Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 05:17 PM EDT

PDB ID	:	2MMZ
BMRB ID	:	19872
Title	:	Solution structure of the apo form of human glutaredoxin 5
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Deposited on	:	2014-03-25

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

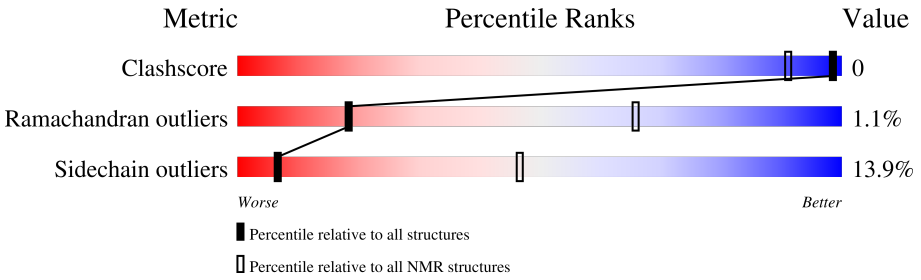
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	121	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:42-A:150 (109)	0.61	12

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1840 atoms, of which 915 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Glutaredoxin-related protein 5, mitochondrial.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	121	1840	586	915	157	178	4	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q86SX6
A	2	SER	-	expression tag	UNP Q86SX6
A	3	PHE	-	expression tag	UNP Q86SX6
A	4	THR	-	expression tag	UNP Q86SX6
A	5	MET	-	expression tag	UNP Q86SX6

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: Glutaredoxin-related protein 5, mitochondrial

Chain A: 74% 14% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 K53 V54 V55 V56 F57 L58 Q66 F69 R78 R83 D84 Y85 R97 N105 W106 I109 F118 V119 L126 V135 L148 D149 E150

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: Glutaredoxin-related protein 5, mitochondrial

Chain A: 76% 11% • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L45 K53 V54 V55 V56 F57 L58 E63 Q66 R78 R83 D84 Y85 Y103 W106 I109 F118 V119 L126 E150

4.2.2 Score per residue for model 2

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

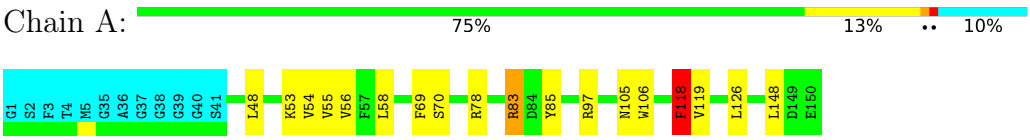
Chain A: 74% 16% • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 D52 K53 V54 V55 V56 F57 L58 K59 E63 C67 R78 Y85 N105 W106 P107 T108 F118 V119 L126 D133 L134 V135 E150

4.2.3 Score per residue for model 3

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

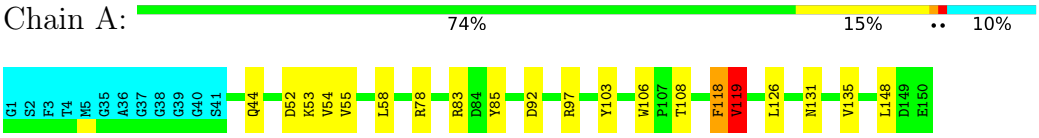
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

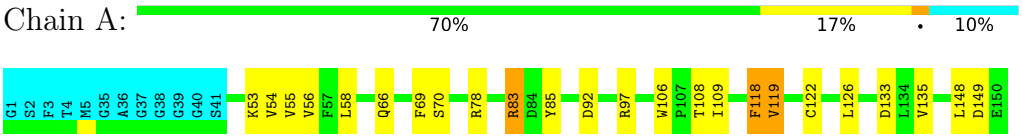
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

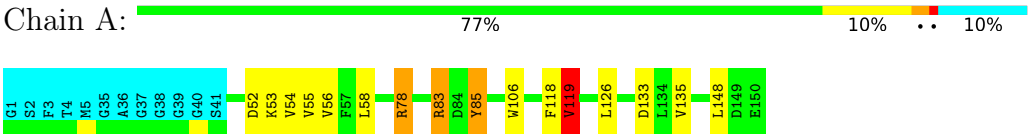
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

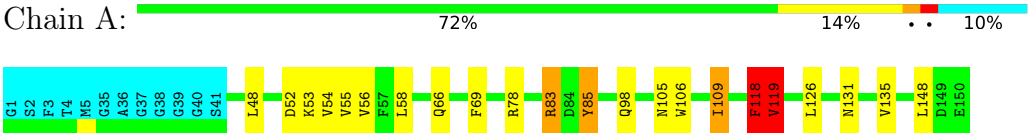
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 73% 15% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 K50 K53 V54 V55 V56 F57 L58 Q66 F69 R78 R83 D84 Y85 R97 Q98 N105 W106 Q111 F118 V119 L126 N131 V135 E150

4.2.9 Score per residue for model 9

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 70% 17% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 K53 V54 V55 V56 F57 L58 Q66 F69 R78 R83 D84 Y85 N89 V90 L91 D92 N105 W106 I109 F118 V119 L126 N131 K139 L148 D149 E150

4.2.10 Score per residue for model 10

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 74% 13% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 D52 K53 V54 V55 V56 F57 L58 Q66 R78 R83 D84 Y85 R97 W106 F118 V119 L126 N131 V135 L148 D149 E150

4.2.11 Score per residue for model 11

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 72% 16% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 K51 D52 K53 V54 V55 V56 F57 L58 F69 R78 R83 D84 Y85 D92 R97 Y103 W106 Q111 F118 V119 L126 V135 L148 D149 E150

4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 74% 16% • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 Q44 L48 K53 V54 V55 V56 F57 L58 K59 Q66 R78 R83 D84 Y85 R97 W106 V119 L126 D133 L134 V135 K139 L148 D149 E150

4.2.13 Score per residue for model 13

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 76% 12% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 K53 V54 V55 V56 F57 L58 Q66 F69 R83 D84 Y85 R97 N105 W106 F118 V119 L126 D133 E150

4.2.14 Score per residue for model 14

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 75% 12% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 K53 V54 V55 V56 F57 L58 Q66 F69 R83 D84 Y85 N105 W106 I109 F118 V119 L126 V135 L148 D149 E150

4.2.15 Score per residue for model 15

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 74% 14% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 K51 D52 K53 V54 V55 V56 F57 L58 F69 R78 R83 D84 Y85 D92 R97 Q98 W106 I109 F118 V119 L126 V135 E136 L148 D149 E150

4.2.16 Score per residue for model 16

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A: 70% 17% • • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 D52 K53 V54 V55 V56 F57 L58 Q66 F69 S70 N71 R78 R83 D84 Y85 R97 Q98 N105 W106 F118 V119 C122 L125 L126 V135 L148 D149 E150

4.2.17 Score per residue for model 17

• Molecule 1: Glutaredoxin-related protein 5, mitochondrial

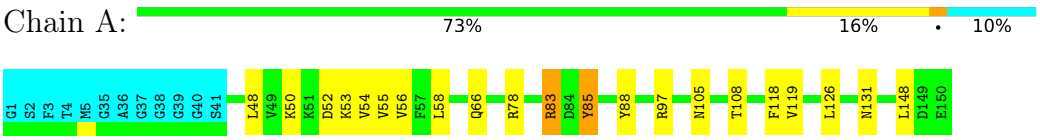
Chain A: 74% 13% • 10%

G1 S2 F3 T4 M5 G35 A36 G37 G38 G39 G40 S41 L48 V49 K50 K53 V54 V55 V56 F57 L58 R83 D84 Y85 R97 W106 I109 Y113 V119 L126 N131 K139 L148 D149 E150

4.2.18 Score per residue for model 18

- Molecule 1: Glutaredoxin-related protein 5, mitochondrial

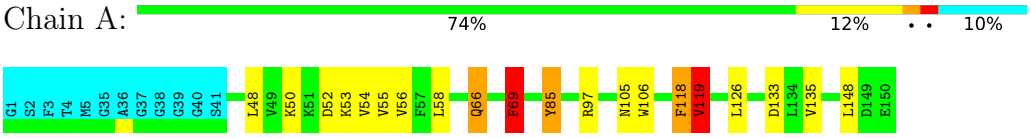
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Glutaredoxin-related protein 5, mitochondrial

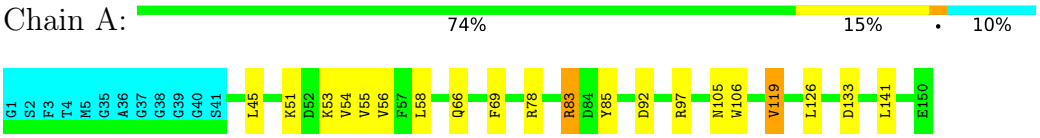
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Glutaredoxin-related protein 5, mitochondrial

Chain A:



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
CYANA	structure solution	
Amber	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1274
Number of shifts mapped to atoms	1274
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.65±0.01	0±0/874 (0.0± 0.0%)	1.19±0.03	8±2/1185 (0.6± 0.1%)
All	All	0.65	0/17480 (0.0%)	1.19	151/23700 (0.6%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.6±1.2
All	All	0	53

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	83	ARG	NE-CZ-NH1	9.64	125.12	120.30	9	18
1	A	97	ARG	NE-CZ-NH1	9.02	124.81	120.30	17	14
1	A	78	ARG	NE-CZ-NH1	7.96	124.28	120.30	9	16
1	A	85	TYR	CB-CG-CD1	-7.91	116.26	121.00	17	18
1	A	118	PHE	CB-CG-CD2	-7.67	115.43	120.80	3	11
1	A	85	TYR	CB-CG-CD2	-7.55	116.47	121.00	18	2
1	A	69	PHE	CB-CG-CD2	-6.79	116.05	120.80	16	6
1	A	118	PHE	CB-CG-CD1	6.39	125.27	120.80	5	5
1	A	69	PHE	CB-CG-CD1	-6.36	116.35	120.80	5	3
1	A	55	VAL	CG1-CB-CG2	-6.16	101.04	110.90	6	13
1	A	135	VAL	CG1-CB-CG2	-6.06	101.20	110.90	19	13
1	A	119	VAL	CA-CB-CG1	5.99	119.89	110.90	4	10
1	A	56	VAL	CG1-CB-CG2	-5.76	101.68	110.90	18	19
1	A	97	ARG	NE-CZ-NH2	-5.54	117.53	120.30	11	1
1	A	119	VAL	CG1-CB-CG2	-5.36	102.33	110.90	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	122	CYS	CA-CB-SG	-5.09	104.84	114.00	5	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	118	PHE	Peptide	15
1	A	119	VAL	Peptide	13
1	A	85	TYR	Sidechain	10
1	A	109	ILE	Peptide	4
1	A	103	TYR	Sidechain	3
1	A	69	PHE	Sidechain	3
1	A	78	ARG	Sidechain	2
1	A	97	ARG	Sidechain	1
1	A	113	TYR	Sidechain	1
1	A	88	TYR	Sidechain	1

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	858	855	855	0±1
All	All	17160	17100	17100	5

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:91:LEU:H	1:A:91:LEU:HD23	0.70	1.45	9	1
1:A:91:LEU:H	1:A:91:LEU:CD2	0.62	2.08	9	1
1:A:89:ASN:ND2	1:A:91:LEU:HD21	0.57	2.15	9	1
1:A:91:LEU:HD23	1:A:91:LEU:N	0.54	2.17	9	1
1:A:69:PHE:CD2	1:A:122:CYS:HB3	0.43	2.49	16	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	108/121 (89%)	100±2 (93±2%)	6±2 (6±2%)	1±1 (1±1%)	18	66
All	All	2160/2420 (89%)	2010 (93%)	126 (6%)	24 (1%)	18	66

All 6 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	119	VAL	14
1	A	69	PHE	4
1	A	108	THR	2
1	A	66	GLN	2
1	A	67	CYS	1
1	A	149	ASP	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	94/99 (95%)	81±2 (86±3%)	13±2 (14±3%)	7	47
All	All	1880/1980 (95%)	1618 (86%)	262 (14%)	7	47

