	0.4	0	0.0	0.0
Backbone-Sidechain	172	32.3	27	15.7	5.1	4	2.3	0.8
Sidechain-Sidechain	7	1.3	2	28.6	0.4	1	14.3	0.2
Medium range ($i-j >1$ & $i-j <5$)	92	17.3	21	22.8	3.9	9	9.8	1.7
Backbone-Backbone	27	5.1	6	22.2	1.1	2	7.4	0.4
Backbone-Sidechain	49	9.2	6	12.2	1.1	4	8.2	0.8
Sidechain-Sidechain	16	3.0	9	56.2	1.7	3	18.8	0.6
Long range ($i-j \geq 5$)	51	9.6	13	25.5	2.4	4	7.8	0.8
Backbone-Backbone	2	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	12	2.3	2	16.7	0.4	1	8.3	0.2
Sidechain-Sidechain	37	6.9	11	29.7	2.1	3	8.1	0.6
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	533	100.0	75	14.1	14.1	22	4.1	4.1
Backbone-Backbone	65	12.2	8	12.3	1.5	2	3.1	0.4
Backbone-Sidechain	397	74.5	45	11.3	8.4	13	3.3	2.4
Sidechain-Sidechain	71	13.3	22	31.0	4.1	7	9.9	1.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	6	13	15	6	0	40	0.94	7.62	1.49	0.33
2	6	15	15	5	0	41	0.95	7.58	1.47	0.32
3	5	16	12	7	0	40	0.93	7.87	1.54	0.34
4	6	12	13	5	0	36	1.03	7.68	1.57	0.4
5	5	15	12	6	0	38	0.94	7.82	1.56	0.34
6	6	11	12	5	0	34	1.07	7.59	1.58	0.39
7	6	15	14	6	0	41	0.9	7.56	1.47	0.29
8	6	13	13	5	0	37	1.02	7.7	1.54	0.35
9	7	10	14	5	0	36	1.01	7.87	1.6	0.34
10	7	16	16	8	0	47	0.95	7.85	1.46	0.31

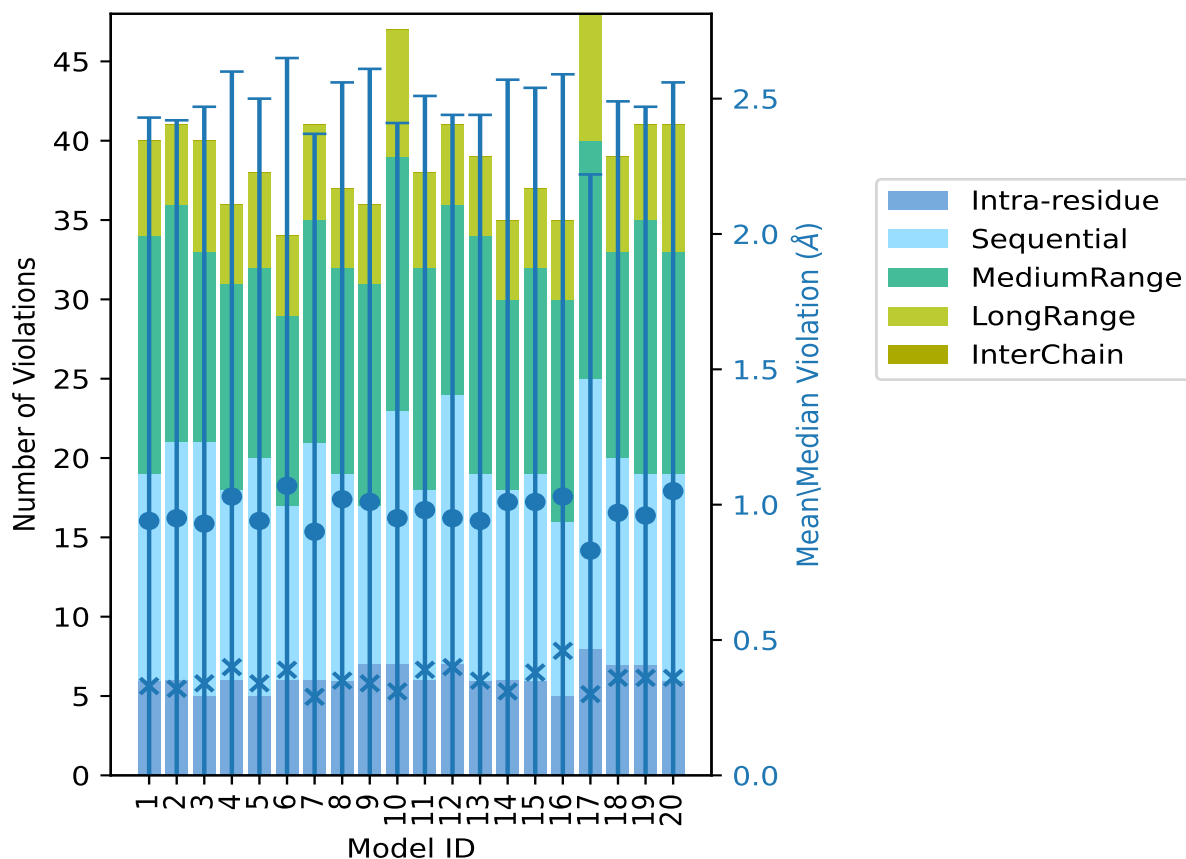
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
11	6	12	14	6	0	38	0.98	7.64	1.53	0.39
12	7	17	12	5	0	41	0.95	7.72	1.49	0.4
13	6	13	15	5	0	39	0.94	7.78	1.5	0.35
14	6	12	12	5	0	35	1.01	7.56	1.56	0.31
15	6	13	13	5	0	37	1.01	7.72	1.53	0.38
16	5	11	14	5	0	35	1.03	7.64	1.56	0.46
17	8	17	15	8	0	48	0.83	7.57	1.39	0.3
18	7	13	13	6	0	39	0.97	7.7	1.52	0.36
19	7	12	16	6	0	41	0.96	7.76	1.51	0.36
20	6	13	14	8	0	41	1.05	7.84	1.51	0.36

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

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



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

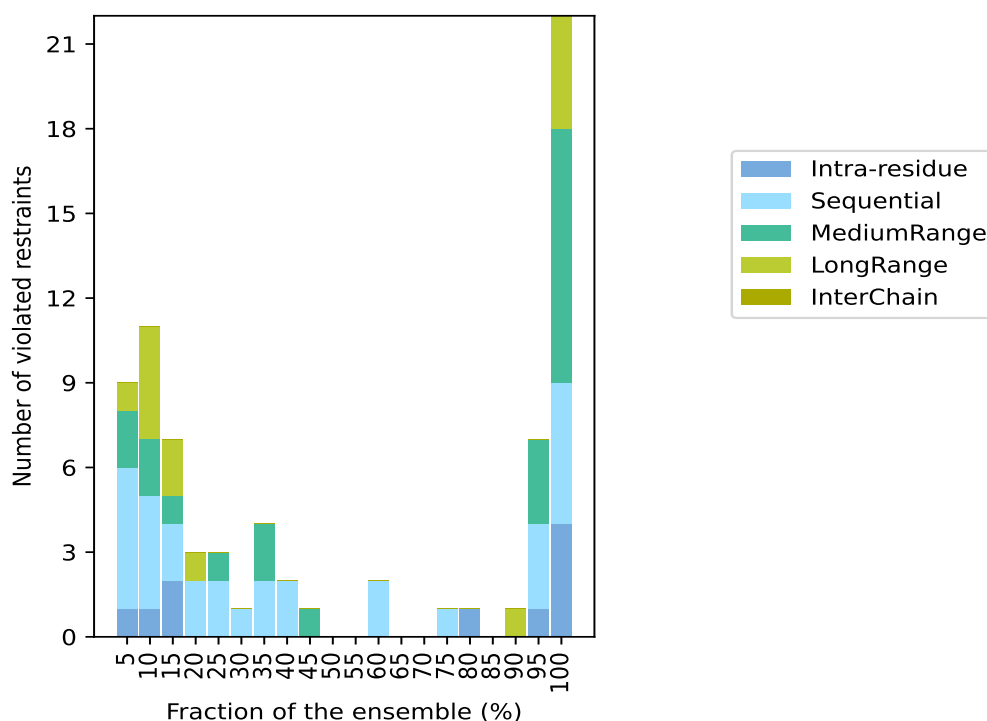
9.3 Distance violation statistics for the ensemble

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, 458(IR:165, SQ:184, MR:71, LR:38, 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	%
1	5	2	1	0	9	1	5.0
1	4	2	4	0	11	2	10.0
2	2	1	2	0	7	3	15.0
0	2	0	1	0	3	4	20.0
0	2	1	0	0	3	5	25.0
0	1	0	0	0	1	6	30.0
0	2	2	0	0	4	7	35.0
0	2	0	0	0	2	8	40.0
0	0	1	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	2	0	0	0	2	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	1	0	0	0	1	15	75.0
1	0	0	0	0	1	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	1	0	1	18	90.0
1	3	3	0	0	7	19	95.0
4	5	9	4	0	22	20	100.0

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

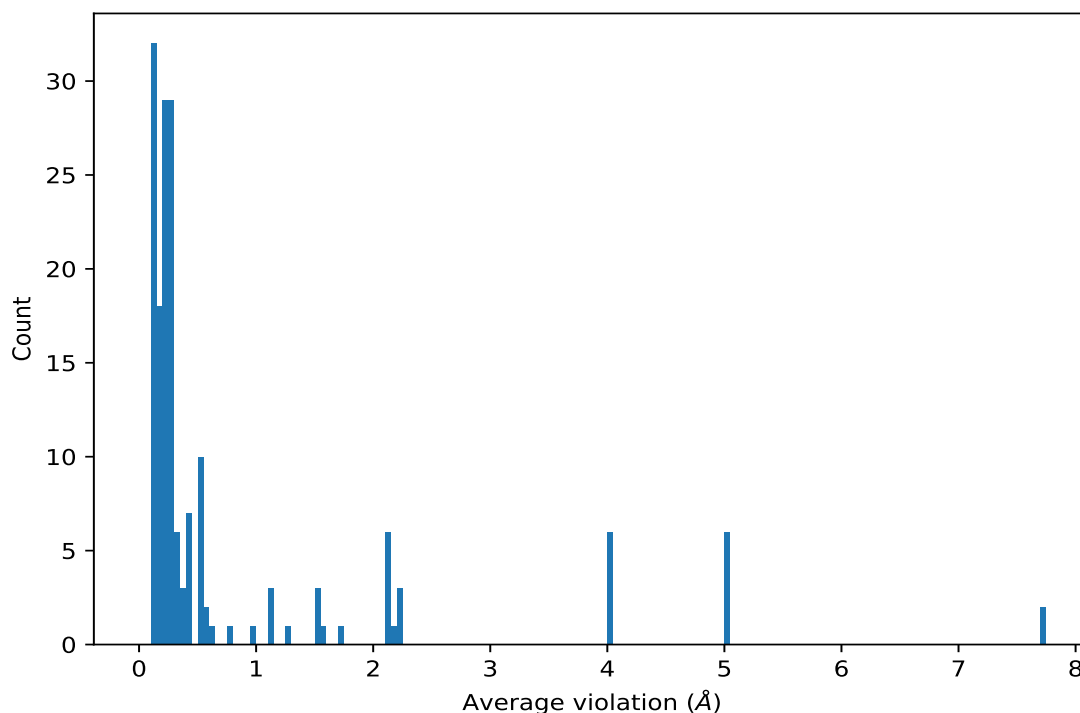
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

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

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



9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	20	7.7	0.11	7.7
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	20	7.7	0.11	7.7
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	20	5.05	0.09	5.04
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	20	5.05	0.09	5.04
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	20	5.05	0.09	5.04
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	20	5.05	0.09	5.04
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	20	5.05	0.09	5.04
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	20	5.05	0.09	5.04
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	20	4.01	0.09	4.0
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	20	4.01	0.09	4.0
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	20	4.01	0.09	4.0
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	20	4.01	0.09	4.0
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	20	4.01	0.09	4.0
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	20	4.01	0.09	4.0
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	20	2.23	0.25	2.23
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	20	2.23	0.25	2.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	20	2.23	0.25	2.23
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	20	2.15	0.14	2.21
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	20	2.12	0.17	2.11
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	20	2.12	0.17	2.11
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	20	2.12	0.17	2.11
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	20	1.72	0.21	1.7
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	20	1.25	0.09	1.25
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	20	1.13	0.17	1.12
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	20	1.13	0.17	1.12
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	20	1.13	0.17	1.12
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	20	0.96	0.2	1.03
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	20	0.75	0.18	0.75
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	20	0.62	0.04	0.6
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	20	0.41	0.19	0.35
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	20	0.41	0.19	0.35
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	20	0.41	0.19	0.35
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	20	0.41	0.07	0.41
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	20	0.41	0.07	0.41
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	20	0.4	0.03	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	20	0.4	0.03	0.4
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	20	0.37	0.12	0.34
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	20	0.37	0.12	0.34
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	20	0.37	0.12	0.34
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	20	0.31	0.07	0.32
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	20	0.31	0.07	0.32
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	20	0.3	0.05	0.29
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	20	0.3	0.05	0.29
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	20	0.27	0.07	0.3
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	20	0.27	0.07	0.3
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	20	0.27	0.07	0.3
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	20	0.26	0.04	0.26
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	20	0.26	0.04	0.26
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	20	0.26	0.04	0.26
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	20	0.26	0.04	0.26
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	20	0.26	0.04	0.26
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	20	0.26	0.04	0.26
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	20	0.23	0.04	0.23
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	20	0.23	0.08	0.24
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	20	0.23	0.08	0.24
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	19	0.58	0.03	0.58
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	19	0.58	0.03	0.58
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	19	0.54	0.18	0.51

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	19	0.54	0.18	0.51
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	19	0.54	0.18	0.51
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	19	0.29	0.07	0.31
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	19	0.29	0.07	0.31
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	19	0.29	0.07	0.31
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	19	0.29	0.07	0.31
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	19	0.29	0.07	0.31
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	19	0.29	0.07	0.31
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	19	0.25	0.06	0.25
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	19	0.18	0.03	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	19	0.18	0.03	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	19	0.18	0.03	0.19
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	19	0.18	0.02	0.18
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	19	0.18	0.02	0.18
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	19	0.17	0.05	0.15
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	19	0.17	0.05	0.15
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	18	0.3	0.13	0.3
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	18	0.3	0.13	0.3
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	18	0.3	0.13	0.3
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	16	0.5	0.08	0.49
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	15	0.18	0.05	0.18
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	15	0.18	0.05	0.18
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	12	0.32	0.15	0.25
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	12	0.32	0.15	0.25
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	12	0.21	0.07	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	12	0.21	0.07	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	12	0.21	0.07	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	12	0.21	0.07	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	12	0.21	0.07	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	12	0.21	0.07	0.21
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	9	0.17	0.04	0.17
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	8	0.51	0.04	0.52
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	8	0.51	0.04	0.52
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	8	0.51	0.04	0.52
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	8	0.51	0.04	0.52
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	8	0.51	0.04	0.52
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	8	0.51	0.04	0.52
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	8	0.23	0.04	0.24
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	8	0.23	0.04	0.24
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	7	0.28	0.02	0.29
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	7	0.22	0.07	0.2
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	7	0.22	0.07	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	7	0.2	0.03	0.2
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	7	0.2	0.03	0.2
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	7	0.2	0.03	0.2
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	7	0.13	0.01	0.14
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	7	0.13	0.01	0.14
(1,149)	1:80:A:THR:HG21	1:81:A:VAL:H	6	0.2	0.04	0.2
(1,149)	1:80:A:THR:HG22	1:81:A:VAL:H	6	0.2	0.04	0.2
(1,149)	1:80:A:THR:HG23	1:81:A:VAL:H	6	0.2	0.04	0.2
(1,424)	1:82:A:ARG:HG2	1:83:A:ARG:H	5	0.26	0.06	0.23
(1,424)	1:82:A:ARG:HG3	1:83:A:ARG:H	5	0.26	0.06	0.23
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD2	5	0.23	0.05	0.22
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD3	5	0.23	0.05	0.22
(1,391)	1:153:A:VAL:HB	1:154:A:ASP:H	5	0.12	0.02	0.11
(1,506)	1:141:A:LEU:HD11	1:146:A:TYR:HE1	4	0.22	0.08	0.18
(1,506)	1:141:A:LEU:HD12	1:146:A:TYR:HE1	4	0.22	0.08	0.18
(1,506)	1:141:A:LEU:HD13	1:146:A:TYR:HE1	4	0.22	0.08	0.18
(1,506)	1:141:A:LEU:HD21	1:146:A:TYR:HE1	4	0.22	0.08	0.18
(1,506)	1:141:A:LEU:HD22	1:146:A:TYR:HE1	4	0.22	0.08	0.18
(1,506)	1:141:A:LEU:HD23	1:146:A:TYR:HE1	4	0.22	0.08	0.18
(1,176)	1:88:A:VAL:HB	1:89:A:ARG:H	4	0.14	0.04	0.12
(1,334)	1:135:A:GLU:HA	1:136:A:GLY:H	4	0.11	0.01	0.11
(1,33)	1:56:A:ALA:HB1	1:140:A:TYR:HD2	3	1.52	0.9	2.14
(1,33)	1:56:A:ALA:HB2	1:140:A:TYR:HD2	3	1.52	0.9	2.14
(1,33)	1:56:A:ALA:HB3	1:140:A:TYR:HD2	3	1.52	0.9	2.14
(1,70)	1:56:A:ALA:HB1	1:57:A:GLY:H	3	0.27	0.08	0.28
(1,70)	1:56:A:ALA:HB2	1:57:A:GLY:H	3	0.27	0.08	0.28
(1,70)	1:56:A:ALA:HB3	1:57:A:GLY:H	3	0.27	0.08	0.28
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB2	3	0.27	0.21	0.12
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB3	3	0.27	0.21	0.12
(1,468)	1:122:A:LEU:HB2	1:127:A:PHE:HD1	3	0.17	0.05	0.14
(1,468)	1:122:A:LEU:HB3	1:127:A:PHE:HD1	3	0.17	0.05	0.14
(1,38)	1:138:A:ILE:HD11	1:140:A:TYR:HE1	3	0.16	0.08	0.11
(1,38)	1:138:A:ILE:HD12	1:140:A:TYR:HE1	3	0.16	0.08	0.11
(1,38)	1:138:A:ILE:HD13	1:140:A:TYR:HE1	3	0.16	0.08	0.11
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB2	3	0.16	0.04	0.17
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB3	3	0.16	0.04	0.17
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD2	3	0.14	0.01	0.13
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD3	3	0.14	0.01	0.13
(1,37)	1:56:A:ALA:HB1	1:140:A:TYR:HE2	2	2.1	0.02	2.1
(1,37)	1:56:A:ALA:HB2	1:140:A:TYR:HE2	2	2.1	0.02	2.1
(1,37)	1:56:A:ALA:HB3	1:140:A:TYR:HE2	2	2.1	0.02	2.1
(1,34)	1:56:A:ALA:HA	1:140:A:TYR:HD2	2	1.59	0.02	1.59

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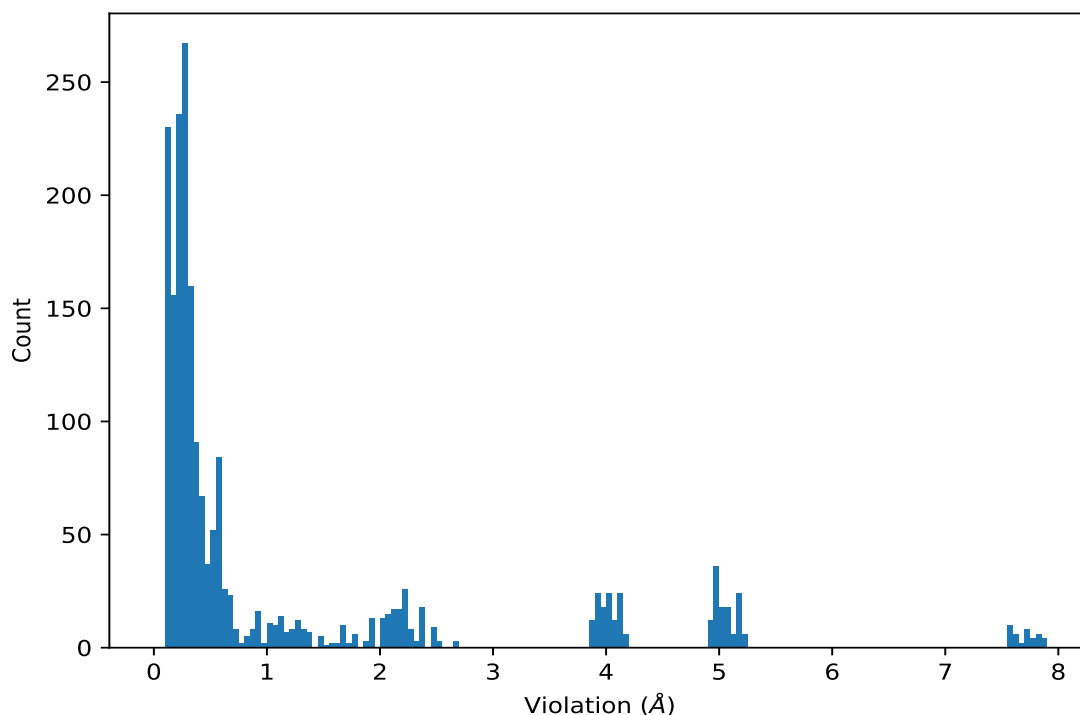
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,163)	1:83:A:ARG:HG2	1:84:A:GLY:H	2	0.33	0.02	0.33
(1,163)	1:83:A:ARG:HG3	1:84:A:GLY:H	2	0.33	0.02	0.33
(1,330)	1:135:A:GLU:H	1:135:A:GLU:HB2	2	0.23	0.06	0.23
(1,330)	1:135:A:GLU:H	1:135:A:GLU:HB3	2	0.23	0.06	0.23
(1,181)	1:86:A:ASP:HA	1:90:A:ALA:H	2	0.16	0.01	0.16
(1,247)	1:110:A:GLU:HG2	1:111:A:ASP:H	2	0.15	0.03	0.15
(1,247)	1:110:A:GLU:HG3	1:111:A:ASP:H	2	0.15	0.03	0.15
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG11	2	0.13	0.0	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG12	2	0.13	0.0	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG13	2	0.13	0.0	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG21	2	0.13	0.0	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG22	2	0.13	0.0	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG23	2	0.13	0.0	0.13
(1,201)	1:93:A:THR:HG21	1:94:A:THR:H	2	0.12	0.01	0.12
(1,201)	1:93:A:THR:HG22	1:94:A:THR:H	2	0.12	0.01	0.12
(1,201)	1:93:A:THR:HG23	1:94:A:THR:H	2	0.12	0.01	0.12
(1,266)	1:113:A:ILE:HA	1:115:A:ALA:H	2	0.12	0.0	0.12
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG11	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG12	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG13	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG21	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG22	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG23	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG11	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG12	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG13	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG21	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG22	2	0.12	0.01	0.12
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG23	2	0.12	0.01	0.12
(1,145)	1:79:A:PRO:HA	1:80:A:THR:H	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)
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	3	7.87
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	3	7.87
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	9	7.87
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	9	7.87
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	10	7.85
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	10	7.85
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	20	7.84
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	20	7.84
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	5	7.82
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	5	7.82
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	13	7.78
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	13	7.78
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	19	7.76
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	19	7.76
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	12	7.72
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	12	7.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	15	7.72
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	15	7.72
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	8	7.7
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	8	7.7
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	18	7.7
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	18	7.7
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	4	7.68
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	4	7.68
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	11	7.64
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	11	7.64
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	16	7.64
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	16	7.64
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	1	7.62
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	1	7.62
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	6	7.59
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	6	7.59
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	2	7.58
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	2	7.58
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	17	7.57
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	17	7.57
