Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 05:08 AM EDT

PDB ID	:	5HUZ
BMRB ID	:	30005
Title	:	Solution structure of coiled coil domain of myosin binding subunit of myosin light chain phosphatase
Authors	:	Sharma, A.K.; Birrane, G.; Anklin, C.; Rigby, A.C.; Pollak, M.; Alper, S.L.
Deposited on	:	2016-01-27

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:

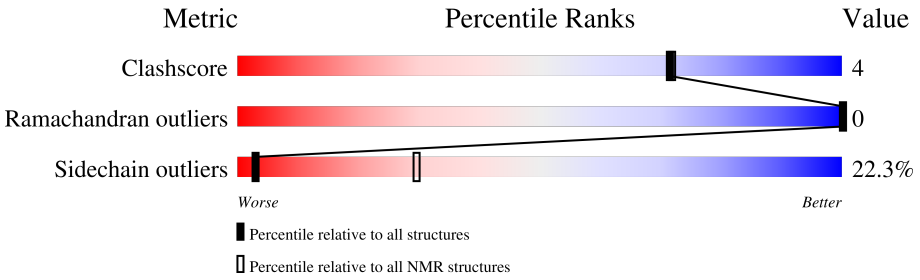
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 45%.

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	48	48% 17% • 25% 8%
1	B	48	52% 17% 23% 8%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:3-A:34, B:102-B:134 (65)	0.39	8

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1518 atoms, of which 768 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein phosphatase 1 regulatory subunit 12A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	44	760	236	385	65	73	1	0
1	B	44	758	236	383	65	73	1	0

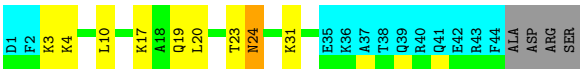
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

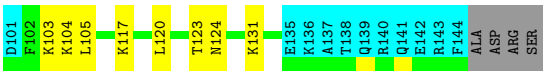
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 48% 17% • 25% 8%



• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 52% 17% 23% 8%



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

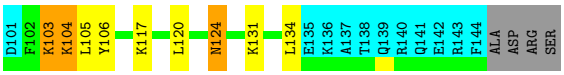
4.2.1 Score per residue for model 1

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 46% 21% 25% 8%

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

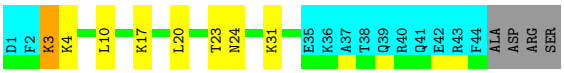
Chain B: 50% 12% 6% 23% 8%



4.2.2 Score per residue for model 2

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 50% 15% • 25% 8%



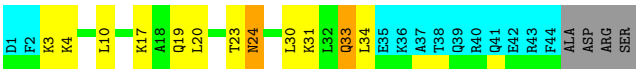
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 50% 12% 6% 23% 8%

4.2.3 Score per residue for model 3

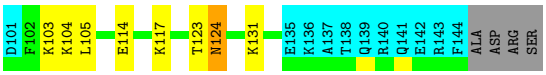
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 42% 21% • 25% 8%



• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

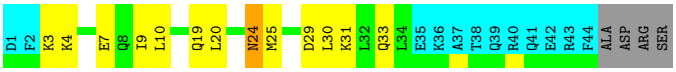
Chain B: 52% 15% • 23% 8%



4.2.4 Score per residue for model 4

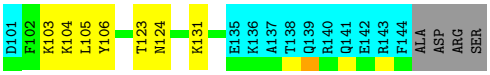
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 40% 25% • 25% 8%



• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

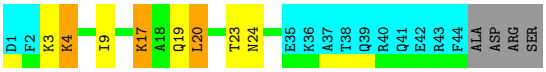
Chain B: 54% 15% 23% 8%



4.2.5 Score per residue for model 5

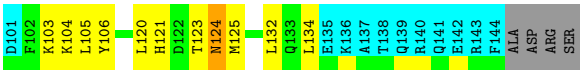
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 50% 10% 6% 25% 8%



• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

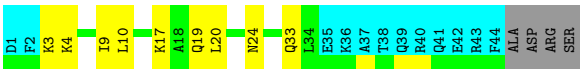
Chain B: 46% 21% • 23% 8%



4.2.6 Score per residue for model 6

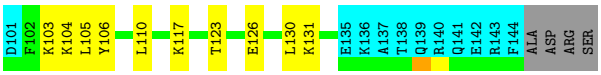
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 48% 19% 25% 8%



• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

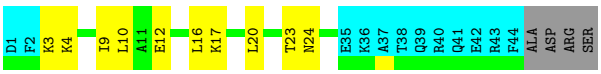
Chain B: 48% 21% 23% 8%



4.2.7 Score per residue for model 7

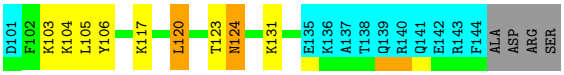
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 46% 21% 25% 8%



• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

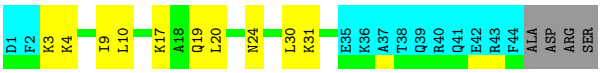
Chain B: 50% 15% • 23% 8%



4.2.8 Score per residue for model 8 (medoid)

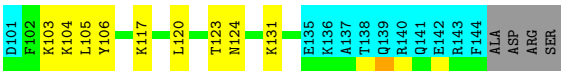
• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 46% 21% 25% 8%



• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 50% 19% 23% 8%



4.2.9 Score per residue for model 9

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 40% 27% 25% 8%

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 50% 17% • 23% 8%

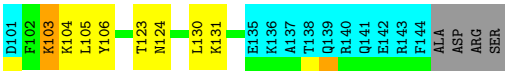
4.2.10 Score per residue for model 10

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 46% 15% 6% 25% 8%

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

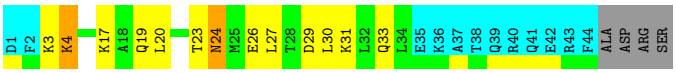
Chain B: 52% 15% • 23% 8%



4.2.11 Score per residue for model 11

- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 40% 23% • 25% 8%



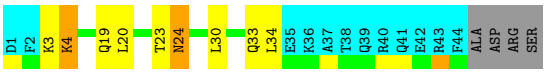
- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 50% 17% • 23% 8%

4.2.12 Score per residue for model 12

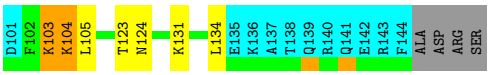
- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 48% 15% • 25% 8%



- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 54% 10% • 23% 8%



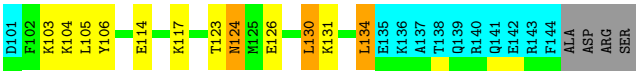
4.2.13 Score per residue for model 13

- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 46% 15% 6% 25% 8%

- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

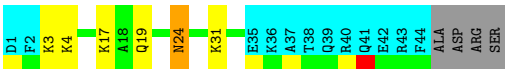
Chain B: 44% 19% 6% 23% 8%



4.2.14 Score per residue for model 14

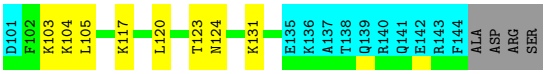
- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 54% 10% • 25% 8%



- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

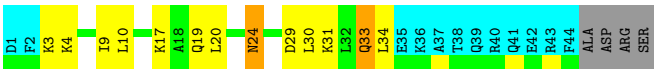
Chain B: 52% 17% 23% 8%



4.2.15 Score per residue for model 15

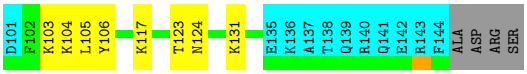
- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 40% 23% • 25% 8%



- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

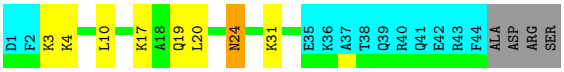
Chain B: 52% 17% 23% 8%



4.2.16 Score per residue for model 16

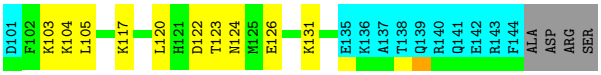
- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 50% 15% • 25% 8%



- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 48% 21% 23% 8%



4.2.17 Score per residue for model 17

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 40% 25% • 25% 8%

D1 F2 K3 K4 L10 K17 A18 Q19 L20 H21 D22 T23 N24 M25 E26 L27 K31 L34 E35 K36 A37 T38 Q39 R40 Q41 E42 R43 F44 ALA ASP ARG SER

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 48% 19% • 23% 8%

D101 F102 K103 K104 L105 L110 D122 T123 N124 M125 E126 K131 L134 E135 K136 A137 T138 Q139 R140 Q141 E142 R143 F144 ALA ASP ARG SER

4.2.18 Score per residue for model 18

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 46% 19% • 25% 8%

D1 F2 K3 K4 L10 Q19 L20 H21 N24 M25 L30 K31 E35 K36 A37 T38 Q39 R40 Q41 E42 R43 F44 ALA ASP ARG SER

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B: 42% 27% 23% 8%

D101 F102 K103 K104 L105 L110 K117 L120 H121 D122 T123 E126 L127 K131 L132 Q133 L134 E135 K136 A137 T138 Q139 R140 Q141 E142 R143 F144 ALA ASP ARG SER