All 37 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	53	LYS	20
1	A	54	VAL	20
1	A	58	LEU	20
1	A	126	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	A	106	TRP	19
1	A	148	LEU	15
1	A	119	VAL	14
1	A	66	GLN	13
1	A	48	LEU	13
1	A	83	ARG	12
1	A	105	ASN	11
1	A	52	ASP	9
1	A	109	ILE	7
1	A	133	ASP	7
1	A	131	ASN	7
1	A	55	VAL	6
1	A	92	ASP	6
1	A	69	PHE	4
1	A	98	GLN	4
1	A	50	LYS	4
1	A	118	PHE	3
1	A	139	LYS	3
1	A	51	LYS	3
1	A	45	LEU	2
1	A	63	GLU	2
1	A	59	LYS	2
1	A	70	SER	2
1	A	44	GLN	2
1	A	108	THR	2
1	A	111	GLN	2
1	A	149	ASP	2
1	A	78	ARG	1
1	A	91	LEU	1
1	A	136	GLU	1
1	A	71	ASN	1
1	A	125	LEU	1
1	A	141	LEU	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 monosaccharides 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 80% for the well-defined parts and 79% 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	1274
Number of shifts mapped to atoms	1274
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	120	0.41 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	106	0.77 ± 0.13	Should be applied
$^{13}C'$	117	0.19 ± 0.23	None needed (< 0.5 ppm)
^{15}N	113	0.68 ± 0.35	None needed (imprecise)

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 80%, i.e. 1201 atoms were assigned a chemical shift out of a possible 1500. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	427/544 (78%)	109/222 (49%)	215/218 (99%)	103/104 (99%)
Sidechain	740/854 (87%)	502/555 (90%)	238/270 (88%)	0/29 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	34/102 (33%)	29/49 (59%)	0/46 (0%)	5/7 (71%)
Overall	1201/1500 (80%)	640/826 (77%)	453/534 (85%)	108/140 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1274 atoms were assigned a chemical shift out of a possible 1605. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	470/610 (77%)	120/252 (48%)	237/242 (98%)	113/116 (97%)
Sidechain	768/883 (87%)	521/575 (91%)	247/279 (89%)	0/29 (0%)
Aromatic	36/112 (32%)	31/54 (57%)	0/51 (0%)	5/7 (71%)
Overall	1274/1605 (79%)	672/881 (76%)	484/572 (85%)	118/152 (78%)

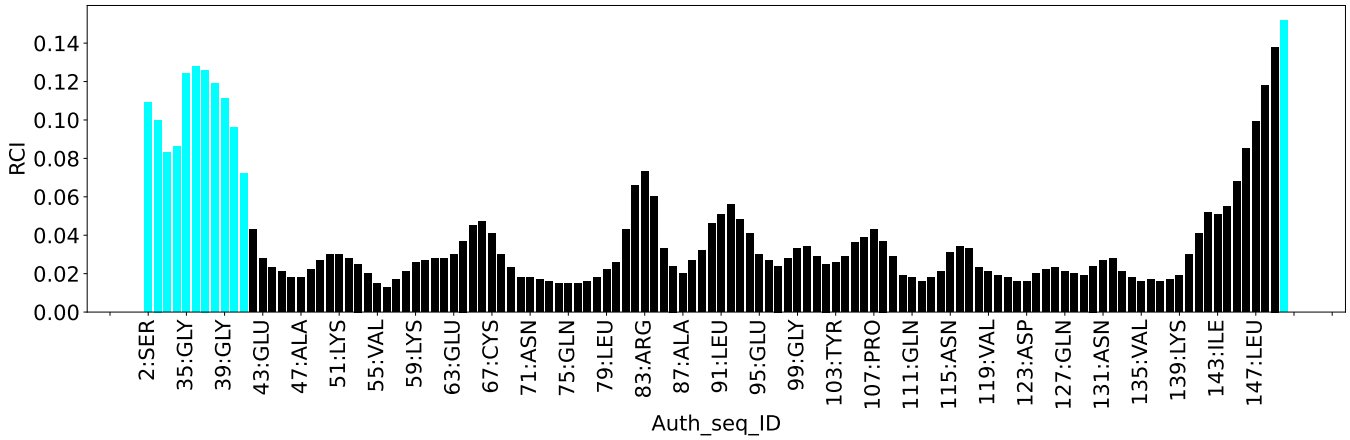
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	1995
Intra-residue (|i-j|=0)	536
Sequential (|i-j|=1)	534
Medium range (|i-j|>1 and |i-j|<5)	391
Long range (|i-j|≥5)	496
Inter-chain	0
Hydrogen bond restraints	38
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.5
Number of long range restraints per residue[1]	4.2

[1]Long 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 (i)

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 (i)

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)	22.2	0.2
0.2-0.5 (Medium)	3.8	0.5
>0.5 (Large)	4.3	1.4

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

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

9 Distance violation analysis (i)

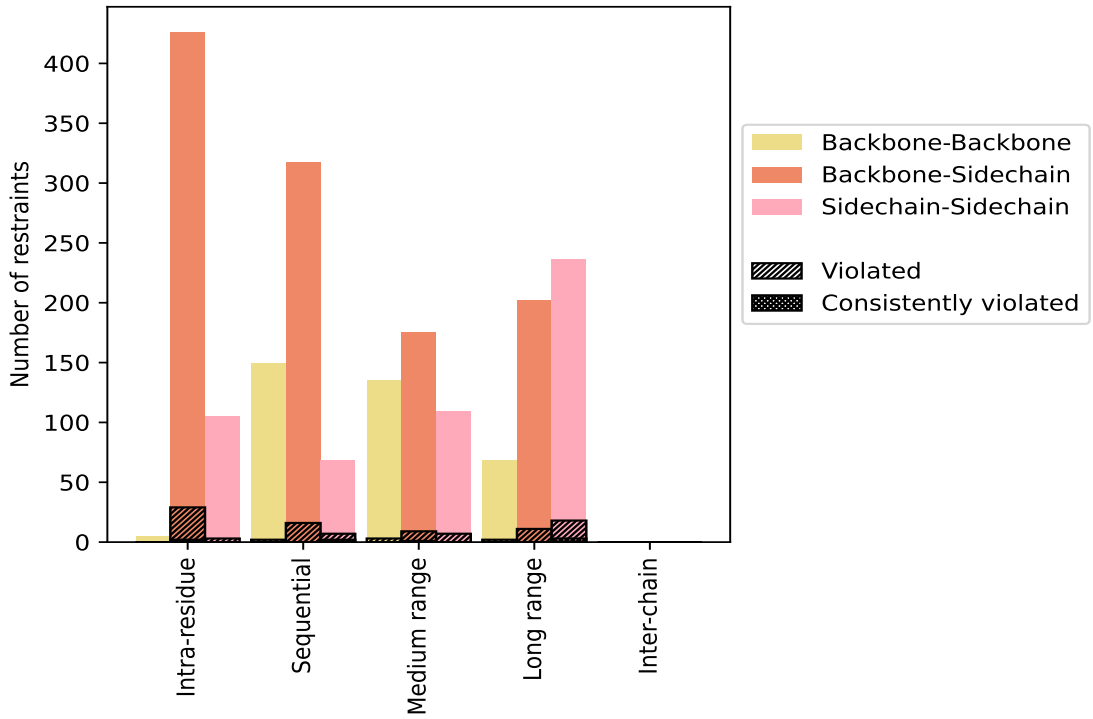
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	536	26.9	32	6.0	1.6	2	0.4	0.1
Backbone-Backbone	5	0.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	426	21.4	29	6.8	1.5	2	0.5	0.1
Sidechain-Sidechain	105	5.3	3	2.9	0.2	0	0.0	0.0
Sequential (|i-j|=1)	534	26.8	25	4.7	1.3	2	0.4	0.1
Backbone-Backbone	149	7.5	2	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	317	15.9	16	5.0	0.8	0	0.0	0.0
Sidechain-Sidechain	68	3.4	7	10.3	0.4	2	2.9	0.1
Medium range (|i-j|>1 & |i-j|<5)	391	19.6	18	4.6	0.9	1	0.3	0.1
Backbone-Backbone	107	5.4	2	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	175	8.8	9	5.1	0.5	1	0.6	0.1
Sidechain-Sidechain	109	5.5	7	6.4	0.4	0	0.0	0.0
Long range (|i-j|≥5)	496	24.9	31	6.2	1.6	3	0.6	0.2
Backbone-Backbone	58	2.9	2	3.4	0.1	0	0.0	0.0
Backbone-Sidechain	202	10.1	11	5.4	0.6	0	0.0	0.0
Sidechain-Sidechain	236	11.8	18	7.6	0.9	3	1.3	0.2
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	38	1.9	1	2.6	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1995	100.0	107	5.4	5.4	8	0.4	0.4
Backbone-Backbone	357	17.9	7	2.0	0.4	0	0.0	0.0
Backbone-Sidechain	1120	56.1	65	5.8	3.3	3	0.3	0.2
Sidechain-Sidechain	518	26.0	35	6.8	1.8	5	1.0	0.3

[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	8	7	3	10	0	28	0.24	1.12	0.23	0.14
2	9	5	4	8	0	26	0.26	0.93	0.23	0.14
3	8	9	4	8	0	29	0.24	1.4	0.27	0.13
4	9	6	3	8	0	26	0.21	0.85	0.16	0.14
5	8	10	7	12	0	37	0.34	1.19	0.33	0.14
6	11	9	4	8	0	32	0.2	0.77	0.17	0.13
7	8	4	5	9	0	26	0.25	0.84	0.23	0.14
8	10	7	6	7	0	30	0.2	0.84	0.15	0.15
9	9	7	5	13	0	34	0.24	0.91	0.21	0.15
10	13	4	3	8	0	28	0.25	0.92	0.23	0.15
11	12	8	3	5	0	28	0.23	0.75	0.19	0.14

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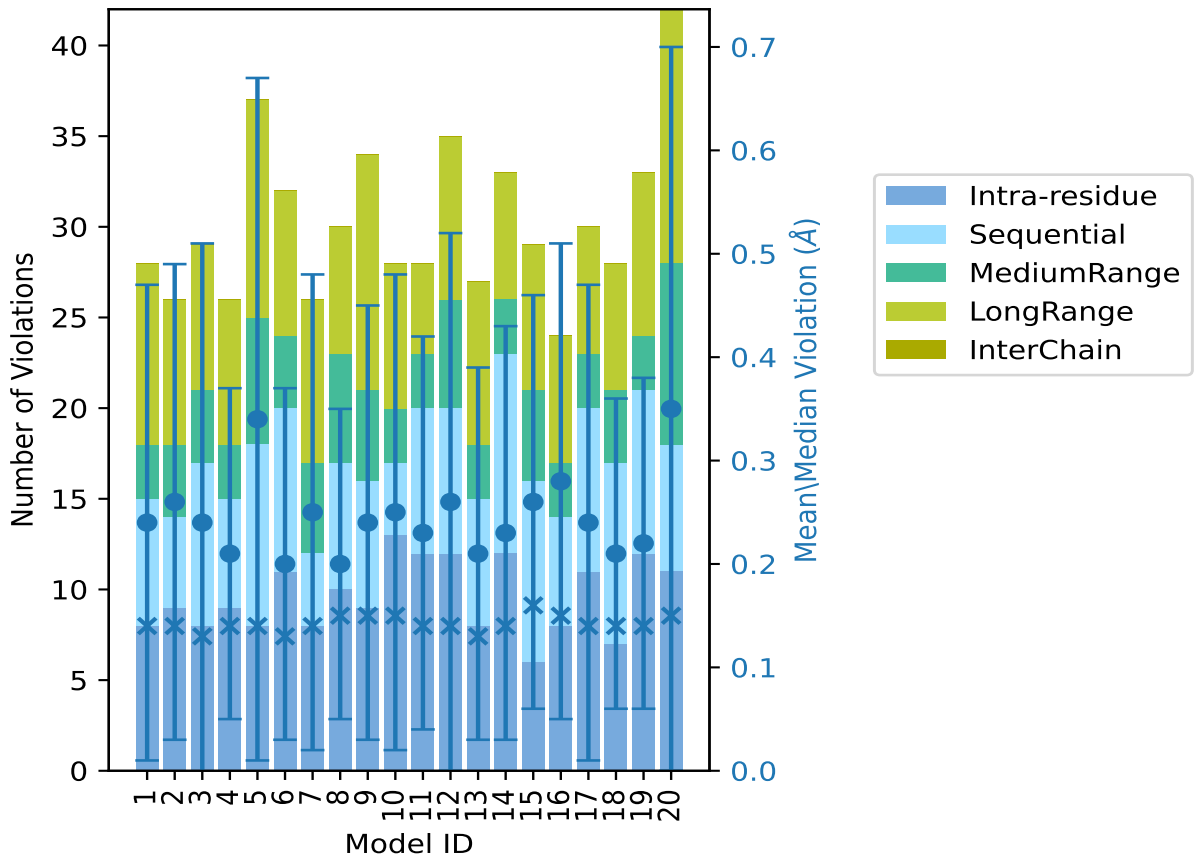
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	12	8	6	9	0	35	0.26	1.32	0.26	0.14
13	8	7	3	9	0	27	0.21	0.7	0.18	0.13
14	12	11	3	7	0	33	0.23	0.77	0.2	0.14
15	6	10	5	8	0	29	0.26	0.9	0.2	0.16
16	8	6	3	7	0	24	0.28	0.88	0.23	0.15
17	11	9	3	7	0	30	0.24	0.89	0.23	0.14
18	7	10	4	7	0	28	0.21	0.74	0.15	0.14
19	12	9	3	9	0	33	0.22	0.78	0.16	0.14
20	11	7	10	14	0	42	0.35	1.4	0.35	0.15