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	7	7.56
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	7	7.56
(1,444)	1:99:A:LEU:HB2	1:117:A:PHE:HZ	14	7.56
(1,444)	1:99:A:LEU:HB3	1:117:A:PHE:HZ	14	7.56
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	19	5.2
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	19	5.2
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	19	5.2
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	19	5.2
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	19	5.2
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	19	5.2
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	9	5.18
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	9	5.18
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	9	5.18
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	9	5.18
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	9	5.18
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	9	5.18
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	11	5.18
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	11	5.18
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	11	5.18
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	11	5.18
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	11	5.18
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	11	5.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	3	5.17
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	3	5.17
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	3	5.17
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	3	5.17
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	3	5.17
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	3	5.17
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	5	5.15
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	5	5.15
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	5	5.15
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	5	5.15
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	5	5.15
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	5	5.15
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	10	5.12
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	10	5.12
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	10	5.12
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	10	5.12
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	10	5.12
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	10	5.12
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	6	5.09
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	6	5.09
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	6	5.09
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	6	5.09
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	6	5.09
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	6	5.09
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	4	5.08
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	4	5.08
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	4	5.08
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	4	5.08
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	4	5.08
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	4	5.08
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	20	5.07
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	20	5.07
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	20	5.07
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	20	5.07
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	20	5.07
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	20	5.07
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	7	5.05
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	7	5.05
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	7	5.05
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	7	5.05
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	7	5.05
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	7	5.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	18	5.04
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	18	5.04
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	18	5.04
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	18	5.04
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	18	5.04
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	18	5.04
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	17	5.02
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	17	5.02
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	17	5.02
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	17	5.02
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	17	5.02
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	17	5.02
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	1	4.99
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	1	4.99
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	1	4.99
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	1	4.99
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	1	4.99
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	1	4.99
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	13	4.99
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	13	4.99
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	13	4.99
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	13	4.99
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	13	4.99
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	13	4.99
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	15	4.98
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	15	4.98
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	15	4.98
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	15	4.98
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	15	4.98
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	15	4.98
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	16	4.97
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	16	4.97
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	16	4.97
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	16	4.97
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	16	4.97
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	16	4.97
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	8	4.96
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	8	4.96
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	8	4.96
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	8	4.96
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	8	4.96
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	8	4.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	12	4.95
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	12	4.95
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	12	4.95
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	12	4.95
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	12	4.95
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	12	4.95
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	2	4.94
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	2	4.94
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	2	4.94
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	2	4.94
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	2	4.94
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	2	4.94
(1,446)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	14	4.9
(1,446)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	14	4.9
(1,446)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	14	4.9
(1,446)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	14	4.9
(1,446)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	14	4.9
(1,446)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	14	4.9
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	19	4.16
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	19	4.16
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	19	4.16
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	19	4.16
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	19	4.16
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	19	4.16
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	9	4.14
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	9	4.14
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	9	4.14
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	9	4.14
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	9	4.14
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	9	4.14
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	11	4.14
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	11	4.14
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	11	4.14
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	11	4.14
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	11	4.14
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	11	4.14
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	3	4.13
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	3	4.13
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	3	4.13
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	3	4.13
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	3	4.13
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	3	4.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	5	4.11
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	5	4.11
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	5	4.11
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	5	4.11
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	5	4.11
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	5	4.11
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	10	4.08
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	10	4.08
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	10	4.08
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	10	4.08
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	10	4.08
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	10	4.08
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	6	4.05
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	6	4.05
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	6	4.05
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	6	4.05
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	6	4.05
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	6	4.05
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	4	4.04
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	4	4.04
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	4	4.04
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	4	4.04
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	4	4.04
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	4	4.04
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	20	4.03
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	20	4.03
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	20	4.03
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	20	4.03
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	20	4.03
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	20	4.03
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	7	4.01
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	7	4.01
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	7	4.01
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	7	4.01
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	7	4.01
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	7	4.01
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	18	4.0
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	18	4.0
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	18	4.0
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	18	4.0
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	18	4.0
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	18	4.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	17	3.98
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	17	3.98
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	17	3.98
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	17	3.98
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	17	3.98
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	17	3.98
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	1	3.95
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	1	3.95
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	1	3.95
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	1	3.95
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	1	3.95
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	1	3.95
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	13	3.95
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	13	3.95
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	13	3.95
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	13	3.95
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	13	3.95
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	13	3.95
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	15	3.94
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	15	3.94
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	15	3.94
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	15	3.94
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	15	3.94
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	15	3.94
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	16	3.93
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	16	3.93
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	16	3.93
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	16	3.93
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	16	3.93
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	16	3.93
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	8	3.92
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	8	3.92
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	8	3.92
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	8	3.92
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	8	3.92
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	8	3.92
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	12	3.91
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	12	3.91
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	12	3.91
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	12	3.91
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	12	3.91
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	12	3.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	2	3.9
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	2	3.9
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	2	3.9
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	2	3.9
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	2	3.9
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	2	3.9
(1,18)	1:99:A:LEU:HD11	1:117:A:PHE:HZ	14	3.86
(1,18)	1:99:A:LEU:HD12	1:117:A:PHE:HZ	14	3.86
(1,18)	1:99:A:LEU:HD13	1:117:A:PHE:HZ	14	3.86
(1,18)	1:99:A:LEU:HD21	1:117:A:PHE:HZ	14	3.86
(1,18)	1:99:A:LEU:HD22	1:117:A:PHE:HZ	14	3.86
(1,18)	1:99:A:LEU:HD23	1:117:A:PHE:HZ	14	3.86
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	17	2.67
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	17	2.67
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	17	2.67
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	2	2.51
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	2	2.51
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	2	2.51
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	8	2.47
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	8	2.47
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	8	2.47
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	12	2.47
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	12	2.47
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	12	2.47
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	19	2.47
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	19	2.47
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	19	2.47
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	1	2.4
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	1	2.4
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	1	2.4
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	12	2.38
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	12	2.38
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	12	2.38
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	4	2.37
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	4	2.37
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	4	2.37
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	14	2.36
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	14	2.36
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	14	2.36
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	1	2.36