4.2.19 Score per residue for model 19

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A: 50% 17% 25% 8%

D1 F2 K3 K4 K17 A18 Q19 N24 D29 L30 K31 L32 Q33 L34 E35 K36 A37 T38 Q39 R40 Q41 E42 R43 F44 ALA ASP ARG SER

• Molecule 1: Protein phosphatase 1 regulatory subunit 12A

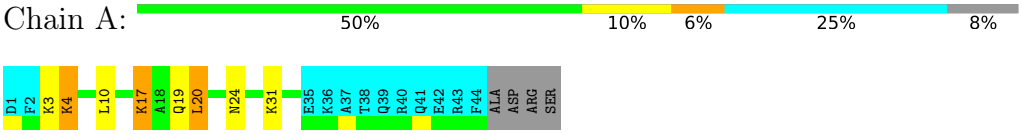
Chain B: 54% 15% 23% 8%

D101 F102 K103 K104 E112 L116 L120 T123 N124 E135 K136 A137 T138 Q139 R140 Q141 E142 R143 F144 ALA ASP ARG SER

4.2.20 Score per residue for model 20

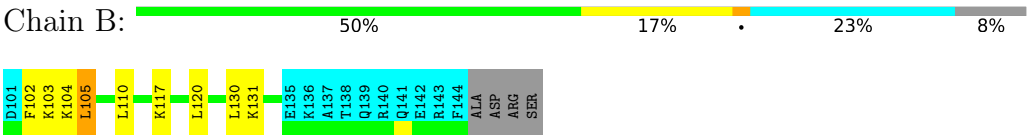
- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain A:



- Molecule 1: Protein phosphatase 1 regulatory subunit 12A

Chain B:



5 Refinement protocol and experimental data overview (i)

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	**Classification**	**Version**
CYANA	structure calculation	3.97
CNS	refinement	1.3

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	602
Number of shifts mapped to atoms	584
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	266	282	281	3±2
1	B	277	291	290	3±1
All	All	10860	11460	11420	78

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HG	1:B:130:LEU:HD12	0.61	1.71	13	1
1:A:27:LEU:HD11	1:B:126:GLU:HB2	0.56	1.76	17	4
1:A:30:LEU:O	1:A:34:LEU:HB2	0.53	2.04	12	2
1:B:117:LYS:HA	1:B:120:LEU:HD23	0.51	1.82	7	2
1:A:24:ASN:ND2	1:B:123:THR:HG21	0.51	2.21	16	17
1:A:17:LYS:HA	1:A:20:LEU:HD23	0.51	1.82	5	2
1:A:30:LEU:HA	1:A:33:GLN:HE21	0.48	1.68	9	1
1:B:114:GLU:HA	1:B:117:LYS:HE2	0.48	1.86	3	1
1:A:23:THR:HG21	1:B:124:ASN:ND2	0.47	2.24	5	10
1:A:3:LYS:HD3	1:A:4:LYS:N	0.47	2.25	10	3
1:A:9:ILE:HD11	1:B:106:TYR:CD2	0.46	2.46	10	4
1:B:121:HIS:O	1:B:125:MET:HG2	0.45	2.10	5	2
1:A:34:LEU:HG	1:B:134:LEU:HD22	0.45	1.87	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:HB3	1:B:130:LEU:HD21	0.45	1.89	9	1
1:A:9:ILE:HD11	1:B:106:TYR:CD1	0.45	2.47	13	5
1:A:21:HIS:O	1:A:25:MET:HG3	0.45	2.12	18	2
1:A:3:LYS:HD3	1:A:4:LYS:H	0.44	1.72	10	2
1:A:26:GLU:O	1:A:30:LEU:HB2	0.43	2.13	10	2
1:B:122:ASP:O	1:B:126:GLU:HG3	0.42	2.13	18	2
1:B:103:LYS:HD3	1:B:104:LYS:N	0.42	2.29	1	2
1:A:12:GLU:O	1:A:16:LEU:HG	0.42	2.14	9	2
1:A:23:THR:HG22	1:B:123:THR:HG22	0.42	1.90	3	3
1:B:112:GLU:O	1:B:116:LEU:HG	0.42	2.14	19	1
1:A:29:ASP:O	1:A:33:GLN:HG2	0.42	2.15	19	2
1:B:126:GLU:O	1:B:130:LEU:HD22	0.41	2.15	6	1
1:A:29:ASP:O	1:A:33:GLN:HG3	0.41	2.16	15	1
1:B:102:PHE:O	1:B:105:LEU:HG	0.41	2.16	20	1
1:B:122:ASP:O	1:B:126:GLU:HG2	0.41	2.16	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	32/48 (67%)	31±1 (96±3%)	1±1 (4±3%)	0±0 (0±0%)	100	100
1	B	33/48 (69%)	33±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100
All	All	1300/1920 (68%)	1272 (98%)	28 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	30/44 (68%)	23±2 (76±6%)	7±2 (24±6%)	2 26
1	B	31/44 (70%)	25±1 (80±4%)	6±1 (20±4%)	3 33
All	All	1220/1760 (69%)	948 (78%)	272 (22%)	3 29

All 26 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	3	LYS	20
1	B	103	LYS	20
1	B	104	LYS	20
1	A	4	LYS	19
1	B	105	LEU	19
1	A	19	GLN	18
1	A	20	LEU	17
1	A	17	LYS	16
1	A	31	LYS	15
1	B	124	ASN	15
1	B	131	LYS	15
1	A	10	LEU	13
1	A	24	ASN	13
1	B	117	LYS	11
1	B	120	LEU	10
1	B	110	LEU	5
1	A	33	GLN	5
1	B	134	LEU	4
1	A	30	LEU	4
1	B	130	LEU	4
1	A	34	LEU	3
1	B	114	GLU	2
1	A	7	GLU	1
1	A	25	MET	1
1	A	29	ASP	1
1	B	133	GLN	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no 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 45% for the well-defined parts and 44% 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	602
Number of shifts mapped to atoms	584
Number of unparsed shifts	0
Number of shifts with mapping errors	18
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 18 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	45	ALA	H	7.792	0.023	.
1	A	45	ALA	CA	54.18	0.000	.
1	A	45	ALA	CB	20.45	0.000	.
1	A	45	ALA	N	130.312	0.210	.
1	A	47	ARG	HA	4.416	0.000	.
1	A	47	ARG	HB2	1.651	0.000	.
1	A	47	ARG	HB3	1.929	0.000	.
1	A	47	ARG	HG2	1.785	0.000	.
1	A	47	ARG	HG3	1.785	0.000	.
1	A	47	ARG	HD2	3.21	0.000	.
1	A	47	ARG	HD3	3.21	0.000	.
1	A	47	ARG	C	174.57	0.000	.
1	A	47	ARG	CA	55.91	0.000	.
1	A	47	ARG	CB	31.02	0.000	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	48	SER	H	7.992	0.028	.
1	A	48	SER	N	122.83	0.227	.
1	A	48	SER	CA	60.29	0.000	.
1	A	48	SER	CB	65.21	0.000	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	47	-1.01 ± 0.27	Should be checked
$^{13}C_{\beta}$	47	-0.03 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	43	-0.55 ± 0.26	Should be applied
^{15}N	46	-0.76 ± 0.35	Should be applied

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 45%, i.e. 440 atoms were assigned a chemical shift out of a possible 968. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	159/325 (49%)	64/130 (49%)	63/130 (48%)	32/65 (49%)
Sidechain	272/599 (45%)	186/386 (48%)	83/193 (43%)	3/20 (15%)
Aromatic	9/44 (20%)	5/21 (24%)	4/19 (21%)	0/4 (0%)
Overall	440/968 (45%)	255/537 (47%)	150/342 (44%)	35/89 (39%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 583 atoms were assigned a chemical shift out of a possible 1316. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	217/440 (49%)	87/176 (49%)	86/176 (49%)	44/88 (50%)
Sidechain	349/802 (44%)	238/510 (47%)	107/254 (42%)	4/38 (11%)
Aromatic	17/74 (23%)	11/36 (31%)	6/34 (18%)	0/4 (0%)
Overall	583/1316 (44%)	336/722 (47%)	199/464 (43%)	48/130 (37%)

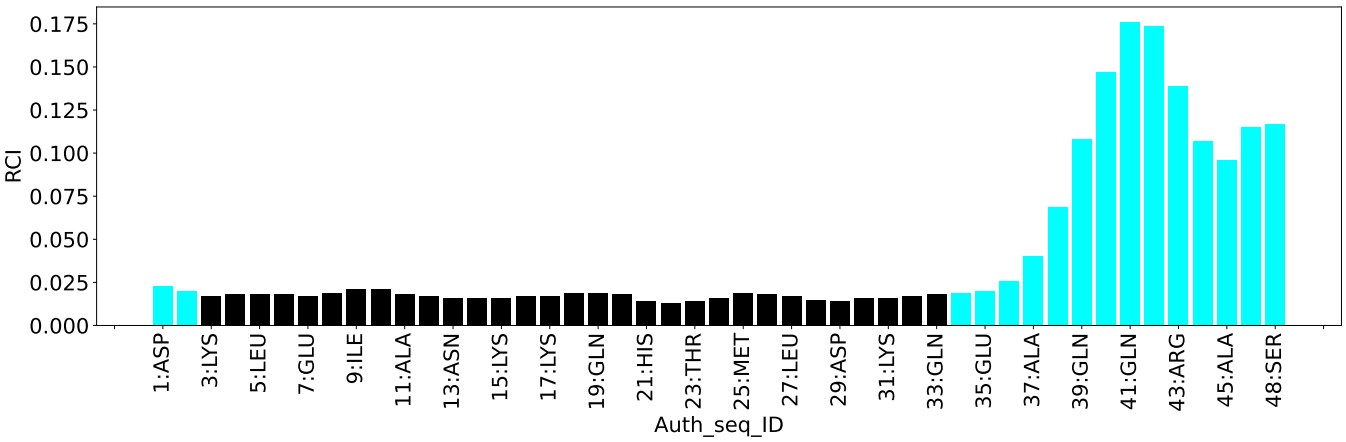
7.1.4 Statistically unusual chemical shifts (i)