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

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



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

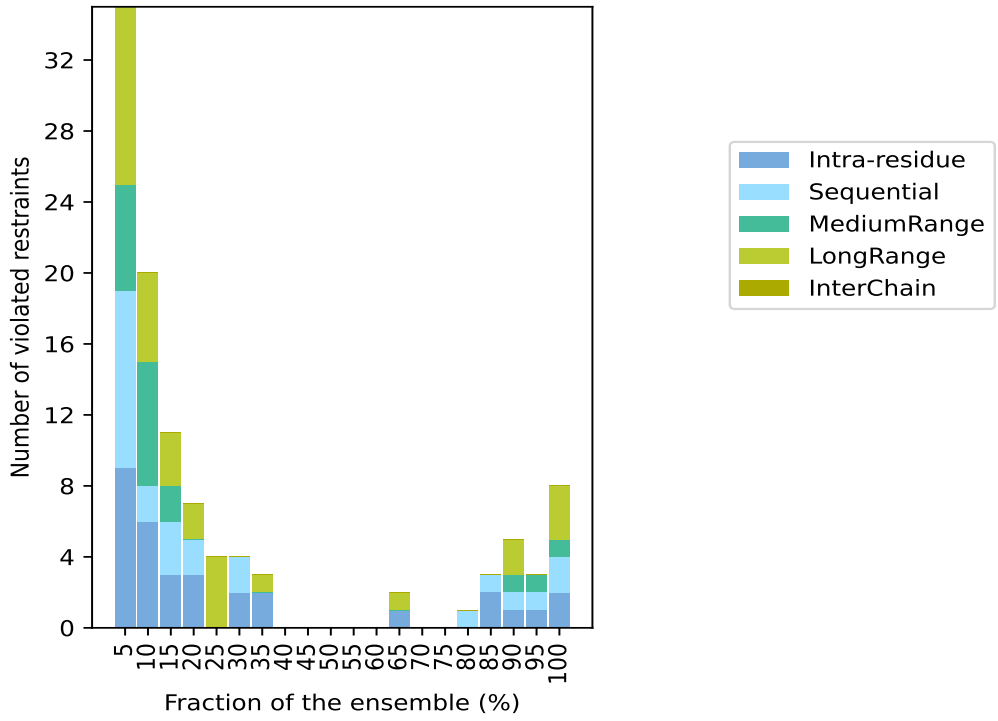
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1851(IR:504, SQ:509, MR:373, LR:465, 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]	%
9	10	6	10	0	35	1	5.0
6	2	7	5	0	20	2	10.0
3	3	2	3	0	11	3	15.0
3	2	0	2	0	7	4	20.0
0	0	0	4	0	4	5	25.0
2	2	0	0	0	4	6	30.0
2	0	0	1	0	3	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
1	0	0	1	0	2	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	1	0	0	0	1	16	80.0
2	1	0	0	0	3	17	85.0
1	1	1	2	0	5	18	90.0
1	1	1	0	0	3	19	95.0
2	2	1	3	0	8	20	100.0

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

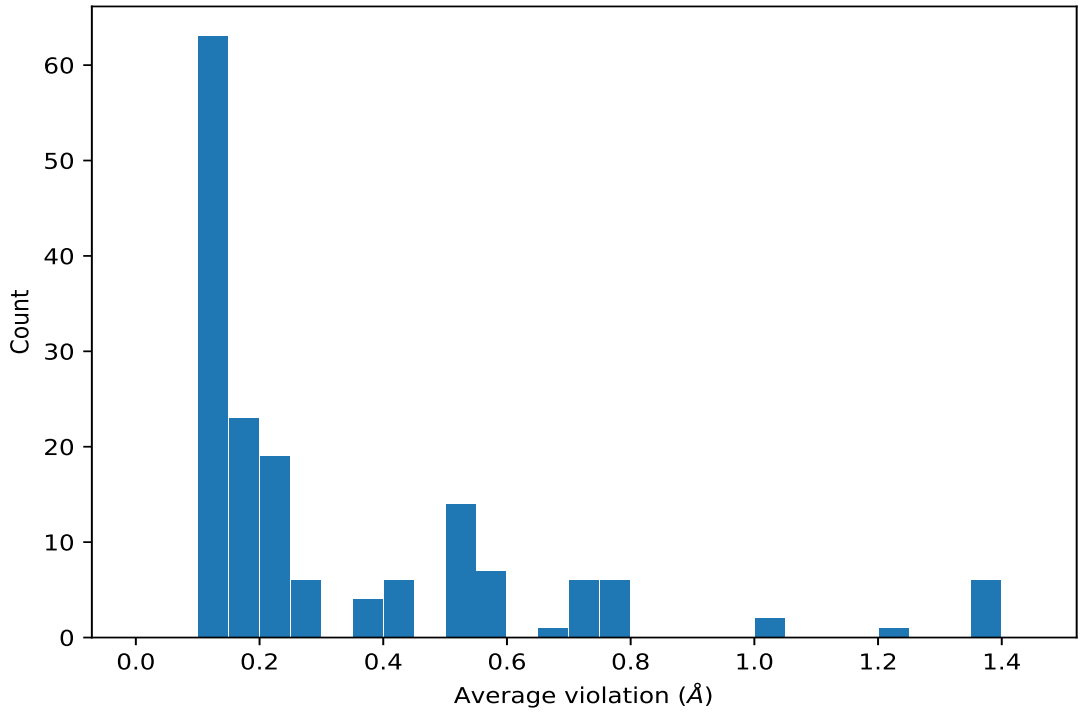
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	20	0.78	0.07	0.76
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	20	0.78	0.07	0.76
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	20	0.78	0.07	0.76
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	20	0.78	0.07	0.76
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	20	0.78	0.07	0.76
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	20	0.78	0.07	0.76
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	20	0.73	0.27	0.75
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	20	0.73	0.27	0.75
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	20	0.73	0.27	0.75
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	20	0.73	0.27	0.75
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	20	0.73	0.27	0.75
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	20	0.73	0.27	0.75
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	20	0.52	0.12	0.54
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	20	0.52	0.12	0.54
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	20	0.52	0.12	0.54
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	20	0.52	0.12	0.54

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	20	0.52	0.12	0.54
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	20	0.52	0.12	0.54
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	20	0.52	0.16	0.54
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	20	0.52	0.16	0.54
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	20	0.52	0.16	0.54
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	20	0.52	0.16	0.54
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	20	0.19	0.02	0.18
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	20	0.14	0.01	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	20	0.14	0.01	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	20	0.14	0.01	0.15
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	20	0.14	0.01	0.14
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	20	0.13	0.01	0.13
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	19	0.29	0.07	0.29
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	19	0.29	0.07	0.29
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	19	0.29	0.07	0.29
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	19	0.29	0.07	0.29
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	19	0.29	0.07	0.29
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	19	0.29	0.07	0.29
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	19	0.14	0.01	0.14
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	19	0.13	0.01	0.13
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	18	0.41	0.14	0.44
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	18	0.41	0.14	0.44
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	18	0.41	0.14	0.44
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	18	0.41	0.14	0.44
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	18	0.41	0.14	0.44
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	18	0.41	0.14	0.44
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	18	0.16	0.03	0.16
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	18	0.15	0.02	0.15
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	18	0.14	0.01	0.14
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	18	0.12	0.01	0.12
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	17	0.15	0.03	0.15
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	17	0.14	0.02	0.14
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	17	0.13	0.02	0.14
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	16	0.23	0.14	0.18