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	1	2.36
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	1	2.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	17	2.35
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	17	2.35
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	17	2.35
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	3	2.34
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	3	2.34
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	3	2.34
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	18	2.3
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	19	2.27
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	19	2.27
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	19	2.27
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	1	2.26
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	11	2.26
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	18	2.26
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	4	2.25
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	2	2.24
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	8	2.24
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	14	2.24
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	5	2.24
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	5	2.24
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	5	2.24
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	2	2.24
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	2	2.24
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	2	2.24
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	6	2.23
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	10	2.23
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	10	2.23
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	10	2.23
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	10	2.23
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	7	2.22
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	7	2.22
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	7	2.22
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	15	2.21
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	16	2.21
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	10	2.21
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	10	2.21
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	10	2.21
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	19	2.2
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	3	2.2
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	3	2.2
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	3	2.2
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	8	2.19
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	8	2.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	8	2.19
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	13	2.18
(1,33)	1:56:A:ALA:HB1	1:140:A:TYR:HD2	10	2.18
(1,33)	1:56:A:ALA:HB2	1:140:A:TYR:HD2	10	2.18
(1,33)	1:56:A:ALA:HB3	1:140:A:TYR:HD2	10	2.18
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	14	2.18
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	14	2.18
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	14	2.18
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	9	2.16
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	6	2.16
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	6	2.16
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	6	2.16
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	15	2.16
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	15	2.16
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	15	2.16
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	16	2.14
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	16	2.14
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	16	2.14
(1,33)	1:56:A:ALA:HB1	1:140:A:TYR:HD2	20	2.14
(1,33)	1:56:A:ALA:HB2	1:140:A:TYR:HD2	20	2.14
(1,33)	1:56:A:ALA:HB3	1:140:A:TYR:HD2	20	2.14
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	12	2.13
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	20	2.12
(1,37)	1:56:A:ALA:HB1	1:140:A:TYR:HE2	10	2.12
(1,37)	1:56:A:ALA:HB2	1:140:A:TYR:HE2	10	2.12
(1,37)	1:56:A:ALA:HB3	1:140:A:TYR:HE2	10	2.12
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	6	2.12
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	6	2.12
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	6	2.12
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	5	2.1
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	5	2.1
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	5	2.1
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	16	2.09
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	16	2.09
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	16	2.09
(1,37)	1:56:A:ALA:HB1	1:140:A:TYR:HE2	20	2.08
(1,37)	1:56:A:ALA:HB2	1:140:A:TYR:HE2	20	2.08
(1,37)	1:56:A:ALA:HB3	1:140:A:TYR:HE2	20	2.08
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	9	2.08
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	9	2.08
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	9	2.08
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	4	2.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	4	2.08
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	4	2.08
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	7	2.06
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	7	2.06
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	7	2.06
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	11	2.02
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	11	2.02
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	11	2.02
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	11	2.02
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	11	2.02
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	11	2.02
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	15	2.01
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	15	2.01
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	15	2.01
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	17	2.0
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	20	2.0
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	20	2.0
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	20	2.0
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	20	1.95
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	18	1.94
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	18	1.94
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	18	1.94
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	9	1.93
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	9	1.93
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	9	1.93
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	18	1.93
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	18	1.93
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	18	1.93
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	3	1.92
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	7	1.92
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	7	1.91
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	6	1.87
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	8	1.87
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	4	1.85
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	3	1.79
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	16	1.75
(1,59)	1:149:A:TYR:H	1:149:A:TYR:HE1	5	1.75
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	20	1.75
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	20	1.75
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	20	1.75
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	12	1.74
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	2	1.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	9	1.69
(1,36)	1:138:A:ILE:HG21	1:140:A:TYR:HE1	13	1.69
(1,36)	1:138:A:ILE:HG22	1:140:A:TYR:HE1	13	1.69
(1,36)	1:138:A:ILE:HG23	1:140:A:TYR:HE1	13	1.69
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	19	1.68
(1,32)	1:138:A:ILE:HG21	1:140:A:TYR:HD1	13	1.68
(1,32)	1:138:A:ILE:HG22	1:140:A:TYR:HD1	13	1.68
(1,32)	1:138:A:ILE:HG23	1:140:A:TYR:HD1	13	1.68
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	10	1.67
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	11	1.67
(1,34)	1:56:A:ALA:HA	1:140:A:TYR:HD2	10	1.61
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	13	1.6
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	14	1.58
(1,34)	1:56:A:ALA:HA	1:140:A:TYR:HD2	20	1.57
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	15	1.52
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	17	1.48
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	13	1.47
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	13	1.47
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	13	1.47
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	5	1.46
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	4	1.38
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	1	1.37
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	18	1.37
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	9	1.36
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	20	1.36
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	20	1.36
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	20	1.36
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	8	1.34
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	8	1.34
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	8	1.34
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	17	1.31
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	18	1.31
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	18	1.31
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	18	1.31
(1,242)	1:106:A:PRO:HA	1:109:A:GLY:H	1	1.3
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	11	1.29
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	15	1.28
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	12	1.26
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	19	1.26
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	10	1.26
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	10	1.26
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	10	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	2	1.25
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	8	1.25
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	2	1.25
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	2	1.25
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	2	1.25
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	10	1.24
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	5	1.24
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	5	1.24
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	5	1.24
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	13	1.23
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	20	1.23
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	14	1.22
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	7	1.21
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	9	1.2
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	9	1.2
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	9	1.2
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	5	1.18
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	1	1.16
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	1	1.16
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	1	1.16
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	6	1.15
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	1	1.14
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	12	1.14
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	12	1.14
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	12	1.14
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	18	1.13
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	4	1.12
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	11	1.12
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	2	1.11
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	14	1.11
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	14	1.11
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	14	1.11
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	14	1.11
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	3	1.1
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	16	1.09
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	8	1.08
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	10	1.08
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	15	1.07
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	15	1.07
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	15	1.07
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	4	1.06
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	4	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	4	1.06
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	6	1.05
(1,235)	1:106:A:PRO:HA	1:108:A:ARG:H	3	1.04
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	15	1.04
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	7	1.04
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	7	1.04
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	7	1.04
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	7	1.03
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	16	1.02
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	19	1.01
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	16	1.0
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	16	1.0
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	16	1.0
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	5	0.98
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	13	0.97
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	9	0.95
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	10	0.94
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	10	0.94
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	10	0.94
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	11	0.94
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	11	0.94
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	11	0.94
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	17	0.93
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	17	0.93
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	17	0.93
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	12	0.92
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	10	0.92
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	6	0.91
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	6	0.91
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	6	0.91
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	2	0.9
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	20	0.88
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	6	0.88
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	3	0.88
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	3	0.88
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	3	0.88
(1,16)	1:115:A:ALA:HB1	1:117:A:PHE:HD2	19	0.88
(1,16)	1:115:A:ALA:HB2	1:117:A:PHE:HD2	19	0.88
(1,16)	1:115:A:ALA:HB3	1:117:A:PHE:HD2	19	0.88
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	17	0.82
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	12	0.81
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	12	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	12	0.81
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	15	0.81
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	4	0.79
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	14	0.77
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	17	0.73
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	1	0.73
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	12	0.73
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	12	0.73
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	12	0.73
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	19	0.71
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	19	0.71
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	19	0.71
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	2	0.7
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	2	0.7
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	2	0.7
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	20	0.7
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	20	0.7
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	20	0.7
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	2	0.7
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	2	0.7
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	2	0.7
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	15	0.7