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	2065
Intra-residue (|i-j|=0)	663
Sequential (|i-j|=1)	469
Medium range (|i-j|>1 and |i-j|<5)	487
Long range (|i-j|≥5)	0
Inter-chain	314
Hydrogen bond restraints	132
Disulfide bond restraints	0
Total dihedral-angle restraints	70
Number of unmapped restraints	0
Number of restraints per residue	22.2
Number of long range restraints per residue[1]	0.0

[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)	37.9	0.2
0.2-0.5 (Medium)	23.9	0.5
>0.5 (Large)	79.3	13.29

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.4	8.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

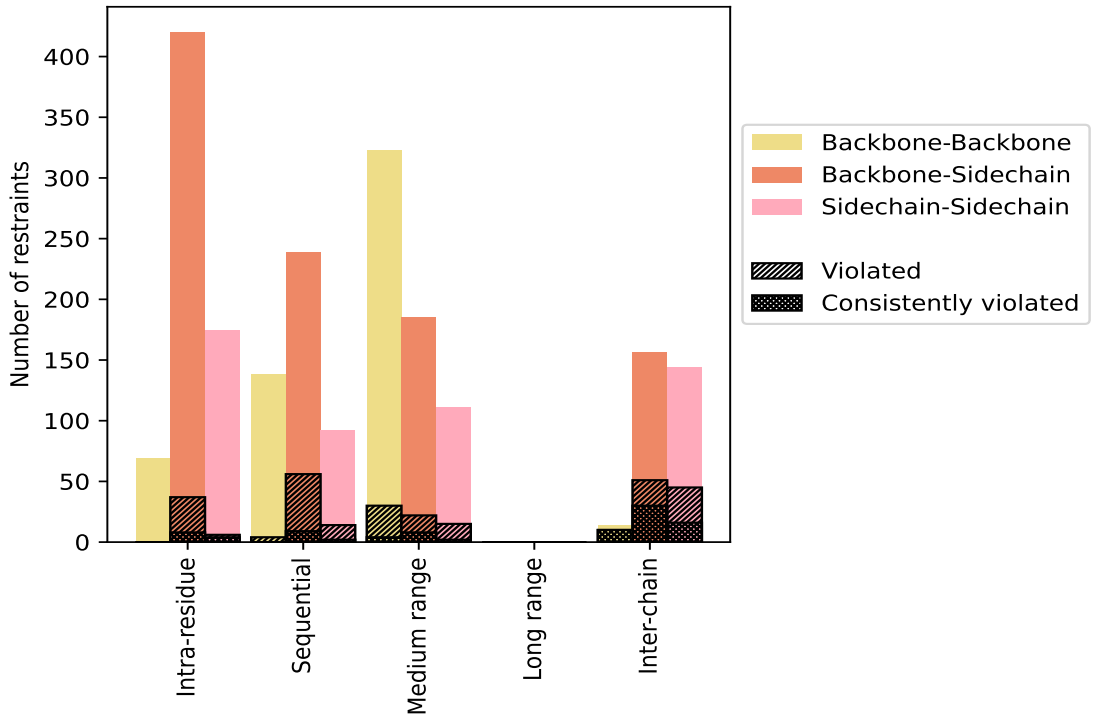
9.1 Summary of distance violations (i)

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)	663	32.1	43	6.5	2.1	12	1.8	0.6
Backbone-Backbone	69	3.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	420	20.3	37	8.8	1.8	8	1.9	0.4
Sidechain-Sidechain	174	8.4	6	3.4	0.3	4	2.3	0.2
Sequential (|i-j|=1)	469	22.7	74	15.8	3.6	11	2.3	0.5
Backbone-Backbone	138	6.7	4	2.9	0.2	0	0.0	0.0
Backbone-Sidechain	239	11.6	56	23.4	2.7	9	3.8	0.4
Sidechain-Sidechain	92	4.5	14	15.2	0.7	2	2.2	0.1
Medium range (|i-j|>1 & |i-j|<5)	487	23.6	43	8.8	2.1	10	2.1	0.5
Backbone-Backbone	191	9.2	6	3.1	0.3	0	0.0	0.0
Backbone-Sidechain	185	9.0	22	11.9	1.1	8	4.3	0.4
Sidechain-Sidechain	111	5.4	15	13.5	0.7	2	1.8	0.1
Long range (|i-j|≥5)	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
Inter-chain	314	15.2	106	33.8	5.1	56	17.8	2.7
Backbone-Backbone	14	0.7	10	71.4	0.5	10	71.4	0.5
Backbone-Sidechain	156	7.6	51	32.7	2.5	30	19.2	1.5
Sidechain-Sidechain	144	7.0	45	31.2	2.2	16	11.1	0.8
Hydrogen bond	132	6.4	24	18.2	1.2	4	3.0	0.2
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2065	100.0	290	14.0	14.0	93	4.5	4.5
Backbone-Backbone	544	26.3	44	8.1	2.1	14	2.6	0.7
Backbone-Sidechain	1000	48.4	166	16.6	8.0	55	5.5	2.7
Sidechain-Sidechain	521	25.2	80	15.4	3.9	24	4.6	1.2

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	19	24	32	0	67	142	3.13	11.9	4.05	0.88
2	19	26	32	0	68	145	3.09	12.67	4.04	0.77
3	18	25	29	0	68	140	3.14	12.3	4.05	0.76
4	13	24	28	0	64	129	3.23	12.2	3.93	0.92
5	19	24	26	0	73	142	3.15	12.17	4.09	0.8
6	18	23	29	0	67	137	3.14	12.63	4.01	0.83
7	20	24	37	0	67	148	2.97	12.65	3.95	0.72
8	18	27	26	0	64	135	3.23	12.64	4.05	0.91
9	18	28	32	0	76	154	2.91	12.02	3.98	0.68
10	19	27	28	0	65	139	2.98	12.16	3.82	0.79
11	20	27	25	0	68	140	3.14	12.8	4.07	0.8

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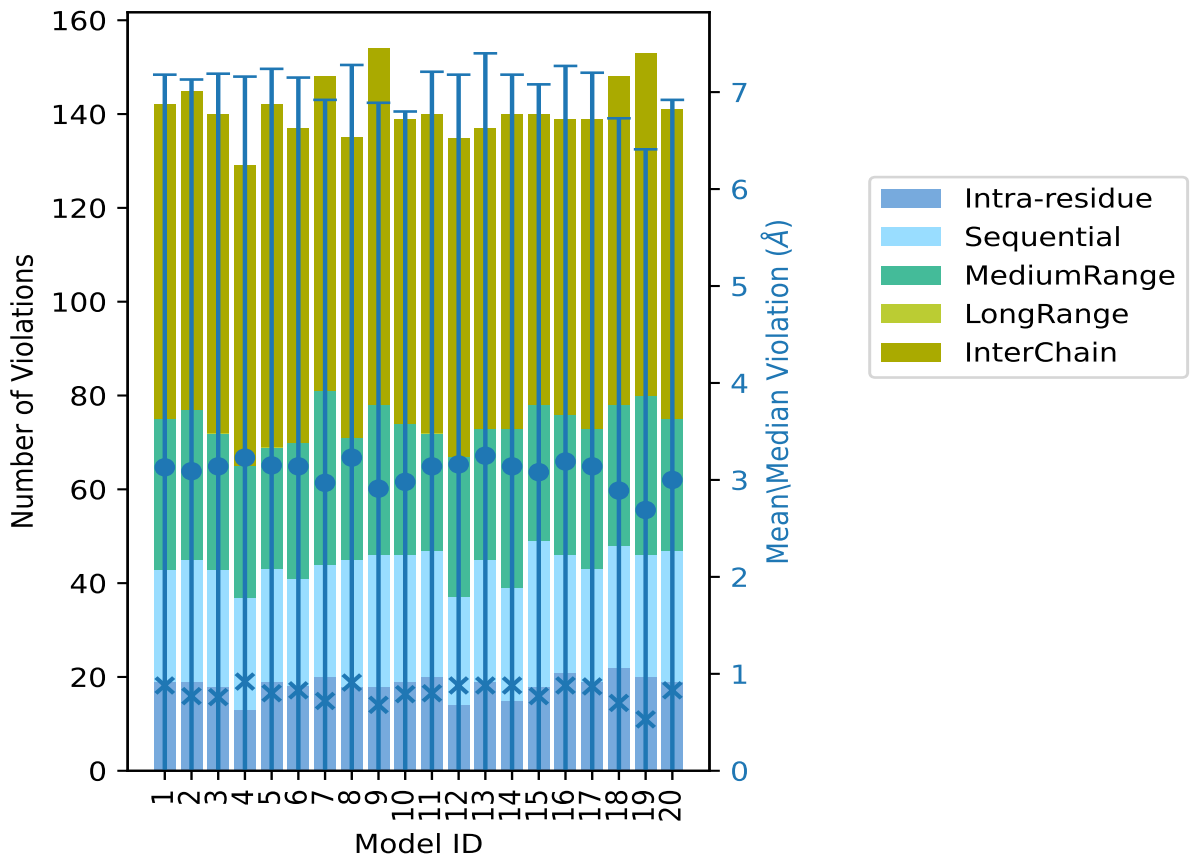
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	14	23	30	0	68	135	3.16	12.01	4.02	0.88
13	19	26	28	0	64	137	3.25	12.86	4.15	0.88
14	15	24	34	0	67	140	3.14	12.42	4.04	0.88
15	18	31	29	0	62	140	3.08	12.51	4.0	0.77
16	21	25	30	0	63	139	3.19	12.65	4.08	0.88
17	19	24	30	0	66	139	3.14	13.29	4.06	0.87
18	22	26	30	0	70	148	2.89	12.88	3.84	0.7
19	20	26	34	0	73	153	2.69	11.74	3.72	0.53
20	19	28	28	0	66	141	3.0	12.84	3.92	0.83