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	16	0.23	0.14	0.18
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	16	0.23	0.14	0.18
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	13	0.52	0.21	0.48
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	13	0.52	0.21	0.48
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	13	0.52	0.21	0.48
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	13	0.52	0.21	0.48
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	13	0.12	0.01	0.12
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	7	0.19	0.05	0.19
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	7	0.19	0.05	0.19
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	7	0.19	0.05	0.19
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	7	0.19	0.05	0.19
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	7	0.19	0.05	0.19
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	7	0.19	0.05	0.19
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	7	0.13	0.01	0.13
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	7	0.11	0.01	0.11
(1,1760)	1:A:50:LYS:HG2	1:A:51:LYS:H	6	0.14	0.02	0.14
(1,1760)	1:A:50:LYS:HG3	1:A:51:LYS:H	6	0.14	0.02	0.14
(1,1431)	1:A:71:ASN:HA	1:A:71:ASN:HD22	6	0.13	0.02	0.12
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG11	6	0.12	0.01	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG12	6	0.12	0.01	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG13	6	0.12	0.01	0.11
(1,1719)	1:A:50:LYS:H	1:A:50:LYS:HB3	6	0.11	0.0	0.11
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD2	5	0.21	0.1	0.15
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD3	5	0.21	0.1	0.15
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD2	5	0.21	0.1	0.15
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD3	5	0.21	0.1	0.15
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD2	5	0.21	0.1	0.15
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD3	5	0.21	0.1	0.15
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD1	5	0.14	0.02	0.13
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD2	5	0.14	0.02	0.13
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD1	5	0.14	0.02	0.13
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD2	5	0.14	0.02	0.13
(1,97)	1:A:112:VAL:H	1:A:119:VAL:HB	5	0.12	0.01	0.11
(1,651)	1:A:58:LEU:HB3	1:A:70:SER:HB3	5	0.12	0.0	0.12
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD1	4	0.12	0.01	0.12
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD2	4	0.12	0.01	0.12
(1,906)	1:A:110:PRO:HG3	1:A:122:CYS:HB3	4	0.12	0.0	0.12
(1,1119)	1:A:53:LYS:HG2	1:A:115:ASN:H	4	0.12	0.0	0.12
(2,27)	1:A:50:LYS:H	1:A:46:ASP:O	4	0.12	0.01	0.11
(1,40)	1:A:117:GLU:HB2	1:A:118:PHE:H	4	0.12	0.0	0.12
(1,1595)	1:A:52:ASP:HB2	1:A:53:LYS:H	4	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD2	4	0.11	0.0	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD3	4	0.11	0.0	0.11
(1,1677)	1:A:117:GLU:HB3	1:A:117:GLU:HG3	4	0.11	0.0	0.11
(1,1462)	1:A:60:GLY:HA3	1:A:89:ASN:HD22	3	0.59	0.29	0.79
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD2	3	0.38	0.09	0.36
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD3	3	0.38	0.09	0.36
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD2	3	0.38	0.09	0.36
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD3	3	0.38	0.09	0.36
(1,1430)	1:A:4:THR:HA	1:A:5:MET:H	3	0.16	0.05	0.15
(1,920)	1:A:145:SER:HB3	1:A:148:LEU:HG	3	0.14	0.01	0.15
(1,527)	1:A:118:PHE:HA	1:A:119:VAL:HB	3	0.13	0.01	0.13
(1,662)	1:A:60:GLY:HA2	1:A:66:GLN:HA	3	0.13	0.01	0.12
(1,1668)	1:A:5:MET:H	1:A:5:MET:HG3	3	0.12	0.0	0.12
(1,32)	1:A:55:VAL:HG21	1:A:86:ALA:H	3	0.11	0.0	0.11
(1,32)	1:A:55:VAL:HG22	1:A:86:ALA:H	3	0.11	0.0	0.11
(1,32)	1:A:55:VAL:HG23	1:A:86:ALA:H	3	0.11	0.0	0.11
(1,466)	1:A:139:LYS:HA	1:A:139:LYS:HG2	3	0.11	0.0	0.11
(1,207)	1:A:53:LYS:HB3	1:A:54:VAL:H	3	0.11	0.0	0.11
(1,938)	1:A:53:LYS:HA	1:A:53:LYS:HG2	3	0.11	0.0	0.11
(1,1091)	1:A:109:ILE:HG21	1:A:111:GLN:HG2	2	1.36	0.04	1.36
(1,1091)	1:A:109:ILE:HG21	1:A:111:GLN:HG3	2	1.36	0.04	1.36
(1,1091)	1:A:109:ILE:HG22	1:A:111:GLN:HG2	2	1.36	0.04	1.36
(1,1091)	1:A:109:ILE:HG22	1:A:111:GLN:HG3	2	1.36	0.04	1.36
(1,1091)	1:A:109:ILE:HG23	1:A:111:GLN:HG2	2	1.36	0.04	1.36
(1,1091)	1:A:109:ILE:HG23	1:A:111:GLN:HG3	2	1.36	0.04	1.36
(1,1213)	1:A:89:ASN:HD22	1:A:91:LEU:H	2	1.21	0.03	1.21
(1,333)	1:A:89:ASN:HD22	1:A:91:LEU:HG	2	1.02	0.04	1.02
(1,1406)	1:A:60:GLY:HA2	1:A:89:ASN:HD22	2	1.0	0.03	1.0
(1,332)	1:A:89:ASN:HD22	1:A:91:LEU:HB2	2	0.68	0.01	0.68
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD11	2	0.55	0.03	0.55
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD12	2	0.55	0.03	0.55
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD13	2	0.55	0.03	0.55
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD21	2	0.55	0.03	0.55
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD22	2	0.55	0.03	0.55
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD23	2	0.55	0.03	0.55
(1,747)	1:A:89:ASN:HB2	1:A:89:ASN:HD22	2	0.2	0.02	0.2
(1,1847)	1:A:56:VAL:HG11	1:A:85:TYR:HD1	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG11	1:A:85:TYR:HD2	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG12	1:A:85:TYR:HD1	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG12	1:A:85:TYR:HD2	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG13	1:A:85:TYR:HD1	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG13	1:A:85:TYR:HD2	2	0.16	0.02	0.16