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	15	0.7
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	15	0.7
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	6	0.68
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	15	0.68
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	3	0.67
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	20	0.67
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	16	0.67
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	12	0.66
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	12	0.66
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	12	0.66
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	11	0.65
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	20	0.65
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	13	0.65
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	17	0.64
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	3	0.64
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	11	0.64
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	11	0.64
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	11	0.64
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	17	0.63
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	17	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	5	0.63
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	12	0.63
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	7	0.63
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	11	0.62
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	18	0.62
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	17	0.61
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	17	0.61
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	17	0.61
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	11	0.61
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	11	0.61
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	5	0.61
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	5	0.61
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	11	0.61
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	11	0.61
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	9	0.61
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	13	0.61
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	13	0.61
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	13	0.61
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	13	0.61
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	12	0.6
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	12	0.6
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	1	0.6
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	8	0.6
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	9	0.6
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	15	0.6
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	15	0.6
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	15	0.6
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	17	0.6
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	17	0.6
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	17	0.6
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	12	0.6
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	2	0.59
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	2	0.59
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	4	0.59
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	4	0.59
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	19	0.59
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	19	0.59
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	2	0.59
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	4	0.59
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	10	0.59
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	14	0.59
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	19	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	6	0.59
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	19	0.58
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	19	0.58
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	19	0.58
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	1	0.58
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	1	0.58
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	3	0.58
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	3	0.58
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	7	0.58
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	7	0.58
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	9	0.58
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	9	0.58
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	7	0.58
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	16	0.58
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	19	0.58
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	7	0.58
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	7	0.58
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	7	0.58
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	16	0.58
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	16	0.58
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	16	0.58
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	13	0.57
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	13	0.57
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	13	0.57
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	13	0.57
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB2	18	0.57
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB3	18	0.57
(1,150)	1:80:A:THR:HB	1:81:A:VAL:H	18	0.57
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	19	0.57
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	1	0.56
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	1	0.56
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	1	0.56
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	1	0.56
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	1	0.56
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	1	0.56
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	8	0.56
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	8	0.56
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	10	0.56
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	10	0.56
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	15	0.56
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	15	0.56
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	18	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	18	0.56
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	12	0.56
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	7	0.56
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	7	0.56
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	7	0.56
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	5	0.55
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	5	0.55
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	5	0.55
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	5	0.55
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	5	0.55
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	5	0.55
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	18	0.55
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	18	0.55
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	18	0.55
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	18	0.55
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	18	0.55
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	18	0.55
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	20	0.55
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	20	0.55
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	8	0.54
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	8	0.54
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	8	0.54
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	14	0.53
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	14	0.53
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	3	0.53
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	3	0.53
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	3	0.53
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	17	0.53
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	17	0.53
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	17	0.53
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	8	0.52
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	8	0.52
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	8	0.52
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	8	0.52
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	8	0.52
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	8	0.52
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	16	0.52
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	16	0.52
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	13	0.52
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	17	0.51
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	17	0.51
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	17	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	17	0.51
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	17	0.51
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	17	0.51
(1,324)	1:130:A:LYS:HG2	1:131:A:PHE:H	16	0.51
(1,324)	1:130:A:LYS:HG3	1:131:A:PHE:H	16	0.51
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	1	0.51
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	1	0.51
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	1	0.51
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	9	0.51
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	13	0.5
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	13	0.5
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	18	0.5
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	18	0.5
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	12	0.5
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	12	0.5
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	12	0.5
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	12	0.5
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	12	0.5
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	12	0.5
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	1	0.5
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	2	0.5
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	12	0.5
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	12	0.5
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	12	0.5
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	14	0.5
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	14	0.5
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	14	0.5
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	8	0.5
(1,24)	1:123:A:TYR:HD2	1:124:A:GLU:HA	20	0.5
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	6	0.49
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	6	0.49
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	4	0.49
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	4	0.49
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	4	0.49
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	2	0.48
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	2	0.48
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	2	0.48
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	2	0.48
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	2	0.48
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	2	0.48
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	8	0.48
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	16	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	16	0.48
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	16	0.48
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	16	0.48
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	7	0.47
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	7	0.47
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	8	0.47
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	8	0.47
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	12	0.47
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	12	0.47
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	10	0.47
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	16	0.46
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	16	0.46
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	11	0.46
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	3	0.46
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	3	0.46
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	3	0.46
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	16	0.45
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	16	0.45
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	10	0.45
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	10	0.45
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	14	0.45
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	6	0.45
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	6	0.45
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	6	0.45
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	17	0.44
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	17	0.44
(1,463)	1:118:A:LEU:HD11	1:119:A:ILE:H	13	0.44
(1,463)	1:118:A:LEU:HD12	1:119:A:ILE:H	13	0.44
(1,463)	1:118:A:LEU:HD13	1:119:A:ILE:H	13	0.44
(1,463)	1:118:A:LEU:HD21	1:119:A:ILE:H	13	0.44
(1,463)	1:118:A:LEU:HD22	1:119:A:ILE:H	13	0.44
(1,463)	1:118:A:LEU:HD23	1:119:A:ILE:H	13	0.44
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	19	0.44
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	19	0.44
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	1	0.43
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	1	0.43
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	19	0.43
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	19	0.43
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	5	0.43
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	5	0.43
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	5	0.43
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	15	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	15	0.43
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	15	0.43
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	3	0.43
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	3	0.43
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	3	0.43
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	6	0.43
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	6	0.43
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	6	0.43
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	2	0.42
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	2	0.42
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	20	0.42
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	20	0.42
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	15	0.42
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	15	0.42
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	15	0.42
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	11	0.42
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	11	0.42
(1,54)	1:149:A:TYR:H	1:149:A:TYR:HD1	5	0.42
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	18	0.41
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	18	0.41
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	18	0.41
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	1	0.41
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	1	0.41
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	11	0.41
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	11	0.41
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	4	0.41
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	17	0.41
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	17	0.41
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	17	0.41
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	5	0.4
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	5	0.4
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	4	0.4
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	4	0.4
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	4	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	3	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	3	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	4	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	4	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	5	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	5	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	12	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	20	0.4
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	20	0.4
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	4	0.4