[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

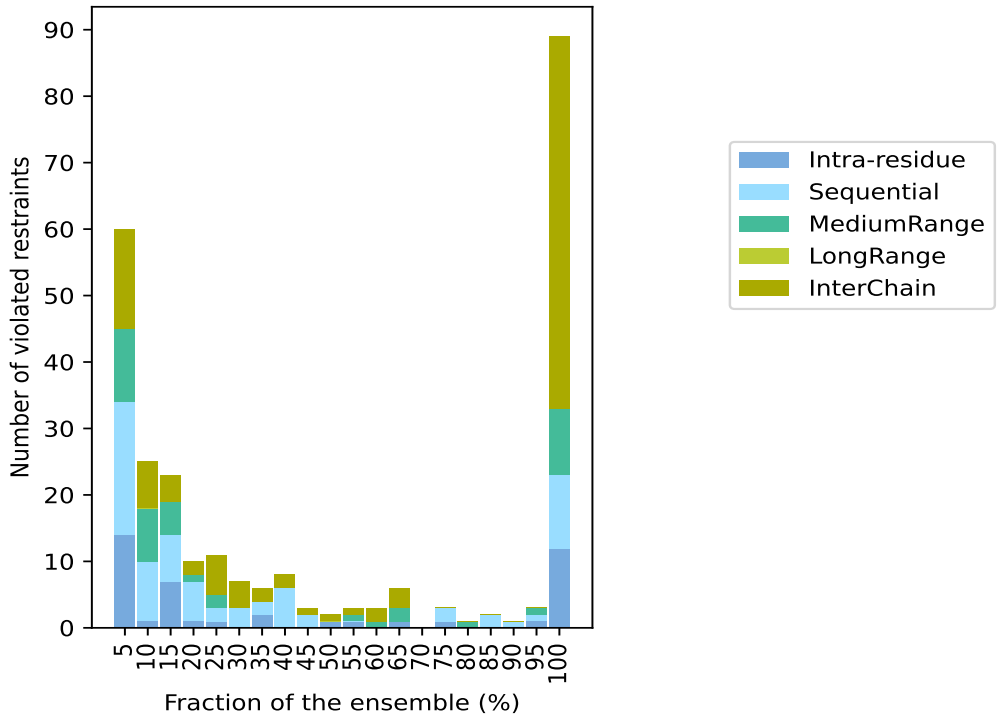
9.3 Distance violation statistics for the ensemble (i)

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, 1667(IR:620, SQ:395, MR:444, LR:0, IC:208) 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]	%
14	20	11	0	15	60	1	5.0
1	9	8	0	7	25	2	10.0
7	7	5	0	4	23	3	15.0
1	6	1	0	2	10	4	20.0
1	2	2	0	6	11	5	25.0
0	3	0	0	4	7	6	30.0
2	2	0	0	2	6	7	35.0
0	6	0	0	2	8	8	40.0
0	2	0	0	1	3	9	45.0
1	0	0	0	1	2	10	50.0
1	0	1	0	1	3	11	55.0
0	0	1	0	2	3	12	60.0
1	0	2	0	3	6	13	65.0
0	0	0	0	0	0	14	70.0
1	2	0	0	0	3	15	75.0
0	0	1	0	0	1	16	80.0
0	2	0	0	0	2	17	85.0
0	1	0	0	0	1	18	90.0
1	1	1	0	0	3	19	95.0
12	11	10	0	56	89	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

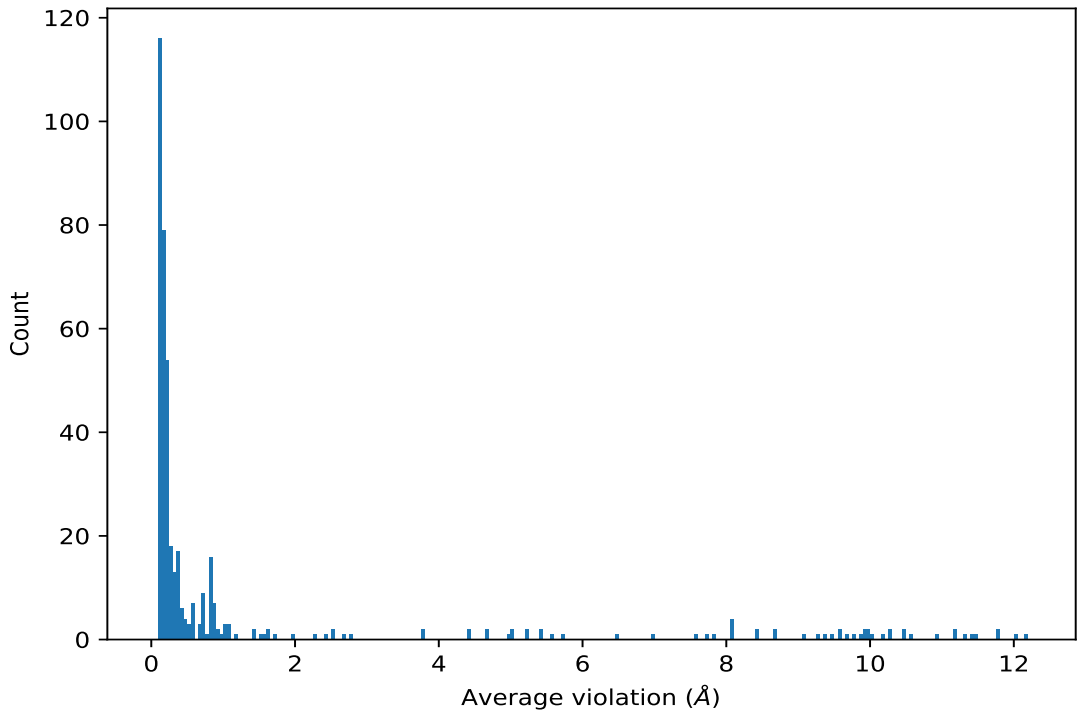
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	20	12.16	0.45	12.18
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	20	12.02	0.25	12.07
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	20	11.76	0.78	11.58
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	20	11.76	0.78	11.58
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	20	11.47	0.15	11.48
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	20	11.42	0.3	11.46
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	20	11.35	0.37	11.46
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	20	11.18	0.82	11.36
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	20	11.16	0.3	11.2
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	20	10.95	0.21	10.97
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	20	10.58	0.49	10.5
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	20	10.48	0.21	10.48
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	20	10.48	0.21	10.48
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	20	10.25	0.2	10.26
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	20	10.25	0.2	10.26
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	20	10.18	0.28	10.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	20	10.02	0.33	10.04
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	20	9.96	0.28	10.02
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	20	9.96	0.28	10.02
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	20	9.93	0.72	9.72
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	20	9.93	0.72	9.72
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	20	9.87	0.89	10.06
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	20	9.79	0.42	9.78
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	20	9.68	0.28	9.76
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	20	9.55	0.5	9.49
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	20	9.55	0.44	9.57
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	20	9.47	0.3	9.48
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	20	9.36	0.64	9.36
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	20	9.28	0.31	9.32
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	20	9.07	0.42	9.06
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	20	8.7	0.23	8.74
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	20	8.7	0.23	8.74
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	20	8.4	0.33	8.38
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	20	8.4	0.33	8.38
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	20	8.08	0.36	8.04
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	20	8.08	0.36	8.04
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	20	8.05	0.9	8.32
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	20	8.05	0.9	8.32
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	20	7.83	0.27	7.86
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	20	7.72	0.39	7.74
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	20	7.56	0.13	7.58
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	20	6.97	0.22	7.02
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	20	6.47	0.11	6.46
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	20	5.73	0.13	5.74
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	20	5.6	0.12	5.6
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	20	5.4	0.36	5.48
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	20	5.4	0.36	5.48
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	20	5.21	0.31	5.26
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	20	5.21	0.31	5.26
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	20	5.05	0.34	5.12
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	20	5.05	0.34	5.12
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	20	4.97	0.29	4.99
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	20	4.67	0.66	4.6
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	20	4.67	0.66	4.6
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	20	4.43	0.41	4.54
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	20	4.43	0.41	4.54
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	20	3.75	0.56	3.78
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	20	3.75	0.56	3.78