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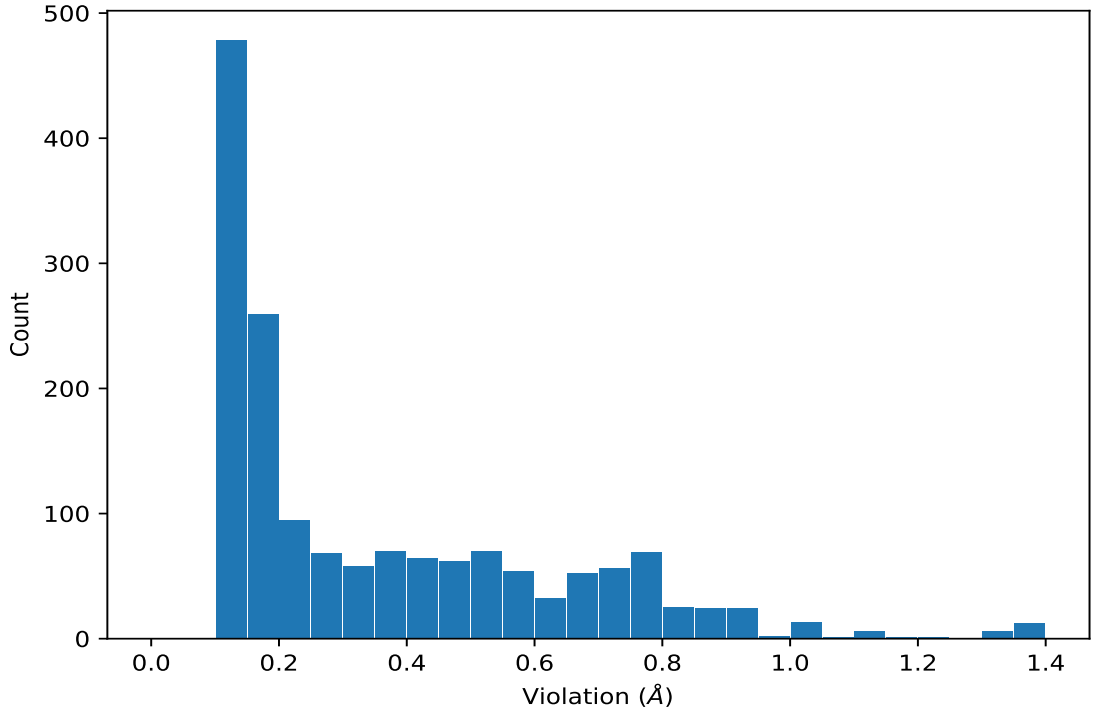
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1847)	1:A:56:VAL:HG21	1:A:85:TYR:HD1	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG21	1:A:85:TYR:HD2	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG22	1:A:85:TYR:HD1	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG22	1:A:85:TYR:HD2	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG23	1:A:85:TYR:HD1	2	0.16	0.02	0.16
(1,1847)	1:A:56:VAL:HG23	1:A:85:TYR:HD2	2	0.16	0.02	0.16
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD11	2	0.14	0.0	0.14
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD12	2	0.14	0.0	0.14
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD13	2	0.14	0.0	0.14
(1,723)	1:A:109:ILE:H	1:A:109:ILE:HB	2	0.12	0.02	0.12
(1,1193)	1:A:83:ARG:H	1:A:83:ARG:HB2	2	0.12	0.0	0.12
(1,1402)	1:A:67:CYS:H	1:A:70:SER:HB2	2	0.12	0.01	0.12
(1,1725)	1:A:50:LYS:HD2	1:A:116:GLY:HA2	2	0.12	0.01	0.12
(1,1484)	1:A:49:VAL:HG11	1:A:116:GLY:HA3	2	0.12	0.0	0.12
(1,1484)	1:A:49:VAL:HG12	1:A:116:GLY:HA3	2	0.12	0.0	0.12
(1,1484)	1:A:49:VAL:HG13	1:A:116:GLY:HA3	2	0.12	0.0	0.12
(1,1671)	1:A:110:PRO:HG2	1:A:122:CYS:HB3	2	0.12	0.0	0.12
(1,605)	1:A:131:ASN:HA	1:A:131:ASN:HD22	2	0.11	0.0	0.11
(1,691)	1:A:47:ALA:H	1:A:48:LEU:HB3	2	0.11	0.0	0.11
(1,1383)	1:A:57:PHE:HB2	1:A:58:LEU:HA	2	0.11	0.0	0.11
(1,1593)	1:A:106:TRP:HB3	1:A:108:THR:HA	2	0.11	0.0	0.11
(1,1594)	1:A:93:ASP:H	1:A:93:ASP:HB3	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard 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)
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	3	1.4
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	3	1.4
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	3	1.4
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	3	1.4
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	3	1.4
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	3	1.4
(1,1091)	1:A:109:ILE:HG21	1:A:111:GLN:HG2	20	1.4
(1,1091)	1:A:109:ILE:HG21	1:A:111:GLN:HG3	20	1.4
(1,1091)	1:A:109:ILE:HG22	1:A:111:GLN:HG2	20	1.4
(1,1091)	1:A:109:ILE:HG22	1:A:111:GLN:HG3	20	1.4
(1,1091)	1:A:109:ILE:HG23	1:A:111:GLN:HG2	20	1.4
(1,1091)	1:A:109:ILE:HG23	1:A:111:GLN:HG3	20	1.4
(1,1091)	1:A:109:ILE:HG21	1:A:111:GLN:HG2	12	1.32
(1,1091)	1:A:109:ILE:HG21	1:A:111:GLN:HG3	12	1.32
(1,1091)	1:A:109:ILE:HG22	1:A:111:GLN:HG2	12	1.32
(1,1091)	1:A:109:ILE:HG22	1:A:111:GLN:HG3	12	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1091)	1:A:109:ILE:HG23	1:A:111:GLN:HG2	12	1.32
(1,1091)	1:A:109:ILE:HG23	1:A:111:GLN:HG3	12	1.32
(1,1213)	1:A:89:ASN:HD22	1:A:91:LEU:H	20	1.24
(1,1213)	1:A:89:ASN:HD22	1:A:91:LEU:H	5	1.19
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	1	1.12
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	1	1.12
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	1	1.12
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	1	1.12
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	1	1.12
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	1	1.12
(1,333)	1:A:89:ASN:HD22	1:A:91:LEU:HG	20	1.06
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	5	1.03
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	5	1.03
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	5	1.03
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	5	1.03
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	5	1.03
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	5	1.03
(1,1406)	1:A:60:GLY:HA2	1:A:89:ASN:HD22	5	1.02
(1,1858)	1:A:144:HIS:HE1	1:A:148:LEU:HD11	20	1.0
(1,1858)	1:A:144:HIS:HE1	1:A:148:LEU:HD12	20	1.0
(1,1858)	1:A:144:HIS:HE1	1:A:148:LEU:HD13	20	1.0
(1,1858)	1:A:144:HIS:HE1	1:A:148:LEU:HD21	20	1.0
(1,1858)	1:A:144:HIS:HE1	1:A:148:LEU:HD22	20	1.0
(1,1858)	1:A:144:HIS:HE1	1:A:148:LEU:HD23	20	1.0
(1,333)	1:A:89:ASN:HD22	1:A:91:LEU:HG	5	0.98
(1,1406)	1:A:60:GLY:HA2	1:A:89:ASN:HD22	20	0.97
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	2	0.93
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	2	0.93
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	2	0.93
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	2	0.93
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	2	0.93
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	2	0.93
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	10	0.92
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	10	0.92
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	10	0.92
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	10	0.92
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	10	0.92
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	10	0.92
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	9	0.91
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	9	0.91
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	9	0.91
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	9	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	9	0.91
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	9	0.91
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	15	0.9
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	15	0.9
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	15	0.9
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	15	0.9
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	15	0.9
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	15	0.9
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	17	0.89
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	17	0.89
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	17	0.89
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	17	0.89
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	17	0.89
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	17	0.89
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	16	0.88
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	16	0.88
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	16	0.88
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	16	0.88
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	16	0.88
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	16	0.88
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	10	0.86
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	10	0.86
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	10	0.86
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	10	0.86
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	10	0.86
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	10	0.86
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	4	0.85
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	4	0.85
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	4	0.85
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	4	0.85
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	4	0.85
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	4	0.85
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	12	0.84
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	12	0.84
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	12	0.84
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	12	0.84
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	7	0.84
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	7	0.84
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	7	0.84
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	7	0.84
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	7	0.84
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	7	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	8	0.84
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	8	0.84
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	8	0.84
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	8	0.84
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	8	0.84
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	8	0.84
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	17	0.83
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	17	0.83
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	17	0.83
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	17	0.83
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	2	0.81
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	2	0.81
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	2	0.81
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	2	0.81
(1,1462)	1:A:60:GLY:HA3	1:A:89:ASN:HD22	5	0.8
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	5	0.79
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	5	0.79
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	5	0.79
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	5	0.79
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	20	0.79
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	20	0.79
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	20	0.79
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	20	0.79
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	20	0.79
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	20	0.79
(1,1462)	1:A:60:GLY:HA3	1:A:89:ASN:HD22	20	0.79
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	19	0.78
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	19	0.78
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	19	0.78
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	19	0.78
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	19	0.78
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	19	0.78
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	6	0.77
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	6	0.77
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	6	0.77
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	6	0.77
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	6	0.77
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	6	0.77
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	2	0.77
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	2	0.77
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	2	0.77
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	2	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	2	0.77
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	2	0.77
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	7	0.77
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	7	0.77
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	7	0.77
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	7	0.77
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	7	0.77
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	7	0.77
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	14	0.77
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	14	0.77
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	14	0.77
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	14	0.77
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	14	0.77
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	14	0.77
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	9	0.76
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	9	0.76
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	9	0.76
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	9	0.76
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	17	0.76
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	17	0.76
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	17	0.76
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	17	0.76
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	17	0.76
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	17	0.76
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	3	0.76
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	3	0.76
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	3	0.76
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	3	0.76
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	3	0.76
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	3	0.76
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	1	0.75
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	1	0.75
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	1	0.75
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	1	0.75
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	1	0.75
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	1	0.75
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	11	0.75
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	11	0.75
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	11	0.75
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	11	0.75
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	11	0.75
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	11	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	7	0.74
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	7	0.74
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	7	0.74
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	7	0.74
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	16	0.74
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	16	0.74
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	16	0.74
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	16	0.74
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	16	0.74
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	16	0.74
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	12	0.74
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	12	0.74
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	12	0.74
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	12	0.74
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	12	0.74
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	12	0.74
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	15	0.74
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	15	0.74
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	15	0.74
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	15	0.74
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	15	0.74
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	15	0.74
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	18	0.74
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	18	0.74
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	18	0.74
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	18	0.74
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	18	0.74
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	18	0.74
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	5	0.73
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	5	0.73
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	5	0.73
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	5	0.73
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	5	0.73
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	5	0.73
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	14	0.72
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	14	0.72
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	14	0.72
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	14	0.72
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	6	0.71
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	6	0.71
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	6	0.71
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	6	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	6	0.71
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	6	0.71
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	13	0.7
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	13	0.7
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	13	0.7
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	13	0.7
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	13	0.7
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	13	0.7
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	13	0.7
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	13	0.7
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	13	0.7
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	13	0.7
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	13	0.7
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	13	0.7
(1,332)	1:A:89:ASN:HD22	1:A:91:LEU:HB2	20	0.69
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	11	0.69
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	11	0.69
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	11	0.69
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	11	0.69
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	11	0.69
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	11	0.69
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	11	0.69
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	11	0.69
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	11	0.69
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	11	0.69
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	11	0.69
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	11	0.69
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	14	0.68
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	14	0.68
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	14	0.68
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	14	0.68
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	14	0.68
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	14	0.68
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	14	0.67
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	14	0.67
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	14	0.67
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	14	0.67
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	14	0.67
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	14	0.67
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	16	0.66
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	16	0.66
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	16	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	16	0.66
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	16	0.66
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	16	0.66
(1,332)	1:A:89:ASN:HD22	1:A:91:LEU:HB2	5	0.66
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	3	0.65
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	3	0.65
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	3	0.65
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	3	0.65
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	3	0.65
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	3	0.65
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	7	0.65
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	7	0.65
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	7	0.65
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	7	0.65
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	16	0.65
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	16	0.65
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	16	0.65
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	16	0.65
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD1	20	0.65
(1,1016)	1:A:55:VAL:HG21	1:A:88:TYR:HD2	20	0.65
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD1	20	0.65
(1,1016)	1:A:55:VAL:HG22	1:A:88:TYR:HD2	20	0.65
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD1	20	0.65
(1,1016)	1:A:55:VAL:HG23	1:A:88:TYR:HD2	20	0.65
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	10	0.63
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	10	0.63
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	10	0.63
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	10	0.63
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	10	0.63
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	10	0.63
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	12	0.62
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	12	0.62
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	12	0.62
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	12	0.62
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	12	0.62
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	12	0.62
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	5	0.61
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	5	0.61
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	5	0.61
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	5	0.61
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	17	0.61
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	17	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	17	0.61
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	17	0.61
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	17	0.61
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	17	0.61
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	9	0.6
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	9	0.6
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	9	0.6
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	9	0.6
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	9	0.6
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	9	0.6
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	11	0.6
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	11	0.6
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	11	0.6
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	11	0.6
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	16	0.59
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	16	0.59
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	16	0.59
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	16	0.59
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	16	0.59
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	16	0.59
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD11	20	0.59
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD12	20	0.59
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD13	20	0.59
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD21	20	0.59
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD22	20	0.59
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD23	20	0.59
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	5	0.58
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	5	0.58
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	5	0.58
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	5	0.58
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	5	0.58
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	5	0.58
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	11	0.58
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	11	0.58
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	11	0.58
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	11	0.58
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	11	0.58
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	11	0.58
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	9	0.58
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	9	0.58
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	9	0.58
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	9	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	6	0.57
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	6	0.57
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	6	0.57
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	6	0.57
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	6	0.57
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	6	0.57
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	10	0.57
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	10	0.57
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	10	0.57
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	10	0.57
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	13	0.57
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	13	0.57
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	13	0.57