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	4	0.4
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	11	0.4
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	11	0.4
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	11	0.4
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	3	0.39
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	3	0.39
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	3	0.39
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	3	0.39
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	3	0.39
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	3	0.39
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	3	0.39
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	3	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	6	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	6	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	13	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	13	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	15	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	15	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	17	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	17	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	18	0.39
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	18	0.39
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	4	0.39
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	6	0.39
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	6	0.39
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	9	0.38
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	9	0.38
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	15	0.38
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	15	0.38
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	9	0.38
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	9	0.38
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	9	0.38
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	11	0.38
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	11	0.38
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	9	0.38
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	9	0.38
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	19	0.37
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	19	0.37
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	16	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	16	0.37
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	16	0.37
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	16	0.37
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	16	0.37
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	16	0.37
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	17	0.37
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	17	0.37
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	17	0.37
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	17	0.37
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	17	0.37
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	17	0.37
(1,424)	1:82:A:ARG:HG2	1:83:A:ARG:H	6	0.37
(1,424)	1:82:A:ARG:HG3	1:83:A:ARG:H	6	0.37
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	17	0.37
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	17	0.37
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	7	0.37
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	7	0.37
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	14	0.37
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	14	0.37
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	19	0.37
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	19	0.37
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	4	0.37
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	4	0.37
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	4	0.37
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	18	0.37
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	20	0.36
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	20	0.36
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	20	0.36
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	20	0.36
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	20	0.36
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	20	0.36
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	3	0.36
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	3	0.36
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	3	0.36
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	2	0.36
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	2	0.36
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	15	0.36
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	15	0.36
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	15	0.36
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	17	0.36
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	17	0.36
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	1	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	1	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	8	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	8	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	10	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	10	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	18	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	18	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	20	0.36
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	20	0.36
(1,70)	1:56:A:ALA:HB1	1:57:A:GLY:H	19	0.36
(1,70)	1:56:A:ALA:HB2	1:57:A:GLY:H	19	0.36
(1,70)	1:56:A:ALA:HB3	1:57:A:GLY:H	19	0.36
(1,60)	1:149:A:TYR:HA	1:149:A:TYR:HE1	15	0.36
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	4	0.35
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	4	0.35
(1,506)	1:141:A:LEU:HD11	1:146:A:TYR:HE1	19	0.35
(1,506)	1:141:A:LEU:HD12	1:146:A:TYR:HE1	19	0.35
(1,506)	1:141:A:LEU:HD13	1:146:A:TYR:HE1	19	0.35
(1,506)	1:141:A:LEU:HD21	1:146:A:TYR:HE1	19	0.35
(1,506)	1:141:A:LEU:HD22	1:146:A:TYR:HE1	19	0.35
(1,506)	1:141:A:LEU:HD23	1:146:A:TYR:HE1	19	0.35
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	9	0.35
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	9	0.35
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	9	0.35
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	9	0.35
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	9	0.35
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	9	0.35
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	13	0.35
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	13	0.35
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	13	0.35
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	10	0.35
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	10	0.35
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG2	8	0.35
(1,204)	1:95:A:GLN:H	1:95:A:GLN:HG3	8	0.35
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	8	0.35
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	8	0.35
(1,163)	1:83:A:ARG:HG2	1:84:A:GLY:H	2	0.35
(1,163)	1:83:A:ARG:HG3	1:84:A:GLY:H	2	0.35
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	13	0.35
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	13	0.35
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	13	0.35
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	13	0.35
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	13	0.35
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	18	0.35
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	18	0.35
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	18	0.35
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	1	0.34
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	1	0.34
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	10	0.34
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	10	0.34
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	14	0.34
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	14	0.34
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	19	0.34
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	19	0.34
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	19	0.34
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	19	0.34
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	19	0.34
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	19	0.34
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	5	0.34
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	5	0.34
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	5	0.34
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	6	0.34
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	6	0.34
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	6	0.34
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	5	0.34
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	5	0.34
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	6	0.34
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	6	0.34
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	6	0.34
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	15	0.34
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	19	0.34
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	19	0.34
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	18	0.33
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	18	0.33
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	18	0.33
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	18	0.33
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	18	0.33
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	18	0.33
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	5	0.33
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	5	0.33
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	5	0.33
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	5	0.33
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	5	0.33
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	7	0.33
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	7	0.33
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	7	0.33
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	20	0.33
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	20	0.33
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	20	0.33
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	18	0.33
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	3	0.33
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	3	0.33
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	19	0.32
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	19	0.32
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	1	0.32
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	1	0.32
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	1	0.32
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	1	0.32
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	1	0.32
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	1	0.32
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	7	0.32
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	7	0.32
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	7	0.32
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	7	0.32
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	7	0.32
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	7	0.32
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	10	0.32
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	10	0.32
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	10	0.32
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	10	0.32
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	10	0.32
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	10	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	1	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	1	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	1	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	1	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	1	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	1	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	6	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	6	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	6	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	6	0.32
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	6	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	6	0.32
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	7	0.32
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	7	0.32
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	5	0.32
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	5	0.32
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	5	0.32
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	9	0.32
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	9	0.32
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	9	0.32
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	6	0.32
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	8	0.32
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	2	0.32
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	2	0.32
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	2	0.32
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	15	0.31
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	15	0.31
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	15	0.31
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	15	0.31
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	15	0.31
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	15	0.31
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	19	0.31
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	19	0.31
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	19	0.31
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	19	0.31
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	19	0.31
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	19	0.31
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	15	0.31
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	15	0.31
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	15	0.31
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	15	0.31
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	15	0.31
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	15	0.31
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	14	0.31
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	14	0.31
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	14	0.31
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	2	0.31
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	2	0.31
(1,163)	1:83:A:ARG:HG2	1:84:A:GLY:H	10	0.31
(1,163)	1:83:A:ARG:HG3	1:84:A:GLY:H	10	0.31
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	20	0.31
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	20	0.31
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	2	0.31
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	2	0.31
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	15	0.31
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	15	0.31
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	17	0.31
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	17	0.31
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD2	19	0.3
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD3	19	0.3
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	2	0.3
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	2	0.3
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	2	0.3
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	2	0.3
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	2	0.3
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	2	0.3
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	13	0.3
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	13	0.3
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	13	0.3
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	13	0.3
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	13	0.3
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	13	0.3
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	4	0.3
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	4	0.3
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	6	0.3
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	6	0.3
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	8	0.3
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	8	0.3
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	18	0.3
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	18	0.3
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	20	0.3
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	20	0.3
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	8	0.3