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	20	2.76	0.47	2.76
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	20	2.66	0.49	2.8
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	20	2.52	0.32	2.56
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	20	2.52	0.32	2.56
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	20	2.43	0.47	2.43
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	20	2.26	0.35	2.28
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	20	1.98	0.18	1.99
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	20	1.73	0.2	1.78
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	20	1.64	0.02	1.64
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	20	1.61	0.02	1.6
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	20	1.58	0.07	1.59
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	20	1.54	0.08	1.55
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	20	1.45	0.09	1.44
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	20	1.43	0.12	1.41
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	20	1.17	0.13	1.15
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	20	1.09	0.17	1.02
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	20	1.03	0.06	1.02
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	20	1.02	0.06	1.02
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	20	1.01	0.22	1.06
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	20	0.96	0.04	0.95
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	20	0.93	0.09	0.93
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	20	0.9	0.01	0.9
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	20	0.89	0.07	0.88
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	20	0.88	0.03	0.89
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	20	0.88	0.01	0.88
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	20	0.87	0.24	0.8
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	20	0.86	0.06	0.87
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	20	0.86	0.06	0.87
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	20	0.86	0.06	0.87
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	20	0.75	0.07	0.76
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	20	0.71	0.18	0.74
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	20	0.71	0.18	0.74
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	20	0.71	0.18	0.74
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	20	0.7	0.07	0.71
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	20	0.67	0.07	0.67
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	20	0.65	0.09	0.66
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	20	0.57	0.06	0.58
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	20	0.53	0.06	0.53
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	20	0.47	0.07	0.46
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	20	0.47	0.07	0.46
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	20	0.44	0.05	0.45
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	20	0.44	0.1	0.44

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	20	0.41	0.05	0.4
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	20	0.31	0.05	0.3
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	20	0.31	0.05	0.3
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	20	0.31	0.05	0.32
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	20	0.3	0.05	0.3
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	20	0.3	0.05	0.3
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	20	0.24	0.06	0.24
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	20	0.24	0.06	0.24
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	20	0.2	0.01	0.2
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	20	0.2	0.04	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	20	0.19	0.01	0.19
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	20	0.19	0.02	0.18
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	20	0.18	0.03	0.19
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	20	0.17	0.03	0.16
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	20	0.16	0.04	0.16
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	20	0.16	0.04	0.16
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	19	0.3	0.14	0.25
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	19	0.22	0.04	0.23
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	19	0.17	0.03	0.18
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	19	0.15	0.03	0.15
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	19	0.15	0.03	0.15
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	18	1.05	0.41	1.25
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	18	0.31	0.05	0.31
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	17	1.09	0.25	1.1
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	17	0.29	0.09	0.33
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	17	0.23	0.07	0.23
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	17	0.18	0.03	0.18
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	16	0.2	0.07	0.2
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	16	0.2	0.07	0.2
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	16	0.2	0.07	0.2
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	16	0.2	0.07	0.2
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	16	0.19	0.04	0.18
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	15	0.25	0.07	0.28
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	15	0.18	0.04	0.18
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	15	0.14	0.03	0.14
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	14	0.24	0.06	0.24
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	13	0.3	0.08	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	13	0.3	0.08	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	13	0.3	0.08	0.32
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	13	0.24	0.1	0.22
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	13	0.2	0.04	0.21
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	13	0.18	0.05	0.18
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	13	0.18	0.05	0.18
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	13	0.18	0.05	0.18
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	13	0.18	0.05	0.17
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	13	0.18	0.05	0.17
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	13	0.16	0.03	0.16
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	13	0.16	0.03	0.16
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	12	0.82	0.34	0.7
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	12	0.82	0.34	0.7
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	12	0.2	0.05	0.2
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	12	0.2	0.05	0.2
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	12	0.2	0.05	0.2
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	12	0.2	0.05	0.2
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	12	0.18	0.04	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	12	0.16	0.02	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	12	0.16	0.02	0.16
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	11	0.15	0.03	0.15
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	11	0.15	0.04	0.13
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	11	0.15	0.04	0.13
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	11	0.15	0.04	0.13
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	11	0.15	0.04	0.13
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	11	0.15	0.04	0.13
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	11	0.15	0.04	0.13
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	11	0.12	0.02	0.12
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	10	0.72	0.24	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	10	0.72	0.24	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	10	0.72	0.24	0.73

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	10	0.72	0.24	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	10	0.72	0.24	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	10	0.72	0.24	0.73
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	10	0.24	0.06	0.24
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	10	0.14	0.03	0.14
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	9	0.36	0.07	0.35
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	9	0.2	0.05	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	9	0.2	0.05	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	9	0.2	0.05	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	9	0.2	0.05	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	9	0.2	0.05	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	9	0.2	0.05	0.21
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	9	0.15	0.03	0.14
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	8	0.18	0.05	0.18
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	8	0.18	0.05	0.18
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	8	0.17	0.06	0.15
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	8	0.17	0.06	0.15
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	8	0.16	0.06	0.13
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	8	0.15	0.03	0.15
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	8	0.15	0.03	0.15
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	8	0.15	0.03	0.15
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	8	0.14	0.03	0.12
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	8	0.12	0.02	0.12
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	8	0.12	0.02	0.12
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	8	0.12	0.02	0.12
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	8	0.12	0.01	0.12
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	7	0.18	0.04	0.18
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	7	0.18	0.04	0.18
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	7	0.18	0.04	0.18
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	7	0.18	0.04	0.18
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	7	0.18	0.04	0.18
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	7	0.18	0.04	0.18
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	7	0.17	0.04	0.17
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	7	0.15	0.02	0.15
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	7	0.14	0.03	0.12
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	7	0.14	0.02	0.13
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	7	0.14	0.02	0.13
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	7	0.13	0.02	0.12
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	7	0.12	0.01	0.12
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	6	0.85	0.44	0.88
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	6	0.85	0.44	0.88
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	6	0.49	0.25	0.43

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	6	0.49	0.25	0.43
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD21	6	0.2	0.08	0.16
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD22	6	0.2	0.08	0.16
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD23	6	0.2	0.08	0.16
(1,1679)	1:A:5:LEU:HD21	1:B:105:LEU:HA	6	0.14	0.02	0.14
(1,1679)	1:A:5:LEU:HD22	1:B:105:LEU:HA	6	0.14	0.02	0.14
(1,1679)	1:A:5:LEU:HD23	1:B:105:LEU:HA	6	0.14	0.02	0.14
(1,1116)	1:B:114:GLU:HG2	1:B:115:LYS:H	6	0.14	0.02	0.14
(1,20)	1:A:2:PHE:HB3	1:A:3:LYS:H	6	0.13	0.02	0.12
(1,1256)	1:B:119:GLN:HG2	1:B:120:LEU:H	6	0.13	0.02	0.13
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	5	0.85	0.5	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	5	0.85	0.5	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	5	0.85	0.5	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	5	0.85	0.5	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	5	0.85	0.5	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	5	0.85	0.5	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	5	0.85	0.5	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	5	0.85	0.5	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	5	0.85	0.5	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	5	0.85	0.5	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	5	0.85	0.5	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	5	0.85	0.5	1.15
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	5	0.39	0.25	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	5	0.39	0.25	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	5	0.39	0.25	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	5	0.39	0.25	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	5	0.39	0.25	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	5	0.39	0.25	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	5	0.39	0.25	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	5	0.39	0.25	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	5	0.39	0.25	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	5	0.39	0.25	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	5	0.39	0.25	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	5	0.39	0.25	0.28
(1,1760)	1:A:24:ASN:HD22	1:B:123:THR:HA	5	0.28	0.1	0.23
(1,286)	1:A:14:GLU:HG2	1:A:15:LYS:HA	5	0.2	0.07	0.19
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG2	5	0.17	0.03	0.16
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG3	5	0.17	0.03	0.16
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG2	5	0.17	0.03	0.16
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG3	5	0.17	0.03	0.16
(1,89)	1:A:4:LYS:HE2	1:A:8:GLN:HG2	5	0.15	0.01	0.15
(1,89)	1:A:4:LYS:HE3	1:A:8:GLN:HG2	5	0.15	0.01	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE21	5	0.14	0.01	0.13
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE22	5	0.14	0.01	0.13
(1,126)	1:A:6:TYR:HA	1:A:9:ILE:HB	5	0.13	0.02	0.12
(2,61)	1:A:32:LEU:O	1:A:36:LYS:H	5	0.13	0.02	0.12
(2,127)	1:A:32:LEU:O	1:A:36:LYS:H	5	0.13	0.02	0.12
(2,59)	1:A:31:LYS:O	1:A:35:GLU:H	5	0.13	0.02	0.13
(2,125)	1:A:31:LYS:O	1:A:35:GLU:H	5	0.13	0.02	0.13
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG21	5	0.13	0.02	0.13
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG22	5	0.13	0.02	0.13
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG23	5	0.13	0.02	0.13
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	4	0.5	0.29	0.42
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	4	0.5	0.29	0.42
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG2	4	0.24	0.06	0.26
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG3	4	0.24	0.06	0.26
(1,148)	1:A:7:GLU:HB2	1:A:8:GLN:HE21	4	0.22	0.1	0.18
(1,1630)	1:B:141:GLN:HG2	1:B:142:GLU:H	4	0.21	0.03	0.2
(1,1630)	1:B:141:GLN:HG3	1:B:142:GLU:H	4	0.21	0.03	0.2
(1,797)	1:A:41:GLN:HE21	1:A:43:ARG:H	4	0.18	0.06	0.18
(1,797)	1:A:41:GLN:HE22	1:A:43:ARG:H	4	0.18	0.06	0.18
(1,776)	1:A:40:ARG:HG2	1:A:41:GLN:H	4	0.15	0.03	0.15
(1,776)	1:A:40:ARG:HG3	1:A:41:GLN:H	4	0.15	0.03	0.15
(1,1659)	1:B:144:PHE:H	1:B:144:PHE:HB2	4	0.14	0.04	0.13
(1,984)	1:B:107:GLU:HB3	1:B:108:GLN:HE21	4	0.13	0.02	0.13
(1,1883)	1:B:123:THR:HG21	1:A:24:ASN:HB3	4	0.12	0.01	0.12
(1,1883)	1:B:123:THR:HG22	1:A:24:ASN:HB3	4	0.12	0.01	0.12
(1,1883)	1:B:123:THR:HG23	1:A:24:ASN:HB3	4	0.12	0.01	0.12
(1,751)	1:A:39:GLN:H	1:A:40:ARG:H	4	0.11	0.0	0.11
(1,741)	1:A:38:THR:H	1:A:38:THR:HG21	3	0.4	0.05	0.39
(1,741)	1:A:38:THR:H	1:A:38:THR:HG22	3	0.4	0.05	0.39
(1,741)	1:A:38:THR:H	1:A:38:THR:HG23	3	0.4	0.05	0.39
(1,521)	1:A:25:MET:H	1:A:25:MET:HG2	3	0.33	0.03	0.33
(1,1675)	1:A:5:LEU:HD21	1:A:3:LYS:H	3	0.33	0.13	0.28
(1,1675)	1:A:5:LEU:HD22	1:A:3:LYS:H	3	0.33	0.13	0.28
(1,1675)	1:A:5:LEU:HD23	1:A:3:LYS:H	3	0.33	0.13	0.28
(1,918)	1:B:104:LYS:HD2	1:B:108:GLN:HG2	3	0.23	0.09	0.2
(1,918)	1:B:104:LYS:HD3	1:B:108:GLN:HG2	3	0.23	0.09	0.2
(2,75)	1:A:6:TYR:O	1:A:10:LEU:H	3	0.23	0.02	0.22
(1,87)	1:A:4:LYS:HD2	1:A:8:GLN:HG2	3	0.21	0.06	0.18
(1,87)	1:A:4:LYS:HD3	1:A:8:GLN:HG2	3	0.21	0.06	0.18
(1,745)	1:A:38:THR:HG21	1:A:39:GLN:H	3	0.19	0.0	0.19
(1,745)	1:A:38:THR:HG22	1:A:39:GLN:H	3	0.19	0.0	0.19
(1,745)	1:A:38:THR:HG23	1:A:39:GLN:H	3	0.19	0.0	0.19