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	13	0.57
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	13	0.57
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	13	0.57
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	15	0.55
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	15	0.55
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	15	0.55
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	15	0.55
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	9	0.55
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	9	0.55
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	9	0.55
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	9	0.55
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	9	0.55
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	9	0.55
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	1	0.54
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	1	0.54
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	1	0.54
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	1	0.54
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	1	0.54
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	1	0.54
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	2	0.54
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	2	0.54
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	2	0.54
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	2	0.54
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	2	0.54
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	2	0.54
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	1	0.54
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	1	0.54
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	1	0.54
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	1	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	20	0.54
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	20	0.54
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	20	0.54
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	20	0.54
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	9	0.54
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	9	0.54
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	9	0.54
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	9	0.54
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	9	0.54
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	9	0.54
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	12	0.53
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	12	0.53
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	12	0.53
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	12	0.53
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	12	0.53
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	12	0.53
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	19	0.53
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	19	0.53
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	19	0.53
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	19	0.53
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	14	0.52
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	14	0.52
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	14	0.52
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	14	0.52
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	14	0.52
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	14	0.52
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	18	0.52
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	18	0.52
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	18	0.52
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	18	0.52
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	18	0.52
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	18	0.52
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD11	19	0.52
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD12	19	0.52
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD13	19	0.52
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD21	19	0.52
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD22	19	0.52
(1,1852)	1:A:145:SER:H	1:A:148:LEU:HD23	19	0.52
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	10	0.51
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	10	0.51
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	10	0.51
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	10	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	10	0.51
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	10	0.51
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD2	15	0.5
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD3	15	0.5
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD2	15	0.5
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD3	15	0.5
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	5	0.5
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	5	0.5
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	5	0.5
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	5	0.5
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	5	0.5
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	5	0.5
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	19	0.49
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	19	0.49
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	19	0.49
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	19	0.49
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	19	0.49
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	19	0.49
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	17	0.48
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	17	0.48
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	17	0.48
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	17	0.48
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	17	0.48
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	17	0.48
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	16	0.48
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	16	0.48
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	16	0.48
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	16	0.48
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	8	0.48
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	8	0.48
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	8	0.48
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	8	0.48
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	8	0.48
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	8	0.48
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	12	0.47
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	12	0.47
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	12	0.47
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	12	0.47
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	12	0.47
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	12	0.47
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	7	0.46
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	7	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	7	0.46
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	7	0.46
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	7	0.46
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	7	0.46
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	11	0.46
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	11	0.46
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	11	0.46
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	11	0.46
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	11	0.46
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	11	0.46
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	15	0.46
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	15	0.46
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	15	0.46
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	15	0.46
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	15	0.46
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	15	0.46
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	4	0.45
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	4	0.45
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	4	0.45
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	4	0.45
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	4	0.45
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	4	0.45
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	15	0.45
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	15	0.45
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	15	0.45
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	15	0.45
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	15	0.45
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	15	0.45
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	13	0.45
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	13	0.45
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	13	0.45
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	13	0.45
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	2	0.44
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	2	0.44
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	2	0.44
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	2	0.44
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	20	0.43
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	20	0.43
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	20	0.43
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	20	0.43
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	20	0.43
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	3	0.43
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	3	0.43
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	3	0.43
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	3	0.43
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	19	0.43
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	19	0.43
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	19	0.43
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	19	0.43
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	15	0.42
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	15	0.42
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	15	0.42
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	15	0.42
(1,775)	1:A:135:VAL:HG11	1:A:136:GLU:HG2	15	0.42
(1,775)	1:A:135:VAL:HG11	1:A:136:GLU:HG3	15	0.42
(1,775)	1:A:135:VAL:HG12	1:A:136:GLU:HG2	15	0.42
(1,775)	1:A:135:VAL:HG12	1:A:136:GLU:HG3	15	0.42
(1,775)	1:A:135:VAL:HG13	1:A:136:GLU:HG2	15	0.42
(1,775)	1:A:135:VAL:HG13	1:A:136:GLU:HG3	15	0.42
(1,1522)	1:A:91:LEU:HD21	1:A:97:ARG:HD2	9	0.42
(1,1522)	1:A:91:LEU:HD21	1:A:97:ARG:HD3	9	0.42
(1,1522)	1:A:91:LEU:HD22	1:A:97:ARG:HD2	9	0.42
(1,1522)	1:A:91:LEU:HD22	1:A:97:ARG:HD3	9	0.42
(1,1522)	1:A:91:LEU:HD23	1:A:97:ARG:HD2	9	0.42
(1,1522)	1:A:91:LEU:HD23	1:A:97:ARG:HD3	9	0.42
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	12	0.41
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	12	0.41
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	12	0.41
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	12	0.41
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	19	0.41
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	19	0.41
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	19	0.41
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	19	0.41
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	19	0.41
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	19	0.41
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	8	0.4
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	8	0.4
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	8	0.4
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	8	0.4
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	18	0.4
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	18	0.4
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	18	0.4
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	18	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	18	0.4
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	18	0.4
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	18	0.4
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	18	0.4
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	18	0.4
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	18	0.4
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	18	0.4
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	18	0.4
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	18	0.4
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	18	0.4
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	18	0.4
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	18	0.4
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	1	0.39
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	1	0.39
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	1	0.39
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	1	0.39
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	1	0.39
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	1	0.39
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	8	0.39
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	8	0.39
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	8	0.39
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	8	0.39
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	8	0.39
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	8	0.39
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	11	0.39
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	11	0.39
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	11	0.39
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	11	0.39
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	11	0.39
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	11	0.39
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	2	0.38
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	2	0.38
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	2	0.38
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	2	0.38
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	2	0.38
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	2	0.38
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	4	0.37
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	4	0.37
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	4	0.37
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	4	0.37
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	3	0.37
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	3	0.37
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	3	0.37
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	3	0.37
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	3	0.37
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	1	0.36
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	1	0.36
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	1	0.36
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	1	0.36
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	4	0.36
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	4	0.36
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	4	0.36
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	4	0.36
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	4	0.36
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	4	0.36
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD2	12	0.36
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD3	12	0.36
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD2	12	0.36
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD3	12	0.36
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	6	0.35
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	6	0.35
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	6	0.35
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	6	0.35
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	18	0.35
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	18	0.35
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	18	0.35
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	18	0.35
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	18	0.35
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	18	0.35
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	4	0.35
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	4	0.35
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	4	0.35
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	4	0.35
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	4	0.35
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	4	0.35
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD2	14	0.35
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD3	14	0.35
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD2	14	0.35
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD3	14	0.35
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD2	14	0.35
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD3	14	0.35
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	18	0.34
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	18	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	18	0.34
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	18	0.34
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	18	0.34
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	18	0.34
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	13	0.33
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	13	0.33
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	13	0.33
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	13	0.33
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	13	0.33
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	13	0.33
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	19	0.32
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	19	0.32
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	19	0.32
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	19	0.32
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	19	0.32
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	19	0.32
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	1	0.32
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	1	0.32
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	1	0.32
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	1	0.32
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	1	0.32
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	1	0.32
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	17	0.32
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	17	0.32
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	17	0.32
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	17	0.32
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	17	0.32
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	17	0.32
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	6	0.31
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	6	0.31
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	6	0.31
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	6	0.31
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	6	0.31
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	6	0.31
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	10	0.3
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	10	0.3
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	10	0.3
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	10	0.3
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD11	4	0.3
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD12	4	0.3
(1,1831)	1:A:57:PHE:HD1	1:A:96:LEU:HD13	4	0.3
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD11	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD12	4	0.3
(1,1831)	1:A:57:PHE:HD2	1:A:96:LEU:HD13	4	0.3
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	7	0.3
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	7	0.3
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	7	0.3
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	7	0.3
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	7	0.3
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	7	0.3
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	16	0.3
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	16	0.3
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	16	0.3
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	16	0.3
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	16	0.3
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	16	0.3
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	2	0.29
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	2	0.29
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	2	0.29
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	2	0.29
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	2	0.29
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	2	0.29
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	8	0.29
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	8	0.29
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	8	0.29
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	8	0.29
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	8	0.29
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	8	0.29
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	8	0.29
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	8	0.29
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	8	0.29
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	8	0.29
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	8	0.29
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	8	0.29
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD2	9	0.29
(1,1715)	1:A:136:GLU:HG2	1:A:139:LYS:HD3	9	0.29
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD2	9	0.29
(1,1715)	1:A:136:GLU:HG3	1:A:139:LYS:HD3	9	0.29
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	12	0.29
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	12	0.29
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	12	0.29
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	12	0.29
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	12	0.29
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	14	0.29
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	14	0.29
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	14	0.29
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	14	0.29
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	14	0.29
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	14	0.29
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD2	13	0.29
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD3	13	0.29
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD2	13	0.29
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD3	13	0.29
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD2	13	0.29
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD3	13	0.29
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	20	0.28
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	20	0.28
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	20	0.28
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	20	0.28
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	2	0.28
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	2	0.28
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	2	0.28
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	2	0.28
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	2	0.28
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	2	0.28
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	10	0.28
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	10	0.28
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	10	0.28
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	10	0.28
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	10	0.28