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	8	0.3
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	8	0.3
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	16	0.3
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	16	0.3
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	16	0.3
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	13	0.3
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	9	0.3
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	9	0.3
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	9	0.3
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	11	0.3
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	11	0.3
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	14	0.3
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	14	0.3
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	14	0.3
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	8	0.3
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	3	0.29
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	3	0.29
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	3	0.29
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	3	0.29
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	3	0.29
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	3	0.29
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	14	0.29
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	14	0.29
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	14	0.29
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	14	0.29
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	14	0.29
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	14	0.29
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	3	0.29
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	3	0.29
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	3	0.29
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	3	0.29
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	3	0.29
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	3	0.29
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	8	0.29
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	8	0.29
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	8	0.29
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	16	0.29
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	16	0.29
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	11	0.29
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	11	0.29
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	11	0.29
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	17	0.29
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	7	0.29
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	10	0.29
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	20	0.29
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	8	0.28
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	8	0.28
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	8	0.28
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	8	0.28
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	8	0.28
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	8	0.28
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	17	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	17	0.28
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	17	0.28
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	17	0.28
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	17	0.28
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	17	0.28
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	10	0.28
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	10	0.28
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	10	0.28
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	6	0.28
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	6	0.28
(1,330)	1:135:A:GLU:H	1:135:A:GLU:HB2	17	0.28
(1,330)	1:135:A:GLU:H	1:135:A:GLU:HB3	17	0.28
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	3	0.28
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	3	0.28
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	7	0.28
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	7	0.28
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	14	0.28
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	14	0.28
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	3	0.28
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	3	0.28
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	6	0.28
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	6	0.28
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	14	0.28
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	14	0.28
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	14	0.28
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	11	0.28
(1,70)	1:56:A:ALA:HB1	1:57:A:GLY:H	17	0.28
(1,70)	1:56:A:ALA:HB2	1:57:A:GLY:H	17	0.28
(1,70)	1:56:A:ALA:HB3	1:57:A:GLY:H	17	0.28
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	19	0.28
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	19	0.28
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	19	0.28
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	15	0.28
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	4	0.27
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	4	0.27
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	4	0.27
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	4	0.27
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	4	0.27
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	4	0.27
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	12	0.27
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	12	0.27
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	12	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	12	0.27
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	12	0.27
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	12	0.27
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	1	0.27
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	1	0.27
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	1	0.27
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	1	0.27
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	1	0.27
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	1	0.27
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	11	0.27
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	11	0.27
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	11	0.27
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	3	0.27
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	4	0.27
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	4	0.27
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	20	0.27
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	20	0.27
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	19	0.27
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	19	0.27
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	1	0.27
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	1	0.27
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	15	0.27
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	15	0.27
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	20	0.27
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	7	0.27
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	7	0.27
(1,38)	1:138:A:ILE:HD11	1:140:A:TYR:HE1	10	0.27
(1,38)	1:138:A:ILE:HD12	1:140:A:TYR:HE1	10	0.27
(1,38)	1:138:A:ILE:HD13	1:140:A:TYR:HE1	10	0.27
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	2	0.27
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	1	0.27
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	1	0.27
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	1	0.27
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	9	0.27
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	9	0.27
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	9	0.27
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	11	0.26
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	11	0.26
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD2	11	0.26
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD3	11	0.26
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG2	11	0.26
(1,511)	1:144:A:GLU:H	1:144:A:GLU:HG3	11	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	2	0.26
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	2	0.26
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	2	0.26
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	2	0.26
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	2	0.26
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	2	0.26
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	5	0.26
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	5	0.26
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	5	0.26
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	5	0.26
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	5	0.26
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	5	0.26
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	9	0.26
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	9	0.26
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	9	0.26
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	9	0.26
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	9	0.26
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	9	0.26
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	11	0.26
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	11	0.26
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	11	0.26
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	11	0.26
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	11	0.26
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	11	0.26
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	12	0.26
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	12	0.26
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	12	0.26
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	12	0.26
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	12	0.26
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	12	0.26
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	20	0.26
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	20	0.26
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	9	0.26
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	9	0.26
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	16	0.26
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	16	0.26
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	16	0.26
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	2	0.26
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	2	0.26
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	17	0.26
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	5	0.26
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	12	0.26
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	12	0.26
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	8	0.26
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	8	0.26
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	4	0.26
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	4	0.26
(1,149)	1:80:A:THR:HG21	1:81:A:VAL:H	12	0.26
(1,149)	1:80:A:THR:HG22	1:81:A:VAL:H	12	0.26
(1,149)	1:80:A:THR:HG23	1:81:A:VAL:H	12	0.26
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	16	0.26
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	4	0.26
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	4	0.26
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	4	0.26
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	13	0.25
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	13	0.25
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	13	0.25
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	13	0.25
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	13	0.25
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	13	0.25
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	8	0.25
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	8	0.25
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	8	0.25
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	8	0.25
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	8	0.25
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	8	0.25
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	20	0.25
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	20	0.25
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	20	0.25
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	20	0.25
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	20	0.25
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	20	0.25
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	12	0.25
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	12	0.25
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	13	0.25
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	13	0.25
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	6	0.25
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	6	0.25
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	18	0.25
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	18	0.25
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	1	0.25
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	13	0.25
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	9	0.25
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	9	0.25
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	15	0.25
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	15	0.25
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	2	0.25
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	2	0.25
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	17	0.25
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	17	0.25
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	5	0.25
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	4	0.25
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	4	0.25
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	4	0.25
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	8	0.25
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	8	0.25
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	8	0.25
(1,33)	1:56:A:ALA:HB1	1:140:A:TYR:HD2	17	0.25
(1,33)	1:56:A:ALA:HB2	1:140:A:TYR:HD2	17	0.25
(1,33)	1:56:A:ALA:HB3	1:140:A:TYR:HD2	17	0.25
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	8	0.25
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	8	0.25
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	8	0.25
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	7	0.24
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	7	0.24
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	7	0.24
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	7	0.24
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	7	0.24
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	7	0.24
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	10	0.24
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	10	0.24
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	10	0.24
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	10	0.24
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	10	0.24
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	10	0.24
(1,468)	1:122:A:LEU:HB2	1:127:A:PHE:HD1	3	0.24
(1,468)	1:122:A:LEU:HB3	1:127:A:PHE:HD1	3	0.24
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	8	0.24
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	8	0.24
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	7	0.24
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	8	0.24
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	15	0.24
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	15	0.24
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	15	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:95:A:GLN:HG2	1:97:A:CYS:H	13	0.24
(1,213)	1:95:A:GLN:HG3	1:97:A:CYS:H	13	0.24
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	1	0.24
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	1	0.24
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	9	0.24
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	9	0.24
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	19	0.24
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	19	0.24
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	19	0.24
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	9	0.24
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	5	0.24
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	5	0.24
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	16	0.24
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	16	0.24