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG2	3	0.19	0.06	0.21
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG3	3	0.19	0.06	0.21
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG2	3	0.19	0.06	0.21
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG3	3	0.19	0.06	0.21
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG2	3	0.19	0.06	0.21
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG3	3	0.19	0.06	0.21
(1,799)	1:A:41:GLN:HG2	1:A:42:GLU:H	3	0.19	0.07	0.17
(1,799)	1:A:41:GLN:HG3	1:A:42:GLU:H	3	0.19	0.07	0.17
(1,1593)	1:B:139:GLN:HG2	1:B:140:ARG:H	3	0.14	0.02	0.15
(1,1593)	1:B:139:GLN:HG3	1:B:140:ARG:H	3	0.14	0.02	0.15
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE1	3	0.14	0.02	0.13
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE2	3	0.14	0.02	0.13
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE1	3	0.14	0.02	0.13
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE2	3	0.14	0.02	0.13
(1,1168)	1:B:116:LEU:HA	1:B:116:LEU:HG	3	0.13	0.02	0.14
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB1	3	0.13	0.02	0.13
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB2	3	0.13	0.02	0.13
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB3	3	0.13	0.02	0.13
(1,1789)	1:A:37:ALA:HB1	1:B:134:LEU:HA	3	0.13	0.01	0.13
(1,1789)	1:A:37:ALA:HB2	1:B:134:LEU:HA	3	0.13	0.01	0.13
(1,1789)	1:A:37:ALA:HB3	1:B:134:LEU:HA	3	0.13	0.01	0.13
(1,61)	1:A:4:LYS:H	1:A:4:LYS:HG2	3	0.12	0.02	0.11
(1,128)	1:A:7:GLU:H	1:A:7:GLU:HB2	3	0.12	0.0	0.12
(1,699)	1:A:34:LEU:HG	1:A:35:GLU:H	3	0.12	0.01	0.12
(1,892)	1:A:4:LYS:H	1:A:4:LYS:HG2	3	0.12	0.02	0.11
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE1	3	0.12	0.0	0.12
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE2	3	0.12	0.0	0.12
(1,370)	1:A:17:LYS:H	1:A:19:GLN:HG2	3	0.12	0.0	0.12
(1,983)	1:B:107:GLU:HB3	1:B:108:GLN:H	3	0.12	0.01	0.12
(1,1768)	1:A:30:LEU:HB2	1:B:130:LEU:HG	3	0.12	0.01	0.12
(1,288)	1:A:14:GLU:HG3	1:A:15:LYS:H	3	0.11	0.0	0.11
(1,560)	1:A:27:LEU:HB2	1:A:27:LEU:HG	3	0.11	0.0	0.11
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD11	2	0.59	0.15	0.59
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD12	2	0.59	0.15	0.59
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD13	2	0.59	0.15	0.59
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD21	2	0.59	0.15	0.59
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD22	2	0.59	0.15	0.59
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD23	2	0.59	0.15	0.59
(1,1474)	1:B:131:LYS:HD2	1:B:135:GLU:HG2	2	0.36	0.09	0.36
(1,1474)	1:B:131:LYS:HD2	1:B:135:GLU:HG3	2	0.36	0.09	0.36
(1,1474)	1:B:131:LYS:HD3	1:B:135:GLU:HG2	2	0.36	0.09	0.36
(1,1474)	1:B:131:LYS:HD3	1:B:135:GLU:HG3	2	0.36	0.09	0.36

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1576)	1:B:138:THR:HG21	1:B:139:GLN:H	2	0.35	0.03	0.35
(1,1576)	1:B:138:THR:HG22	1:B:139:GLN:H	2	0.35	0.03	0.35
(1,1576)	1:B:138:THR:HG23	1:B:139:GLN:H	2	0.35	0.03	0.35
(1,1547)	1:B:135:GLU:HG2	1:B:136:LYS:H	2	0.32	0.05	0.32
(1,1547)	1:B:135:GLU:HG3	1:B:136:LYS:H	2	0.32	0.05	0.32
(1,1425)	1:B:129:ASP:H	1:B:131:LYS:HG2	2	0.23	0.02	0.23
(1,1425)	1:B:129:ASP:H	1:B:131:LYS:HG3	2	0.23	0.02	0.23
(1,1602)	1:B:140:ARG:HA	1:B:141:GLN:H	2	0.2	0.07	0.2
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD11	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD12	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD13	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD21	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD22	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD23	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD11	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD12	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD13	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD21	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD22	2	0.2	0.03	0.2
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD23	2	0.2	0.03	0.2
(1,1769)	1:A:30:LEU:HB3	1:B:130:LEU:HG	2	0.2	0.09	0.2
(1,760)	1:A:39:GLN:HE21	1:A:40:ARG:HG2	2	0.18	0.06	0.18
(1,760)	1:A:39:GLN:HE21	1:A:40:ARG:HG3	2	0.18	0.06	0.18
(1,760)	1:A:39:GLN:HE22	1:A:40:ARG:HG2	2	0.18	0.06	0.18
(1,760)	1:A:39:GLN:HE22	1:A:40:ARG:HG3	2	0.18	0.06	0.18
(1,920)	1:B:104:LYS:HE2	1:B:108:GLN:HG2	2	0.17	0.03	0.17
(1,920)	1:B:104:LYS:HE3	1:B:108:GLN:HG2	2	0.17	0.03	0.17
(1,1635)	1:B:141:GLN:HG2	1:B:143:ARG:HD2	2	0.16	0.02	0.16
(1,1635)	1:B:141:GLN:HG2	1:B:143:ARG:HD3	2	0.16	0.02	0.16
(1,1635)	1:B:141:GLN:HG3	1:B:143:ARG:HD2	2	0.16	0.02	0.16
(1,1635)	1:B:141:GLN:HG3	1:B:143:ARG:HD3	2	0.16	0.02	0.16
(1,774)	1:A:40:ARG:HD2	1:A:41:GLN:HG2	2	0.16	0.02	0.16
(1,774)	1:A:40:ARG:HD2	1:A:41:GLN:HG3	2	0.16	0.02	0.16
(1,774)	1:A:40:ARG:HD3	1:A:41:GLN:HG2	2	0.16	0.02	0.16
(1,774)	1:A:40:ARG:HD3	1:A:41:GLN:HG3	2	0.16	0.02	0.16
(1,811)	1:A:42:GLU:H	1:A:43:ARG:HG2	2	0.16	0.02	0.16
(1,811)	1:A:42:GLU:H	1:A:43:ARG:HG3	2	0.16	0.02	0.16
(1,968)	1:B:107:GLU:HA	1:B:110:LEU:HB3	2	0.16	0.05	0.16
(1,1842)	1:B:109:ILE:HG21	1:A:6:TYR:HE1	2	0.16	0.01	0.16
(1,1842)	1:B:109:ILE:HG21	1:A:6:TYR:HE2	2	0.16	0.01	0.16
(1,1842)	1:B:109:ILE:HG22	1:A:6:TYR:HE1	2	0.16	0.01	0.16
(1,1842)	1:B:109:ILE:HG22	1:A:6:TYR:HE2	2	0.16	0.01	0.16