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	10	0.28
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	19	0.28
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	19	0.28
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	19	0.28
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	19	0.28
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	19	0.28
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	19	0.28
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	8	0.25
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	8	0.25
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	8	0.25
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	8	0.25
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	8	0.25
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	8	0.25
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	9	0.24
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	9	0.24
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	9	0.24
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	9	0.24
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	9	0.24
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	9	0.23
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	20	0.23
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	20	0.23
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	20	0.23
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	20	0.23
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	20	0.23
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	20	0.23
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	12	0.23
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	12	0.23
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	12	0.23
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	12	0.23
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	12	0.23
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	12	0.23
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	12	0.23
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	12	0.23
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	12	0.23
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	12	0.23
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	12	0.23
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	12	0.23
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	15	0.23
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	15	0.23
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	15	0.23
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	15	0.23
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	15	0.23
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	15	0.23
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD1	8	0.22
(1,949)	1:A:58:LEU:HD11	1:A:85:TYR:HD2	8	0.22
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD1	8	0.22
(1,949)	1:A:58:LEU:HD12	1:A:85:TYR:HD2	8	0.22
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD1	8	0.22
(1,949)	1:A:58:LEU:HD13	1:A:85:TYR:HD2	8	0.22
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	17	0.22
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	7	0.22
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	7	0.22
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	7	0.22
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	7	0.22
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	7	0.22
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1430)	1:A:4:THR:HA	1:A:5:MET:H	14	0.22
(1,747)	1:A:89:ASN:HB2	1:A:89:ASN:HD22	20	0.21
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	7	0.21
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	19	0.21
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	2	0.21
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	10	0.21
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	1	0.21
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	1	0.21
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	1	0.21
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	1	0.21
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	1	0.21
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	1	0.21
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	1	0.21
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	1	0.21
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	1	0.21
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	1	0.21
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	1	0.21
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	1	0.21
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	20	0.21
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	20	0.21
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	20	0.21
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	20	0.21
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	20	0.21
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	20	0.21
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	20	0.21
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	20	0.21
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	20	0.21
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	20	0.21
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	20	0.21
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	20	0.21
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB2	6	0.2
(1,879)	1:A:43:GLU:HG2	1:A:44:GLN:HB3	6	0.2
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB2	6	0.2
(1,879)	1:A:43:GLU:HG3	1:A:44:GLN:HB3	6	0.2
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	4	0.2
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	8	0.2
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	14	0.2
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	12	0.2
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	15	0.2
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	3	0.2
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	3	0.2
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	3	0.2
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	3	0.2
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	3	0.2
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	6	0.2
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	6	0.2
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	6	0.2
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	6	0.2
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	6	0.2
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	6	0.2
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	1	0.19
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	15	0.19
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	16	0.19
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	16	0.19
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	5	0.19
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	5	0.19
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	5	0.19
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	5	0.19
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	5	0.19
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	5	0.19
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	5	0.19
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	5	0.19
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	5	0.19
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	5	0.19
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	5	0.19
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	5	0.19
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	5	0.19
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	5	0.19
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	5	0.19
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	5	0.19
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	5	0.19
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	5	0.19
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	6	0.19
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	6	0.19
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	6	0.19
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	6	0.19
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	6	0.19
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	6	0.19
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	6	0.19
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	6	0.19
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	6	0.19
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	6	0.19
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	6	0.19
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	8	0.19
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	14	0.19
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	16	0.19
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	4	0.19
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	15	0.19
(1,747)	1:A:89:ASN:HB2	1:A:89:ASN:HD22	5	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	2	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	3	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	5	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	6	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	12	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	18	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	20	0.18
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	4	0.18
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	19	0.18
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	19	0.18
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	19	0.18
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	19	0.18
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	19	0.18
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	19	0.18
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	3	0.18
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	3	0.18
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	3	0.18
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	3	0.18
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	3	0.18
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	3	0.18
(1,1847)	1:A:56:VAL:HG11	1:A:85:TYR:HD1	6	0.18
(1,1847)	1:A:56:VAL:HG11	1:A:85:TYR:HD2	6	0.18
(1,1847)	1:A:56:VAL:HG12	1:A:85:TYR:HD1	6	0.18
(1,1847)	1:A:56:VAL:HG12	1:A:85:TYR:HD2	6	0.18
(1,1847)	1:A:56:VAL:HG13	1:A:85:TYR:HD1	6	0.18
(1,1847)	1:A:56:VAL:HG13	1:A:85:TYR:HD2	6	0.18
(1,1847)	1:A:56:VAL:HG21	1:A:85:TYR:HD1	6	0.18
(1,1847)	1:A:56:VAL:HG21	1:A:85:TYR:HD2	6	0.18
(1,1847)	1:A:56:VAL:HG22	1:A:85:TYR:HD1	6	0.18
(1,1847)	1:A:56:VAL:HG22	1:A:85:TYR:HD2	6	0.18
(1,1847)	1:A:56:VAL:HG23	1:A:85:TYR:HD1	6	0.18
(1,1847)	1:A:56:VAL:HG23	1:A:85:TYR:HD2	6	0.18
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	9	0.18
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	10	0.18
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	13	0.17
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	17	0.17
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	17	0.17
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	17	0.17
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	17	0.17
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	17	0.17
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	17	0.17
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	17	0.17
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	17	0.17
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	17	0.17
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	17	0.17
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	17	0.17
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	17	0.17
(1,1462)	1:A:60:GLY:HA3	1:A:89:ASN:HD22	9	0.17
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	18	0.17
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	18	0.17
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	18	0.17
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	18	0.17
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	18	0.17
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	18	0.17
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	7	0.17
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	17	0.17
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	14	0.17
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	16	0.17
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	20	0.16
(1,731)	1:A:85:TYR:HB3	1:A:87:ALA:HA	11	0.16
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	11	0.16
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	11	0.16
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	11	0.16
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	6	0.16
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	9	0.16
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	11	0.16
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	20	0.16
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	5	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	3	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	3	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	3	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	3	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	3	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	3	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	3	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	3	0.16
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	3	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	3	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	3	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	4	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	4	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	4	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	4	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	4	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	4	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	4	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	4	0.16
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	4	0.16
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	4	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	4	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	4	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	9	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	9	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	9	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	9	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	9	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	9	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	9	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	9	0.16
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	9	0.16
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	9	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	9	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	9	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	15	0.16
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	15	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	15	0.16
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	15	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	15	0.16
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	15	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	15	0.16
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	15	0.16
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	15	0.16
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	15	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	15	0.16
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	15	0.16
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	10	0.16
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1760)	1:A:50:LYS:HG2	1:A:51:LYS:H	18	0.16
(1,1760)	1:A:50:LYS:HG3	1:A:51:LYS:H	18	0.16
(1,1760)	1:A:50:LYS:HG2	1:A:51:LYS:H	19	0.16
(1,1760)	1:A:50:LYS:HG3	1:A:51:LYS:H	19	0.16
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	2	0.16
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	19	0.16
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	2	0.16
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	5	0.16
(1,1431)	1:A:71:ASN:HA	1:A:71:ASN:HD22	17	0.16
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD1	15	0.16
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD2	15	0.16
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD1	15	0.16
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD2	15	0.16
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	6	0.16
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	10	0.16
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	15	0.16
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	8	0.16
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	12	0.16
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	6	0.16
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	17	0.16
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	18	0.16
(1,920)	1:A:145:SER:HB3	1:A:148:LEU:HG	7	0.15
(1,920)	1:A:145:SER:HB3	1:A:148:LEU:HG	8	0.15
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	10	0.15
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	3	0.15
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	8	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	1	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	1	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	1	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	6	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	6	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	6	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	8	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	8	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	8	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	10	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	10	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	10	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	14	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	14	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	14	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	16	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	16	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	17	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	17	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	17	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	18	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	18	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	18	0.15
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	20	0.15
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	20	0.15
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	20	0.15
(1,321)	1:A:89:ASN:HD21	1:A:91:LEU:HB2	9	0.15
(1,287)	1:A:60:GLY:H	1:A:91:LEU:HB2	9	0.15
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	13	0.15
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	13	0.15
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	13	0.15
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	13	0.15
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	13	0.15
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	13	0.15
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	13	0.15
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	13	0.15
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	13	0.15
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	13	0.15
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	13	0.15
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	13	0.15
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	4	0.15
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	11	0.15
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	15	0.15
(1,1760)	1:A:50:LYS:HG2	1:A:51:LYS:H	8	0.15
(1,1760)	1:A:50:LYS:HG3	1:A:51:LYS:H	8	0.15
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	12	0.15
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	16	0.15
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	18	0.15
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	20	0.15
(1,1642)	1:A:136:GLU:HB2	1:A:137:GLU:H	15	0.15
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	14	0.15
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	15	0.15
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	8	0.15
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	16	0.15
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	20	0.15
(1,1430)	1:A:4:THR:HA	1:A:5:MET:H	15	0.15
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD1	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD2	12	0.15
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD1	12	0.15
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD2	12	0.15
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	1	0.15
(1,1244)	1:A:60:GLY:H	1:A:89:ASN:HD22	20	0.15
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	3	0.15
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	5	0.15
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	20	0.15
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD2	15	0.15
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD3	15	0.15
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD2	15	0.15
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD3	15	0.15
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD2	15	0.15
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD3	15	0.15
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	9	0.15
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	12	0.15
(1,97)	1:A:112:VAL:H	1:A:119:VAL:HB	18	0.14
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	7	0.14
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	10	0.14
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	11	0.14
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	16	0.14
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	11	0.14
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	12	0.14
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	16	0.14
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG2	8	0.14
(1,803)	1:A:59:LYS:HG2	1:A:66:GLN:HG3	8	0.14
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG2	8	0.14
(1,803)	1:A:59:LYS:HG3	1:A:66:GLN:HG3	8	0.14
(1,723)	1:A:109:ILE:H	1:A:109:ILE:HB	12	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	2	0.14
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	2	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	2	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	4	0.14
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	4	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	4	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	5	0.14
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	5	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	5	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	7	0.14
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	7	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	7	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	9	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	9	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	12	0.14
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	12	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	12	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	13	0.14
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	13	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	13	0.14
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	15	0.14
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	15	0.14
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	15	0.14
(1,662)	1:A:60:GLY:HA2	1:A:66:GLN:HA	7	0.14
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	5	0.14
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	8	0.14
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	13	0.14
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	14	0.14