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	9	0.24
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	9	0.24
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	9	0.24
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	20	0.24
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	20	0.24
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	20	0.24
(1,424)	1:82:A:ARG:HG2	1:83:A:ARG:H	5	0.23
(1,424)	1:82:A:ARG:HG3	1:83:A:ARG:H	5	0.23
(1,424)	1:82:A:ARG:HG2	1:83:A:ARG:H	7	0.23
(1,424)	1:82:A:ARG:HG3	1:83:A:ARG:H	7	0.23
(1,424)	1:82:A:ARG:HG2	1:83:A:ARG:H	20	0.23
(1,424)	1:82:A:ARG:HG3	1:83:A:ARG:H	20	0.23
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	16	0.23
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	16	0.23
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	2	0.23
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	2	0.23
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	2	0.23
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	19	0.23
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	19	0.23
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	2	0.23
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	9	0.23
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	14	0.23
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	20	0.23
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	2	0.23
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	2	0.23
(1,149)	1:80:A:THR:HG21	1:81:A:VAL:H	11	0.23
(1,149)	1:80:A:THR:HG22	1:81:A:VAL:H	11	0.23
(1,149)	1:80:A:THR:HG23	1:81:A:VAL:H	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	19	0.23
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	7	0.23
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	7	0.23
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	7	0.23
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	19	0.23
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	9	0.23
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	9	0.23
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	12	0.23
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	12	0.23
(1,10)	1:85:A:TRP:HE3	1:88:A:VAL:HB	17	0.23
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	19	0.23
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	19	0.23
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	19	0.23
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD2	16	0.22
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD3	16	0.22
(1,509)	1:141:A:LEU:HD11	1:149:A:TYR:HD2	7	0.22
(1,509)	1:141:A:LEU:HD12	1:149:A:TYR:HD2	7	0.22
(1,509)	1:141:A:LEU:HD13	1:149:A:TYR:HD2	7	0.22
(1,509)	1:141:A:LEU:HD21	1:149:A:TYR:HD2	7	0.22
(1,509)	1:141:A:LEU:HD22	1:149:A:TYR:HD2	7	0.22
(1,509)	1:141:A:LEU:HD23	1:149:A:TYR:HD2	7	0.22
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	16	0.22
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	16	0.22
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	16	0.22
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	16	0.22
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	16	0.22
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	16	0.22
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	20	0.22
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	20	0.22
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	20	0.22
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	20	0.22
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	20	0.22
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	20	0.22
(1,424)	1:82:A:ARG:HG2	1:83:A:ARG:H	12	0.22
(1,424)	1:82:A:ARG:HG3	1:83:A:ARG:H	12	0.22
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	7	0.22
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	7	0.22
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	7	0.22
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	7	0.22
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	7	0.22
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	7	0.22
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	3	0.22
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	12	0.22
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	12	0.22
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	5	0.22
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	10	0.22
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	11	0.22
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	19	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	1	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	1	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	1	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	14	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	14	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	14	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	17	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	17	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	17	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	19	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	19	0.22
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	19	0.22
(1,149)	1:80:A:THR:HG21	1:81:A:VAL:H	3	0.22
(1,149)	1:80:A:THR:HG22	1:81:A:VAL:H	3	0.22
(1,149)	1:80:A:THR:HG23	1:81:A:VAL:H	3	0.22
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	10	0.22
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	10	0.22
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	10	0.22
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	10	0.22
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	10	0.22
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	10	0.22
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	10	0.22
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	19	0.22
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	19	0.22
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	19	0.22
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	10	0.22
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	10	0.22
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	10	0.22
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	14	0.22
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	14	0.22
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	14	0.22
(1,506)	1:141:A:LEU:HD11	1:146:A:TYR:HE1	17	0.21
(1,506)	1:141:A:LEU:HD12	1:146:A:TYR:HE1	17	0.21
(1,506)	1:141:A:LEU:HD13	1:146:A:TYR:HE1	17	0.21
(1,506)	1:141:A:LEU:HD21	1:146:A:TYR:HE1	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:141:A:LEU:HD22	1:146:A:TYR:HE1	17	0.21
(1,506)	1:141:A:LEU:HD23	1:146:A:TYR:HE1	17	0.21
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	14	0.21
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	14	0.21
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	14	0.21
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	14	0.21
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	14	0.21
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	14	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	10	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	10	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	10	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	10	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	10	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	10	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	16	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	16	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	16	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	16	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	16	0.21
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	16	0.21
(1,343)	1:56:A:ALA:HB1	1:141:A:LEU:H	1	0.21
(1,343)	1:56:A:ALA:HB2	1:141:A:LEU:H	1	0.21
(1,343)	1:56:A:ALA:HB3	1:141:A:LEU:H	1	0.21
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	10	0.21
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	10	0.21
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	6	0.21
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	6	0.21
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	6	0.21
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	9	0.21
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	9	0.21
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	9	0.21
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	5	0.21
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	5	0.21
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	17	0.21
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	17	0.21
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	16	0.21
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	1	0.21
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	1	0.21
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	1	0.21
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	18	0.21
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	18	0.21
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	1	0.2
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	1	0.2
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	19	0.2
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	19	0.2
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	1	0.2
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	1	0.2
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	10	0.2
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	10	0.2
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	17	0.2
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	17	0.2
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB2	3	0.2
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB3	3	0.2
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	6	0.2
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	6	0.2
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	6	0.2
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	6	0.2
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	6	0.2
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	6	0.2
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	7	0.2
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	7	0.2
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	13	0.2
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	13	0.2
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	12	0.2
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	10	0.2
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	10	0.2
(1,176)	1:88:A:VAL:HB	1:89:A:ARG:H	17	0.2
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	13	0.2
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	18	0.2
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	18	0.2
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	18	0.2
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	13	0.2
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	13	0.2
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	1	0.2
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	1	0.2
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	1	0.2
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	10	0.2
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	10	0.2
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	10	0.2
(1,31)	1:138:A:ILE:HD11	1:140:A:TYR:HD1	18	0.2
(1,31)	1:138:A:ILE:HD12	1:140:A:TYR:HD1	18	0.2
(1,31)	1:138:A:ILE:HD13	1:140:A:TYR:HD1	18	0.2
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	5	0.2
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	5	0.2
(1,6)	1:74:A:THR:HG21	1:75:A:PHE:HD1	18	0.2
(1,6)	1:74:A:THR:HG22	1:75:A:PHE:HD1	18	0.2
(1,6)	1:74:A:THR:HG23	1:75:A:PHE:HD1	18	0.2
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	4	0.19
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	4	0.19
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	8	0.19
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	8	0.19
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	11	0.19
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	11	0.19
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	15	0.19
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	15	0.19
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	18	0.19
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	18	0.19
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	4	0.19
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	4	0.19
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	4	0.19
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	4	0.19
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	4	0.19
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	4	0.19
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	15	0.19
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	15	0.19
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	15	0.19
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	15	0.19
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	15	0.19
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	15	0.19
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	15	0.19
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	15	0.19
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	4	0.19
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	4	0.19
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	4	0.19
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	4	0.19
(1,323)	1:130:A:LYS:HD2	1:131:A:PHE:H	6	0.19
(1,323)	1:130:A:LYS:HD3	1:131:A:PHE:H	6	0.19
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	4	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	3	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	3	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	3	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	4	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	4	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	8	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	8	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	8	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	18	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	18	0.19
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	18	0.19
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	18	0.19
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	18	0.19
(1,149)	1:80:A:THR:HG21	1:81:A:VAL:H	15	0.19
(1,149)	1:80:A:THR:HG22	1:81:A:VAL:H	15	0.19
(1,149)	1:80:A:THR:HG23	1:81:A:VAL:H	15	0.19
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	1	0.19
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	1	0.19
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	7	0.19
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	2	0.19
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	2	0.19
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	2	0.19
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	3	0.19
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	3	0.19
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	3	0.19
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	5	0.19
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	5	0.19
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	5	0.19
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	2	0.18
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	2	0.18
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	9	0.18
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	9	0.18
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	10	0.18
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	10	0.18
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	14	0.18
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	14	0.18
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	13	0.18
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	13	0.18
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD2	18	0.18
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD3	18	0.18
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	3	0.18
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	3	0.18
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	7	0.18
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	7	0.18
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	6	0.18
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	5	0.18
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	5	0.18
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	7	0.18
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	7	0.18
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	7	0.18
(1,247)	1:110:A:GLU:HG2	1:111:A:ASP:H	14	0.18
(1,247)	1:110:A:GLU:HG3	1:111:A:ASP:H	14	0.18
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	14	0.18
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	14	0.18
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	14	0.18