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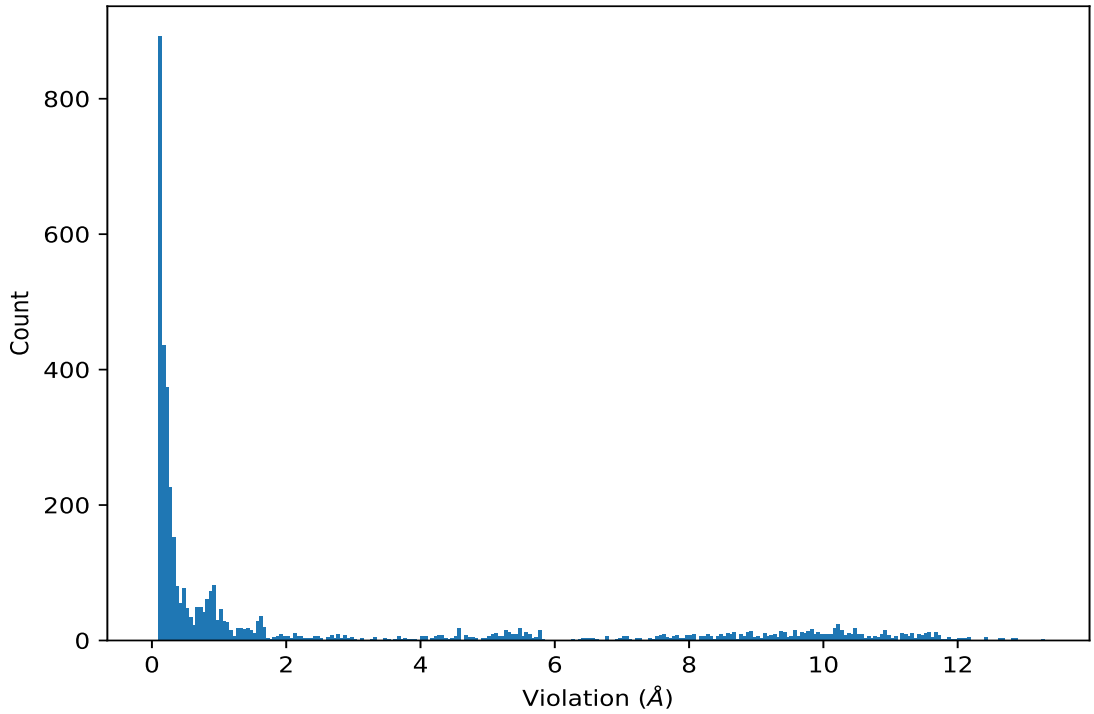
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1842)	1:B:109:ILE:HG23	1:A:6:TYR:HE1	2	0.16	0.01	0.16
(1,1842)	1:B:109:ILE:HG23	1:A:6:TYR:HE2	2	0.16	0.01	0.16
(1,1656)	1:B:143:ARG:HB2	1:B:144:PHE:H	2	0.15	0.01	0.15
(1,1656)	1:B:143:ARG:HB3	1:B:144:PHE:H	2	0.15	0.01	0.15
(1,201)	1:A:9:ILE:HG21	1:A:10:LEU:H	2	0.14	0.01	0.14
(1,201)	1:A:9:ILE:HG22	1:A:10:LEU:H	2	0.14	0.01	0.14
(1,201)	1:A:9:ILE:HG23	1:A:10:LEU:H	2	0.14	0.01	0.14
(1,658)	1:A:32:LEU:HA	1:A:35:GLU:HG2	2	0.14	0.02	0.14
(1,658)	1:A:32:LEU:HA	1:A:35:GLU:HG3	2	0.14	0.02	0.14
(1,970)	1:B:107:GLU:HA	1:B:111:ALA:H	2	0.14	0.01	0.14
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD11	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD12	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD13	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD21	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD22	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD23	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD11	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD12	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD13	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD21	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD22	2	0.13	0.02	0.13
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD23	2	0.13	0.02	0.13
(1,828)	1:A:44:PHE:H	1:A:44:PHE:HB2	2	0.12	0.02	0.12
(1,1924)	1:A:41:GLN:HE21	1:B:141:GLN:HE22	2	0.12	0.02	0.12
(1,804)	1:A:41:GLN:HG2	1:A:43:ARG:HD2	2	0.12	0.01	0.12
(1,804)	1:A:41:GLN:HG2	1:A:43:ARG:HD3	2	0.12	0.01	0.12
(1,804)	1:A:41:GLN:HG3	1:A:43:ARG:HD2	2	0.12	0.01	0.12
(1,804)	1:A:41:GLN:HG3	1:A:43:ARG:HD3	2	0.12	0.01	0.12
(1,131)	1:A:7:GLU:H	1:A:8:GLN:H	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD11	1:A:19:GLN:HB2	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD11	1:A:19:GLN:HB3	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD12	1:A:19:GLN:HB2	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD12	1:A:19:GLN:HB3	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD13	1:A:19:GLN:HB2	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD13	1:A:19:GLN:HB3	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD21	1:A:19:GLN:HB2	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD21	1:A:19:GLN:HB3	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD22	1:A:19:GLN:HB2	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD22	1:A:19:GLN:HB3	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD23	1:A:19:GLN:HB2	2	0.11	0.0	0.11
(1,1873)	1:B:120:LEU:HD23	1:A:19:GLN: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)
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	17	13.29
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	17	13.29
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	18	12.88
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	18	12.88
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	13	12.86
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	20	12.84
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	20	12.84
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	11	12.8
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	2	12.67
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	7	12.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	16	12.65
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	8	12.64
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	8	12.64
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	6	12.63
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	6	12.63
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	15	12.51
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	14	12.42
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	17	12.42
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	7	12.41
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	7	12.41
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	6	12.41
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	13	12.36
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	3	12.3
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	17	12.27
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	15	12.24
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	4	12.2
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	5	12.17
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	14	12.16
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	5	12.16
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	10	12.16
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	16	12.14
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	11	12.13
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	5	12.11
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	4	12.08
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	6	12.08
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	10	12.06
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	9	12.02
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	8	12.01
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	12	12.01
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	14	11.96
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	14	11.96
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	5	11.94
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	1	11.9
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	9	11.89
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	1	11.87
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	13	11.87
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	2	11.86
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	20	11.86
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	18	11.83
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	13	11.82
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	3	11.78
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	9	11.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	13	11.74
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	9	11.74
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	19	11.74
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	20	11.74
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	1	11.74
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	1	11.73
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	3	11.73
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	5	11.72
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	1	11.69
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	8	11.69
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	11	11.69
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	11	11.68
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	11	11.68
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	8	11.68
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	5	11.68
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	9	11.66
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	12	11.65
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	12	11.65
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	16	11.65
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	3	11.65
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	2	11.65
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	12	11.64
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	11	11.63
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	7	11.62
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	13	11.62
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	2	11.61
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	17	11.6
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	17	11.6
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	14	11.59
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	5	11.59
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	5	11.59
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	11	11.59
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	16	11.57
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	16	11.57
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	3	11.57
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	15	11.57
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	12	11.57
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	16	11.56
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	7	11.54
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	3	11.53
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	3	11.53
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	14	11.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	3	11.53
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	15	11.52
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	11	11.51
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	9	11.51
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	9	11.51
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	7	11.51
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	9	11.51
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	2	11.49
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	12	11.49
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	16	11.49
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	12	11.49
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	15	11.47
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	15	11.47
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	8	11.46
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	14	11.46
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	1	11.44
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	1	11.44
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	16	11.44
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	6	11.44
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	8	11.44
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	17	11.43
(1,879)	1:B:103:LYS:HD3	1:A:4:LYS:H	18	11.43
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	18	11.42
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	12	11.41
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	5	11.4
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	16	11.39
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	20	11.36
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	15	11.36
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	17	11.35
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	17	11.35
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	18	11.35
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	14	11.34
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	9	11.33
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	12	11.33
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	6	11.32
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	17	11.31
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	4	11.3
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	2	11.3
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	6	11.3
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	8	11.28
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	13	11.28
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	1	11.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,899)	1:B:104:LYS:HA	1:A:4:LYS:HG2	19	11.27
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	20	11.27
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	4	11.27
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	8	11.26
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	6	11.24
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	13	11.23
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	13	11.23
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	11	11.23
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	10	11.23
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	13	11.22
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	10	11.22
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	7	11.22
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	14	11.22
(1,891)	1:A:4:LYS:H	1:B:104:LYS:HA	19	11.21
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	3	11.2
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	15	11.2
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	3	11.2
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	5	11.19
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	17	11.19
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	9	11.19
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	7	11.18
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	11	11.16
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	1	11.16
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	15	11.15
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	20	11.15
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	1	11.14
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	5	11.1
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	20	11.09
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	14	11.08
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	4	11.06
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	18	11.06
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	17	11.05
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	4	11.04
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	16	11.03
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	6	11.02
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	4	10.99
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	4	10.99
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	6	10.99
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	10	10.99
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	20	10.98
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	3	10.97
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	10	10.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	10	10.96
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	18	10.95
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	18	10.95
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	2	10.95
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	10	10.95
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	10	10.95
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	8	10.94
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	12	10.94
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	18	10.94
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	9	10.93
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	9	10.93
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	20	10.92
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	20	10.92
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	8	10.92
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	4	10.91
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	12	10.91
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	8	10.89
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	8	10.89
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	2	10.89
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	7	10.89
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	13	10.88
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	1	10.87
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	5	10.86
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	5	10.86
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	15	10.86
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	6	10.85
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	6	10.85
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	19	10.84
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	18	10.8
(1,876)	1:B:103:LYS:HD2	1:A:4:LYS:H	19	10.8
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	2	10.79
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	2	10.79
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	5	10.79
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	13	10.78
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	13	10.78
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	1	10.77
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	20	10.76
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	2	10.74
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	18	10.73
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	4	10.72
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	1	10.7
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	1	10.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	2	10.7
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	2	10.7
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	9	10.65
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	9	10.65
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	17	10.62
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	2	10.62
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	16	10.61
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	16	10.61
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	14	10.6
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	7	10.6
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	7	10.6
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	3	10.6
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	3	10.6
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	13	10.6
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	11	10.59
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	7	10.56
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	3	10.56
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	17	10.53
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	17	10.53
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	8	10.53
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	5	10.52
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	5	10.52
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	14	10.51
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	20	10.51
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	1	10.5
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	1	10.5
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	11	10.49
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	17	10.49
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	14	10.49
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	14	10.49
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	15	10.49
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	15	10.49
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	7	10.49
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	7	10.48
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	7	10.48
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	18	10.48
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	11	10.47
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	11	10.47
(1,900)	1:B:104:LYS:HA	1:A:4:LYS:HG3	19	10.46
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	16	10.46
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	16	10.46
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	8	10.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	8	10.46
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	11	10.46
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	11	10.46
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	17	10.43
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	17	10.43
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	12	10.43
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	12	10.43
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	13	10.42
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	13	10.42
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	14	10.41
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	14	10.41
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	13	10.4
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	2	10.39
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	6	10.38
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	6	10.38
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	17	10.37
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	17	10.37
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	11	10.37
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	13	10.37
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	16	10.36
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	16	10.36
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	2	10.36
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	9	10.36
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	11	10.35
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	2	10.35
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	3	10.33
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	3	10.33
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	19	10.32
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	19	10.32
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	8	10.31
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	12	10.3