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	18	0.14
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	19	0.14
(1,527)	1:A:118:PHE:HA	1:A:119:VAL:HB	17	0.14
(1,387)	1:A:135:VAL:HA	1:A:136:GLU:HG2	15	0.14
(1,387)	1:A:135:VAL:HA	1:A:136:GLU:HG3	15	0.14
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	11	0.14
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	20	0.14
(1,1847)	1:A:56:VAL:HG11	1:A:85:TYR:HD1	19	0.14
(1,1847)	1:A:56:VAL:HG11	1:A:85:TYR:HD2	19	0.14
(1,1847)	1:A:56:VAL:HG12	1:A:85:TYR:HD1	19	0.14
(1,1847)	1:A:56:VAL:HG12	1:A:85:TYR:HD2	19	0.14
(1,1847)	1:A:56:VAL:HG13	1:A:85:TYR:HD1	19	0.14
(1,1847)	1:A:56:VAL:HG13	1:A:85:TYR:HD2	19	0.14
(1,1847)	1:A:56:VAL:HG21	1:A:85:TYR:HD1	19	0.14
(1,1847)	1:A:56:VAL:HG21	1:A:85:TYR:HD2	19	0.14
(1,1847)	1:A:56:VAL:HG22	1:A:85:TYR:HD1	19	0.14
(1,1847)	1:A:56:VAL:HG22	1:A:85:TYR:HD2	19	0.14
(1,1847)	1:A:56:VAL:HG23	1:A:85:TYR:HD1	19	0.14
(1,1847)	1:A:56:VAL:HG23	1:A:85:TYR:HD2	19	0.14
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	19	0.14
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	19	0.14
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	19	0.14
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	19	0.14
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	19	0.14
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	19	0.14
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	19	0.14
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	19	0.14
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	19	0.14
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	19	0.14
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	19	0.14
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	3	0.14
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	5	0.14
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	9	0.14
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	16	0.14
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	17	0.14
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	1	0.14
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	4	0.14
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	6	0.14
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	14	0.14
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	17	0.14
(1,166)	1:A:133:ASP:HB2	1:A:134:LEU:H	11	0.14
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	14	0.14
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	1	0.14
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	5	0.14
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	18	0.14
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	19	0.14
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	20	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	1	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	3	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	4	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	7	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	9	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	10	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	11	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	13	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	14	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	15	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	18	0.14
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	19	0.14
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	2	0.14
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	13	0.14
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	1	0.14
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	10	0.14
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	13	0.14
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	16	0.14
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	19	0.14
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD11	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD12	12	0.14
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD13	12	0.14
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD11	20	0.14
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD12	20	0.14
(1,1114)	1:A:109:ILE:HA	1:A:109:ILE:HD13	20	0.14
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	2	0.14
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	5	0.14
(2,27)	1:A:50:LYS:H	1:A:46:ASP:O	20	0.13
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG11	11	0.13
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG12	11	0.13
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG13	11	0.13
(1,920)	1:A:145:SER:HB3	1:A:148:LEU:HG	3	0.13
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	4	0.13
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	12	0.13
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	17	0.13
(1,906)	1:A:110:PRO:HG3	1:A:122:CYS:HB3	9	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	1	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	2	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	3	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	5	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	6	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	8	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	12	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	13	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	14	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	15	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	17	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	18	0.13
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	20	0.13
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	6	0.13
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	7	0.13
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	10	0.13
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	14	0.13
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	15	0.13
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	19	0.13
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	3	0.13
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	3	0.13
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	3	0.13
(1,702)	1:A:56:VAL:HG21	1:A:57:PHE:HB2	19	0.13
(1,702)	1:A:56:VAL:HG22	1:A:57:PHE:HB2	19	0.13
(1,702)	1:A:56:VAL:HG23	1:A:57:PHE:HB2	19	0.13
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,650)	1:A:58:LEU:HB2	1:A:110:PRO:HG2	3	0.13
(1,527)	1:A:118:PHE:HA	1:A:119:VAL:HB	18	0.13
(1,449)	1:A:108:THR:HA	1:A:109:ILE:H	20	0.13
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	7	0.13
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	7	0.13
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	7	0.13
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	7	0.13
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	7	0.13
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	7	0.13
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	7	0.13
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG2	14	0.13
(1,1813)	1:A:74:VAL:HG11	1:A:75:GLN:HG3	14	0.13
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG2	14	0.13
(1,1813)	1:A:74:VAL:HG12	1:A:75:GLN:HG3	14	0.13
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG2	14	0.13
(1,1813)	1:A:74:VAL:HG13	1:A:75:GLN:HG3	14	0.13
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG2	14	0.13
(1,1813)	1:A:74:VAL:HG21	1:A:75:GLN:HG3	14	0.13
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG2	14	0.13
(1,1813)	1:A:74:VAL:HG22	1:A:75:GLN:HG3	14	0.13
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG2	14	0.13
(1,1813)	1:A:74:VAL:HG23	1:A:75:GLN:HG3	14	0.13
(1,1806)	1:A:61:THR:HA	1:A:87:ALA:HB1	5	0.13
(1,1806)	1:A:61:THR:HA	1:A:87:ALA:HB2	5	0.13
(1,1806)	1:A:61:THR:HA	1:A:87:ALA:HB3	5	0.13
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	6	0.13
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	12	0.13
(1,1725)	1:A:50:LYS:HD2	1:A:116:GLY:HA2	6	0.13
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	3	0.13
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	5	0.13
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	9	0.13
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	11	0.13
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	13	0.13
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	18	0.13
(1,1493)	1:A:69:PHE:HB2	1:A:110:PRO:HD2	5	0.13
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	13	0.13
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	17	0.13
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	2	0.13
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	6	0.13
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	12	0.13
(1,1440)	1:A:100:ILE:HA	1:A:100:ILE:HG12	17	0.13
(1,1431)	1:A:71:ASN:HA	1:A:71:ASN:HD22	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1431)	1:A:71:ASN:HA	1:A:71:ASN:HD22	10	0.13
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	14	0.13
(1,1402)	1:A:67:CYS:H	1:A:70:SER:HB2	8	0.13
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD1	14	0.13
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD2	14	0.13
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD1	19	0.13
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD2	19	0.13
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD1	14	0.13
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD2	14	0.13
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD1	14	0.13
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD2	14	0.13
(1,1290)	1:A:48:LEU:HD11	1:A:50:LYS:H	20	0.13
(1,1290)	1:A:48:LEU:HD12	1:A:50:LYS:H	20	0.13
(1,1290)	1:A:48:LEU:HD13	1:A:50:LYS:H	20	0.13
(1,1290)	1:A:48:LEU:HD21	1:A:50:LYS:H	20	0.13
(1,1290)	1:A:48:LEU:HD22	1:A:50:LYS:H	20	0.13
(1,1290)	1:A:48:LEU:HD23	1:A:50:LYS:H	20	0.13
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	4	0.13
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	2	0.13
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	4	0.13
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	6	0.13
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	9	0.13
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	14	0.13
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	17	0.13
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	18	0.13
(1,1119)	1:A:53:LYS:HG2	1:A:115:ASN:H	20	0.13
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD2	1	0.13
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD3	1	0.13
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD2	1	0.13
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD3	1	0.13
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD2	1	0.13
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD3	1	0.13
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	3	0.13
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	7	0.13
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	8	0.13
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	11	0.13
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG11	14	0.12
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG12	14	0.12
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG13	14	0.12
(1,97)	1:A:112:VAL:H	1:A:119:VAL:HB	17	0.12
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	9	0.12
(1,906)	1:A:110:PRO:HG3	1:A:122:CYS:HB3	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:A:110:PRO:HG3	1:A:122:CYS:HB3	7	0.12
(1,906)	1:A:110:PRO:HG3	1:A:122:CYS:HB3	17	0.12
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	4	0.12
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	19	0.12
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	4	0.12
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	5	0.12
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	13	0.12
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	17	0.12
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	18	0.12
(1,662)	1:A:60:GLY:HA2	1:A:66:GLN:HA	13	0.12
(1,662)	1:A:60:GLY:HA2	1:A:66:GLN:HA	18	0.12
(1,651)	1:A:58:LEU:HB3	1:A:70:SER:HB3	4	0.12
(1,651)	1:A:58:LEU:HB3	1:A:70:SER:HB3	10	0.12
(1,651)	1:A:58:LEU:HB3	1:A:70:SER:HB3	19	0.12
(1,551)	1:A:109:ILE:HA	1:A:109:ILE:HG12	14	0.12
(1,527)	1:A:118:PHE:HA	1:A:119:VAL:HB	9	0.12
(1,466)	1:A:139:LYS:HA	1:A:139:LYS:HG2	12	0.12
(1,40)	1:A:117:GLU:HB2	1:A:118:PHE:H	2	0.12
(1,40)	1:A:117:GLU:HB2	1:A:118:PHE:H	19	0.12
(1,32)	1:A:55:VAL:HG21	1:A:86:ALA:H	9	0.12
(1,32)	1:A:55:VAL:HG22	1:A:86:ALA:H	9	0.12
(1,32)	1:A:55:VAL:HG23	1:A:86:ALA:H	9	0.12
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	6	0.12
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	12	0.12
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	14	0.12
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	17	0.12
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	18	0.12
(1,259)	1:A:83:ARG:H	1:A:85:TYR:H	5	0.12
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG11	16	0.12
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG12	16	0.12
(1,1874)	1:A:113:TYR:HD1	1:A:119:VAL:HG13	16	0.12
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG11	16	0.12
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG12	16	0.12
(1,1874)	1:A:113:TYR:HD2	1:A:119:VAL:HG13	16	0.12
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD21	13	0.12
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD22	13	0.12
(1,1870)	1:A:57:PHE:HD1	1:A:96:LEU:HD23	13	0.12
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD21	13	0.12
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD22	13	0.12
(1,1870)	1:A:57:PHE:HD2	1:A:96:LEU:HD23	13	0.12
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	8	0.12
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	19	0.12
(1,1760)	1:A:50:LYS:HG2	1:A:51:LYS:H	14	0.12
(1,1760)	1:A:50:LYS:HG3	1:A:51:LYS:H	14	0.12
(1,1760)	1:A:50:LYS:HG2	1:A:51:LYS:H	17	0.12
(1,1760)	1:A:50:LYS:HG3	1:A:51:LYS:H	17	0.12
(1,1671)	1:A:110:PRO:HG2	1:A:122:CYS:HB3	20	0.12
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	11	0.12
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	13	0.12
(1,1668)	1:A:5:MET:H	1:A:5:MET:HG3	7	0.12
(1,1668)	1:A:5:MET:H	1:A:5:MET:HG3	19	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	1	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	2	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	3	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	5	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	6	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	8	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	9	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	10	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	12	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	16	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	19	0.12
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	20	0.12
(1,1595)	1:A:52:ASP:HB2	1:A:53:LYS:H	16	0.12
(1,1484)	1:A:49:VAL:HG11	1:A:116:GLY:HA3	4	0.12
(1,1484)	1:A:49:VAL:HG12	1:A:116:GLY:HA3	4	0.12
(1,1484)	1:A:49:VAL:HG13	1:A:116:GLY:HA3	4	0.12
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	4	0.12
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	7	0.12
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	11	0.12
(1,1431)	1:A:71:ASN:HA	1:A:71:ASN:HD22	8	0.12
(1,1431)	1:A:71:ASN:HA	1:A:71:ASN:HD22	11	0.12
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD1	3	0.12
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD2	3	0.12
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD1	5	0.12
(1,1379)	1:A:69:PHE:HA	1:A:69:PHE:HD2	5	0.12
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD1	1	0.12
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD2	1	0.12
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD1	1	0.12
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD2	1	0.12
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD1	7	0.12
(1,1330)	1:A:57:PHE:HD1	1:A:88:TYR:HD2	7	0.12
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD1	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:A:57:PHE:HD2	1:A:88:TYR:HD2	7	0.12
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	3	0.12
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	18	0.12
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	19	0.12
(1,1225)	1:A:54:VAL:H	1:A:85:TYR:HB3	3	0.12
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	11	0.12
(1,1208)	1:A:95:GLU:H	1:A:95:GLU:HB3	15	0.12
(1,1193)	1:A:83:ARG:H	1:A:83:ARG:HB2	13	0.12
(1,1193)	1:A:83:ARG:H	1:A:83:ARG:HB2	19	0.12
(1,1119)	1:A:53:LYS:HG2	1:A:115:ASN:H	4	0.12
(1,1119)	1:A:53:LYS:HG2	1:A:115:ASN:H	9	0.12
(1,1119)	1:A:53:LYS:HG2	1:A:115:ASN:H	13	0.12
(2,27)	1:A:50:LYS:H	1:A:46:ASP:O	7	0.11
(2,27)	1:A:50:LYS:H	1:A:46:ASP:O	8	0.11
(2,27)	1:A:50:LYS:H	1:A:46:ASP:O	15	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG11	5	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG12	5	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG13	5	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG11	6	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG12	6	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG13	6	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG11	18	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG12	18	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG13	18	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG11	19	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG12	19	0.11
(1,999)	1:A:134:LEU:H	1:A:135:VAL:HG13	19	0.11
(1,97)	1:A:112:VAL:H	1:A:119:VAL:HB	9	0.11
(1,97)	1:A:112:VAL:H	1:A:119:VAL:HB	12	0.11
(1,97)	1:A:112:VAL:H	1:A:119:VAL:HB	20	0.11
(1,941)	1:A:53:LYS:HG3	1:A:54:VAL:H	12	0.11
(1,938)	1:A:53:LYS:HA	1:A:53:LYS:HG2	2	0.11
(1,938)	1:A:53:LYS:HA	1:A:53:LYS:HG2	6	0.11
(1,938)	1:A:53:LYS:HA	1:A:53:LYS:HG2	7	0.11
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	11	0.11
(1,919)	1:A:148:LEU:H	1:A:148:LEU:HG	16	0.11
(1,843)	1:A:73:VAL:H	1:A:73:VAL:HB	9	0.11
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	1	0.11
(1,832)	1:A:129:HIS:HB2	1:A:130:GLN:HB2	9	0.11
(1,826)	1:A:5:MET:HB2	1:A:5:MET:HG2	8	0.11
(1,723)	1:A:109:ILE:H	1:A:109:ILE:HB	20	0.11
(1,691)	1:A:47:ALA:H	1:A:48:LEU:HB3	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,691)	1:A:47:ALA:H	1:A:48:LEU:HB3	15	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD2	2	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD3	2	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD2	4	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD3	4	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD2	11	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD3	11	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD2	12	0.11
(1,674)	1:A:83:ARG:HA	1:A:83:ARG:HD3	12	0.11
(1,651)	1:A:58:LEU:HB3	1:A:70:SER:HB3	8	0.11
(1,651)	1:A:58:LEU:HB3	1:A:70:SER:HB3	20	0.11
(1,605)	1:A:131:ASN:HA	1:A:131:ASN:HD22	3	0.11
(1,605)	1:A:131:ASN:HA	1:A:131:ASN:HD22	14	0.11
(1,542)	1:A:98:GLN:HA	1:A:100:ILE:H	11	0.11
(1,528)	1:A:118:PHE:HA	1:A:119:VAL:HG11	3	0.11
(1,528)	1:A:118:PHE:HA	1:A:119:VAL:HG12	3	0.11
(1,528)	1:A:118:PHE:HA	1:A:119:VAL:HG13	3	0.11
(1,494)	1:A:136:GLU:HA	1:A:139:LYS:HG3	12	0.11
(1,466)	1:A:139:LYS:HA	1:A:139:LYS:HG2	9	0.11
(1,466)	1:A:139:LYS:HA	1:A:139:LYS:HG2	17	0.11
(1,415)	1:A:49:VAL:HA	1:A:55:VAL:H	5	0.11
(1,40)	1:A:117:GLU:HB2	1:A:118:PHE:H	3	0.11
(1,40)	1:A:117:GLU:HB2	1:A:118:PHE:H	14	0.11
(1,32)	1:A:55:VAL:HG21	1:A:86:ALA:H	13	0.11
(1,32)	1:A:55:VAL:HG22	1:A:86:ALA:H	13	0.11
(1,32)	1:A:55:VAL:HG23	1:A:86:ALA:H	13	0.11
(1,32)	1:A:55:VAL:HG21	1:A:86:ALA:H	17	0.11
(1,32)	1:A:55:VAL:HG22	1:A:86:ALA:H	17	0.11
(1,32)	1:A:55:VAL:HG23	1:A:86:ALA:H	17	0.11
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	2	0.11
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	4	0.11
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	8	0.11
(1,262)	1:A:85:TYR:H	1:A:85:TYR:HB2	10	0.11
(1,24)	1:A:150:GLU:H	1:A:150:GLU:HB3	10	0.11
(1,23)	1:A:150:GLU:H	1:A:150:GLU:HG2	12	0.11
(1,23)	1:A:150:GLU:H	1:A:150:GLU:HG3	12	0.11
(1,207)	1:A:53:LYS:HB3	1:A:54:VAL:H	8	0.11
(1,207)	1:A:53:LYS:HB3	1:A:54:VAL:H	14	0.11
(1,207)	1:A:53:LYS:HB3	1:A:54:VAL:H	18	0.11
(1,18)	1:A:83:ARG:H	1:A:84:ASP:HB2	13	0.11
(1,1783)	1:A:80:HIS:HE1	1:A:135:VAL:HG11	5	0.11
(1,1783)	1:A:80:HIS:HE1	1:A:135:VAL:HG12	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1783)	1:A:80:HIS:HE1	1:A:135:VAL:HG13	5	0.11
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	1	0.11
(1,1767)	1:A:147:LEU:H	1:A:147:LEU:HB3	7	0.11
(1,1760)	1:A:50:LYS:HG2	1:A:51:LYS:H	1	0.11
(1,1760)	1:A:50:LYS:HG3	1:A:51:LYS:H	1	0.11
(1,1756)	1:A:148:LEU:HA	1:A:148:LEU:HG	13	0.11
(1,1725)	1:A:50:LYS:HD2	1:A:116:GLY:HA2	3	0.11
(1,1719)	1:A:50:LYS:H	1:A:50:LYS:HB3	1	0.11
(1,1719)	1:A:50:LYS:H	1:A:50:LYS:HB3	10	0.11
(1,1719)	1:A:50:LYS:H	1:A:50:LYS:HB3	11	0.11
(1,1719)	1:A:50:LYS:H	1:A:50:LYS:HB3	13	0.11
(1,1719)	1:A:50:LYS:H	1:A:50:LYS:HB3	14	0.11
(1,1719)	1:A:50:LYS:H	1:A:50:LYS:HB3	16	0.11
(1,1677)	1:A:117:GLU:HB3	1:A:117:GLU:HG3	6	0.11
(1,1677)	1:A:117:GLU:HB3	1:A:117:GLU:HG3	9	0.11
(1,1677)	1:A:117:GLU:HB3	1:A:117:GLU:HG3	19	0.11
(1,1677)	1:A:117:GLU:HB3	1:A:117:GLU:HG3	20	0.11
(1,1671)	1:A:110:PRO:HG2	1:A:122:CYS:HB3	10	0.11
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	8	0.11
(1,1669)	1:A:78:ARG:H	1:A:78:ARG:HB2	10	0.11
(1,1668)	1:A:5:MET:H	1:A:5:MET:HG3	20	0.11
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	4	0.11
(1,1659)	1:A:129:HIS:HD2	1:A:130:GLN:HB3	17	0.11
(1,1605)	1:A:118:PHE:HD1	1:A:120:GLY:HA3	2	0.11
(1,1605)	1:A:118:PHE:HD2	1:A:120:GLY:HA3	2	0.11
(1,1595)	1:A:52:ASP:HB2	1:A:53:LYS:H	3	0.11
(1,1595)	1:A:52:ASP:HB2	1:A:53:LYS:H	5	0.11
(1,1595)	1:A:52:ASP:HB2	1:A:53:LYS:H	12	0.11
(1,1594)	1:A:93:ASP:H	1:A:93:ASP:HB3	10	0.11
(1,1594)	1:A:93:ASP:H	1:A:93:ASP:HB3	15	0.11
(1,1593)	1:A:106:TRP:HB3	1:A:108:THR:HA	18	0.11
(1,1593)	1:A:106:TRP:HB3	1:A:108:THR:HA	20	0.11
(1,15)	1:A:83:ARG:H	1:A:83:ARG:HB3	8	0.11
(1,1484)	1:A:49:VAL:HG11	1:A:116:GLY:HA3	12	0.11
(1,1484)	1:A:49:VAL:HG12	1:A:116:GLY:HA3	12	0.11
(1,1484)	1:A:49:VAL:HG13	1:A:116:GLY:HA3	12	0.11
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	3	0.11
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	6	0.11
(1,1476)	1:A:129:HIS:HB2	1:A:130:GLN:HG2	16	0.11
(1,1431)	1:A:71:ASN:HA	1:A:71:ASN:HD22	19	0.11
(1,1430)	1:A:4:THR:HA	1:A:5:MET:H	5	0.11
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	6	0.11
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	7	0.11
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	11	0.11
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	17	0.11
(1,1416)	1:A:129:HIS:HA	1:A:129:HIS:HD2	20	0.11
(1,1408)	1:A:83:ARG:HA	1:A:83:ARG:HG2	10	0.11
(1,1408)	1:A:83:ARG:HA	1:A:83:ARG:HG3	10	0.11
(1,1402)	1:A:67:CYS:H	1:A:70:SER:HB2	6	0.11
(1,1383)	1:A:57:PHE:HB2	1:A:58:LEU:HA	6	0.11
(1,1383)	1:A:57:PHE:HB2	1:A:58:LEU:HA	17	0.11
(1,1319)	1:A:118:PHE:H	1:A:118:PHE:HD1	19	0.11
(1,1319)	1:A:118:PHE:H	1:A:118:PHE:HD2	19	0.11
(1,129)	1:A:71:ASN:HB2	1:A:72:ALA:H	6	0.11
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	9	0.11
(1,1284)	1:A:89:ASN:H	1:A:89:ASN:HD22	11	0.11
(1,1275)	1:A:69:PHE:HE1	1:A:122:CYS:HB2	20	0.11
(1,1275)	1:A:69:PHE:HE2	1:A:122:CYS:HB2	20	0.11
(1,1234)	1:A:46:ASP:H	1:A:46:ASP:HB3	2	0.11
(1,1223)	1:A:54:VAL:H	1:A:55:VAL:HG11	12	0.11
(1,1223)	1:A:54:VAL:H	1:A:55:VAL:HG12	12	0.11
(1,1223)	1:A:54:VAL:H	1:A:55:VAL:HG13	12	0.11
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD2	2	0.11
(1,1063)	1:A:90:VAL:HG21	1:A:97:ARG:HD3	2	0.11
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD2	2	0.11
(1,1063)	1:A:90:VAL:HG22	1:A:97:ARG:HD3	2	0.11
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD2	2	0.11
(1,1063)	1:A:90:VAL:HG23	1:A:97:ARG:HD3	2	0.11
(1,1009)	1:A:56:VAL:HG11	1:A:85:TYR:HB3	1	0.11
(1,1009)	1:A:56:VAL:HG12	1:A:85:TYR:HB3	1	0.11
(1,1009)	1:A:56:VAL:HG13	1:A:85:TYR:HB3	1	0.11
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	1	0.11
(1,1)	1:A:146:ALA:H	1:A:148:LEU:HB2	13	0.11

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value