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	18	0.18
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	20	0.18
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	20	0.18
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	20	0.18
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	5	0.17
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	5	0.17
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	12	0.17
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	12	0.17
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	16	0.17
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	16	0.17
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	17	0.17
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	17	0.17
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	20	0.17
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	20	0.17
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD2	13	0.17
(1,519)	1:146:A:TYR:HE2	1:150:A:ARG:HD3	13	0.17
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB2	7	0.17
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB3	7	0.17
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	8	0.17
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	8	0.17
(1,330)	1:135:A:GLU:H	1:135:A:GLU:HB2	19	0.17
(1,330)	1:135:A:GLU:H	1:135:A:GLU:HB3	19	0.17
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	7	0.17
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	7	0.17
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	16	0.17
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	16	0.17
(1,181)	1:86:A:ASP:HA	1:90:A:ALA:H	4	0.17
(1,149)	1:80:A:THR:HG21	1:81:A:VAL:H	17	0.17
(1,149)	1:80:A:THR:HG22	1:81:A:VAL:H	17	0.17
(1,149)	1:80:A:THR:HG23	1:81:A:VAL:H	17	0.17
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	18	0.17
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	2	0.17
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	2	0.17
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	2	0.17
(1,70)	1:56:A:ALA:HB1	1:57:A:GLY:H	12	0.17
(1,70)	1:56:A:ALA:HB2	1:57:A:GLY:H	12	0.17
(1,70)	1:56:A:ALA:HB3	1:57:A:GLY:H	12	0.17
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	7	0.16
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	7	0.16
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	13	0.16
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	13	0.16
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	2	0.16
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	2	0.16
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	2	0.16
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	2	0.16
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	2	0.16
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	2	0.16
(1,382)	1:151:A:GLN:HB2	1:152:A:LEU:H	10	0.16
(1,382)	1:151:A:GLN:HB3	1:152:A:LEU:H	10	0.16
(1,333)	1:135:A:GLU:HG2	1:136:A:GLY:H	12	0.16
(1,333)	1:135:A:GLU:HG3	1:136:A:GLY:H	12	0.16
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	20	0.16
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	20	0.16
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	20	0.16
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	6	0.16
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	6	0.16
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	18	0.16
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	18	0.16
(1,181)	1:86:A:ASP:HA	1:90:A:ALA:H	1	0.16
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD2	17	0.16
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD3	17	0.16
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	9	0.16
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	3	0.16
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	3	0.16
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	3	0.16
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB2	14	0.16
(1,84)	1:67:A:ALA:H	1:70:A:SER:HB3	14	0.16
(1,513)	1:144:A:GLU:HG2	1:145:A:VAL:H	14	0.15
(1,513)	1:144:A:GLU:HG3	1:145:A:VAL:H	14	0.15
(1,506)	1:141:A:LEU:HD11	1:146:A:TYR:HE1	11	0.15
(1,506)	1:141:A:LEU:HD12	1:146:A:TYR:HE1	11	0.15
(1,506)	1:141:A:LEU:HD13	1:146:A:TYR:HE1	11	0.15
(1,506)	1:141:A:LEU:HD21	1:146:A:TYR:HE1	11	0.15
(1,506)	1:141:A:LEU:HD22	1:146:A:TYR:HE1	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,506)	1:141:A:LEU:HD23	1:146:A:TYR:HE1	11	0.15
(1,506)	1:141:A:LEU:HD11	1:146:A:TYR:HE1	16	0.15
(1,506)	1:141:A:LEU:HD12	1:146:A:TYR:HE1	16	0.15
(1,506)	1:141:A:LEU:HD13	1:146:A:TYR:HE1	16	0.15
(1,506)	1:141:A:LEU:HD21	1:146:A:TYR:HE1	16	0.15
(1,506)	1:141:A:LEU:HD22	1:146:A:TYR:HE1	16	0.15
(1,506)	1:141:A:LEU:HD23	1:146:A:TYR:HE1	16	0.15
(1,470)	1:122:A:LEU:HD11	1:125:A:GLN:H	11	0.15
(1,470)	1:122:A:LEU:HD12	1:125:A:GLN:H	11	0.15
(1,470)	1:122:A:LEU:HD13	1:125:A:GLN:H	11	0.15
(1,470)	1:122:A:LEU:HD21	1:125:A:GLN:H	11	0.15
(1,470)	1:122:A:LEU:HD22	1:125:A:GLN:H	11	0.15
(1,470)	1:122:A:LEU:HD23	1:125:A:GLN:H	11	0.15
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	17	0.15
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	17	0.15
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	17	0.15
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	17	0.15
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	17	0.15
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	17	0.15
(1,391)	1:153:A:VAL:HB	1:154:A:ASP:H	18	0.15
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	2	0.15
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	2	0.15
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	17	0.15
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	17	0.15
(1,290)	1:122:A:LEU:HG	1:123:A:TYR:H	16	0.15
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	11	0.15
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	11	0.15
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	11	0.15
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	12	0.15
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	12	0.15
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	12	0.15
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	11	0.15
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	11	0.15
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	15	0.15
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	15	0.15
(1,109)	1:67:A:ALA:HA	1:71:A:ASN:H	3	0.15
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	7	0.15
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	7	0.15
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB2	2	0.14
(1,520)	1:146:A:TYR:HD2	1:150:A:ARG:HB3	2	0.14
(1,468)	1:122:A:LEU:HB2	1:127:A:PHE:HD1	17	0.14
(1,468)	1:122:A:LEU:HB3	1:127:A:PHE:HD1	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	20	0.14
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	20	0.14
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	2	0.14
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	2	0.14
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	2	0.14
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	9	0.14
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	9	0.14
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	11	0.14
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	11	0.14
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	9	0.14
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	9	0.14
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	14	0.14
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	14	0.14
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	17	0.14
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	17	0.14
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB1	12	0.14
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB2	12	0.14
(1,82)	1:66:A:GLN:H	1:67:A:ALA:HB3	12	0.14
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG11	1	0.13
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG12	1	0.13
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG13	1	0.13
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG21	1	0.13
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG22	1	0.13
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG23	1	0.13
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG11	1	0.13
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG12	1	0.13
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG13	1	0.13
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG21	1	0.13
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG22	1	0.13
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG23	1	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG11	3	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG12	3	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG13	3	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG21	3	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG22	3	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG23	3	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG11	7	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG12	7	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG13	7	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG21	7	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG22	7	0.13
(1,476)	1:123:A:TYR:HD1	1:128:A:VAL:HG23	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,471)	1:122:A:LEU:HD11	1:126:A:ASN:H	6	0.13
(1,471)	1:122:A:LEU:HD12	1:126:A:ASN:H	6	0.13
(1,471)	1:122:A:LEU:HD13	1:126:A:ASN:H	6	0.13
(1,471)	1:122:A:LEU:HD21	1:126:A:ASN:H	6	0.13
(1,471)	1:122:A:LEU:HD22	1:126:A:ASN:H	6	0.13
(1,471)	1:122:A:LEU:HD23	1:126:A:ASN:H	6	0.13
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	14	0.13
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	14	0.13
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	14	0.13
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	14	0.13
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	14	0.13
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	14	0.13
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	10	0.13
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	10	0.13
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	10	0.13
(1,240)	1:108:A:ARG:HG2	1:109:A:GLY:H	19	0.13
(1,240)	1:108:A:ARG:HG3	1:109:A:GLY:H	19	0.13
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	3	0.13
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	3	0.13
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	4	0.13
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	4	0.13
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	12	0.13
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	12	0.13
(1,201)	1:93:A:THR:HG21	1:94:A:THR:H	11	0.13
(1,201)	1:93:A:THR:HG22	1:94:A:THR:H	11	0.13
(1,201)	1:93:A:THR:HG23	1:94:A:THR:H	11	0.13
(1,191)	1:92:A:CYS:H	1:93:A:THR:HG21	17	0.13
(1,191)	1:92:A:CYS:H	1:93:A:THR:HG22	17	0.13
(1,191)	1:92:A:CYS:H	1:93:A:THR:HG23	17	0.13
(1,176)	1:88:A:VAL:HB	1:89:A:ARG:H	15	0.13
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD2	7	0.13
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD3	7	0.13
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD2	10	0.13
(1,175)	1:89:A:ARG:H	1:89:A:ARG:HD3	10	0.13
(1,149)	1:80:A:THR:HG21	1:81:A:VAL:H	20	0.13
(1,149)	1:80:A:THR:HG22	1:81:A:VAL:H	20	0.13
(1,149)	1:80:A:THR:HG23	1:81:A:VAL:H	20	0.13
(1,114)	1:67:A:ALA:HB1	1:71:A:ASN:H	12	0.13
(1,114)	1:67:A:ALA:HB2	1:71:A:ASN:H	12	0.13
(1,114)	1:67:A:ALA:HB3	1:71:A:ASN:H	12	0.13
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	13	0.13
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:115:A:ALA:HB1	1:117:A:PHE:HE2	13	0.13
(1,17)	1:115:A:ALA:HB2	1:117:A:PHE:HE2	13	0.13
(1,17)	1:115:A:ALA:HB3	1:117:A:PHE:HE2	13	0.13
(1,468)	1:122:A:LEU:HB2	1:127:A:PHE:HD1	5	0.12
(1,468)	1:122:A:LEU:HB3	1:127:A:PHE:HD1	5	0.12
(1,391)	1:153:A:VAL:HB	1:154:A:ASP:H	10	0.12
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	1	0.12
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	1	0.12
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	5	0.12
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	5	0.12
(1,360)	1:143:A:ARG:HB2	1:144:A:GLU:H	10	0.12
(1,360)	1:143:A:ARG:HB3	1:144:A:GLU:H	10	0.12
(1,334)	1:135:A:GLU:HA	1:136:A:GLY:H	1	0.12
(1,266)	1:113:A:ILE:HA	1:115:A:ALA:H	9	0.12
(1,266)	1:113:A:ILE:HA	1:115:A:ALA:H	20	0.12
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD11	13	0.12
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD12	13	0.12
(1,257)	1:113:A:ILE:H	1:113:A:ILE:HD13	13	0.12
(1,247)	1:110:A:GLU:HG2	1:111:A:ASP:H	3	0.12
(1,247)	1:110:A:GLU:HG3	1:111:A:ASP:H	3	0.12
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB2	9	0.12
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB3	9	0.12
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB2	12	0.12
(1,245)	1:110:A:GLU:H	1:110:A:GLU:HB3	12	0.12
(1,231)	1:107:A:ASP:H	1:107:A:ASP:HB2	17	0.12
(1,231)	1:107:A:ASP:H	1:107:A:ASP:HB3	17	0.12
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	5	0.12
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	5	0.12
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	10	0.12
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	10	0.12
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	20	0.12
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	20	0.12
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	13	0.12
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	13	0.12
(1,176)	1:88:A:VAL:HB	1:89:A:ARG:H	2	0.12
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	10	0.12
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	12	0.12
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	5	0.12
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	5	0.12
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	1	0.12
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	1	0.12
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB2	5	0.11
(1,478)	1:123:A:TYR:HD2	1:124:A:GLU:HB3	5	0.11
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG11	18	0.11
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG12	18	0.11
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG13	18	0.11
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG21	18	0.11
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG22	18	0.11
(1,477)	1:123:A:TYR:HE1	1:128:A:VAL:HG23	18	0.11
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG11	18	0.11
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG12	18	0.11
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG13	18	0.11
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG21	18	0.11
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG22	18	0.11
(1,477)	1:123:A:TYR:HE2	1:128:A:VAL:HG23	18	0.11
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG11	8	0.11
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG12	8	0.11
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG13	8	0.11
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG21	8	0.11
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG22	8	0.11
(1,399)	1:61:A:PHE:H	1:62:A:VAL:HG23	8	0.11
(1,391)	1:153:A:VAL:HB	1:154:A:ASP:H	4	0.11
(1,391)	1:153:A:VAL:HB	1:154:A:ASP:H	12	0.11
(1,334)	1:135:A:GLU:HA	1:136:A:GLY:H	3	0.11
(1,334)	1:135:A:GLU:HA	1:136:A:GLY:H	7	0.11
(1,332)	1:135:A:GLU:HB2	1:136:A:GLY:H	18	0.11
(1,332)	1:135:A:GLU:HB3	1:136:A:GLY:H	18	0.11
(1,208)	1:95:A:GLN:HG2	1:96:A:ASN:H	13	0.11
(1,208)	1:95:A:GLN:HG3	1:96:A:ASN:H	13	0.11
(1,201)	1:93:A:THR:HG21	1:94:A:THR:H	17	0.11
(1,201)	1:93:A:THR:HG22	1:94:A:THR:H	17	0.11
(1,201)	1:93:A:THR:HG23	1:94:A:THR:H	17	0.11
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	12	0.11
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	12	0.11
(1,182)	1:89:A:ARG:HD2	1:90:A:ALA:H	14	0.11
(1,182)	1:89:A:ARG:HD3	1:90:A:ALA:H	14	0.11
(1,176)	1:88:A:VAL:HB	1:89:A:ARG:H	8	0.11
(1,145)	1:79:A:PRO:HA	1:80:A:THR:H	11	0.11
(1,145)	1:79:A:PRO:HA	1:80:A:THR:H	16	0.11
(1,87)	1:66:A:GLN:HB2	1:67:A:ALA:H	15	0.11
(1,87)	1:66:A:GLN:HB3	1:67:A:ALA:H	15	0.11
(1,57)	1:146:A:TYR:HD2	1:150:A:ARG:H	19	0.11
(1,43)	1:55:A:THR:HG21	1:146:A:TYR:HD1	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:55:A:THR:HG22	1:146:A:TYR:HD1	6	0.11
(1,43)	1:55:A:THR:HG23	1:146:A:TYR:HD1	6	0.11
(1,38)	1:138:A:ILE:HD11	1:140:A:TYR:HE1	2	0.11
(1,38)	1:138:A:ILE:HD12	1:140:A:TYR:HE1	2	0.11
(1,38)	1:138:A:ILE:HD13	1:140:A:TYR:HE1	2	0.11
(1,530)	1:152:A:LEU:HB2	1:153:A:VAL:H	3	0.1
(1,530)	1:152:A:LEU:HB3	1:153:A:VAL:H	3	0.1
(1,391)	1:153:A:VAL:HB	1:154:A:ASP:H	5	0.1
(1,334)	1:135:A:GLU:HA	1:136:A:GLY:H	10	0.1
(1,135)	1:75:A:PHE:HA	1:77:A:GLU:H	7	0.1
(1,38)	1:138:A:ILE:HD11	1:140:A:TYR:HE1	17	0.1
(1,38)	1:138:A:ILE:HD12	1:140:A:TYR:HE1	17	0.1
(1,38)	1:138:A:ILE:HD13	1:140:A:TYR:HE1	17	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found