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	9	10.29
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	9	10.29
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	9	10.29
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	13	10.28
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	13	10.28
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	15	10.27
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	15	10.27
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	9	10.27
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	1	10.27
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	13	10.27
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	16	10.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	12	10.26
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	12	10.26
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	18	10.26
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	18	10.26
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	10	10.25
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	5	10.24
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	6	10.24
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	7	10.24
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	7	10.24
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	8	10.24
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	8	10.24
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	14	10.24
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	7	10.24
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	11	10.24
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	9	10.23
(1,909)	1:A:4:LYS:HG2	1:B:108:GLN:HG2	19	10.23
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	2	10.23
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	2	10.23
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	20	10.23
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	20	10.23
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	3	10.23
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	3	10.23
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	18	10.23
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	18	10.23
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	3	10.22
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	6	10.22
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	8	10.21
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	13	10.21
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	5	10.21
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	5	10.21
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	15	10.2
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	14	10.2
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	14	10.2
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	20	10.2
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	20	10.2
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	7	10.19
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	1	10.18
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD2	19	10.17
(1,906)	1:A:4:LYS:HG2	1:B:104:LYS:HD3	19	10.17
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	4	10.17
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	4	10.17
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	5	10.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	7	10.15
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	15	10.15
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	15	10.15
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	15	10.15
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	16	10.15
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	7	10.15
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	12	10.14
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	6	10.12
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	12	10.12
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	1	10.12
(1,877)	1:B:103:LYS:HD2	1:A:4:LYS:HG2	19	10.12
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	7	10.11
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	2	10.11
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	16	10.11
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	16	10.11
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	13	10.09
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	5	10.08
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	6	10.07
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	6	10.07
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	2	10.06
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	2	10.06
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	13	10.05
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	9	10.05
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	9	10.05
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	2	10.04
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	5	10.04
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	16	10.04
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	14	10.03
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	14	10.03
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	1	10.02
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	3	10.02
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	6	10.02
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	6	10.02
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	17	10.02
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	15	9.99
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	12	9.99
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	12	9.99
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	5	9.98
(1,887)	1:B:103:LYS:HG2	1:A:4:LYS:H	10	9.98
(1,887)	1:B:103:LYS:HG3	1:A:4:LYS:H	10	9.98
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	9	9.98
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	16	9.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	18	9.97
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	20	9.95
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	4	9.94
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	10	9.94
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	4	9.94
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	4	9.94
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	16	9.93
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	13	9.92
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	19	9.92
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	3	9.92
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	4	9.91
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	4	9.91
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	2	9.91
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	8	9.89
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	8	9.89
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	8	9.89
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	7	9.89
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	20	9.88
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	9	9.88
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	19	9.87
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	2	9.87
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	11	9.86
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	11	9.86
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	5	9.84
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	5	9.84
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	10	9.84
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	10	9.84
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	11	9.84
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	12	9.84
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	15	9.84
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	1	9.84
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	1	9.83
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	1	9.83
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	3	9.83
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	8	9.83
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	2	9.81
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	13	9.81
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	3	9.81
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	5	9.81
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	13	9.8
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB2	19	9.79
(1,894)	1:A:4:LYS:H	1:B:104:LYS:HB3	19	9.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	4	9.79
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	2	9.79
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	6	9.78
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	17	9.78
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	18	9.77
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	10	9.76
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	11	9.76
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	11	9.76
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	2	9.76
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	12	9.75
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	12	9.75
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	16	9.75
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	20	9.74
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	20	9.74
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	14	9.74
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	6	9.74
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	5	9.73
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	16	9.73
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	14	9.72
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	20	9.71
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	10	9.71
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	10	9.71
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	17	9.71
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	4	9.7
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	13	9.7
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	16	9.68
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	16	9.68
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	4	9.68
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	11	9.68
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	14	9.67
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	15	9.66
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	15	9.66
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	6	9.66
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	6	9.66
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	5	9.65
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	9	9.64
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	9	9.64
(1,880)	1:B:103:LYS:HE2	1:A:4:LYS:H	19	9.63
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	15	9.63
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	3	9.61
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	3	9.61
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	14	9.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	1	9.6
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	1	9.6
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	11	9.6
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	15	9.6
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	3	9.6
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	18	9.59
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	18	9.59
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	8	9.59
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	1	9.58
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	14	9.58
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	1	9.57
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	10	9.57
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	16	9.56
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	19	9.56
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	8	9.55
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	12	9.54
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	19	9.53
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	15	9.53
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	12	9.51
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	17	9.51
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	18	9.5
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	10	9.5
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	9	9.49
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	3	9.48
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	7	9.47
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	9	9.47
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	6	9.47
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	10	9.45
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	7	9.44
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	7	9.44
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	20	9.44
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	19	9.44
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	16	9.44
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	17	9.43
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	7	9.43
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	5	9.43
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	17	9.43
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	14	9.42
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	6	9.41
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	1	9.41
(1,913)	1:A:4:LYS:HG3	1:B:108:GLN:HG2	19	9.39
(1,888)	1:B:103:LYS:HG2	1:A:4:LYS:HG2	19	9.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:B:103:LYS:HG3	1:A:4:LYS:HG2	19	9.39
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	17	9.39
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	14	9.37
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	14	9.37
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	1	9.37
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	9	9.37
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	1	9.37
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	7	9.37
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	14	9.36
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	17	9.36
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	15	9.35
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	9	9.35
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	15	9.34
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	18	9.32
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	13	9.3
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	13	9.3
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	7	9.3
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	7	9.29
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	8	9.29
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	3	9.28
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	20	9.28
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	4	9.27
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	11	9.26
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	15	9.26
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	10	9.26
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	4	9.25
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	4	9.25
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	6	9.24
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	3	9.24
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	12	9.23
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	2	9.22
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	2	9.22
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	8	9.22
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	5	9.22
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	18	9.21
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	11	9.2
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	18	9.17
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	8	9.16
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	4	9.16
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	4	9.16
(1,856)	1:A:3:LYS:H	1:B:103:LYS:HD2	19	9.15
(1,914)	1:A:4:LYS:HG3	1:B:108:GLN:HG3	19	9.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	16	9.14
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	3	9.14
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	16	9.13
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	16	9.13
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	13	9.12
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	13	9.12
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	20	9.11
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	10	9.1
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	10	9.1
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	11	9.1
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	1	9.08
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	1	9.08
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	4	9.07
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	18	9.06
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	17	9.04
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	17	9.04
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	12	9.04
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	8	9.02
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	19	9.01
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	20	9.01
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	20	8.99
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	10	8.99
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	18	8.99
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	12	8.97
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	6	8.96
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	2	8.95
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	2	8.95
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	5	8.94
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	5	8.94
(1,878)	1:B:103:LYS:HD2	1:A:4:LYS:HG3	19	8.94
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	15	8.94
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	5	8.93
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	5	8.93
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	4	8.93
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	6	8.93
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	14	8.93
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	17	8.93
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	3	8.9
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	3	8.9
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	4	8.89
(1,855)	1:A:3:LYS:H	1:B:103:LYS:HB3	20	8.89
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	14	8.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	14	8.88
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	13	8.88
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	13	8.88
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	15	8.87
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	15	8.87
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	14	8.87
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	2	8.86
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	2	8.86
(1,873)	1:B:103:LYS:HB2	1:A:4:LYS:H	10	8.86
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	20	8.83
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	6	8.8
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	6	8.8
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	18	8.8
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	9	8.8
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	9	8.8
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	18	8.8
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	9	8.79
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	9	8.79
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	16	8.79
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	16	8.79
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	1	8.79
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	1	8.79
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	12	8.76
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	12	8.76
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	9	8.75
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	9	8.75
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	11	8.73
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	11	8.73
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	12	8.7
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	12	8.7
(1,857)	1:A:3:LYS:H	1:B:103:LYS:HD3	12	8.69
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	4	8.68
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	4	8.68
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	5	8.68
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	5	8.68
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	13	8.68
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	13	8.68
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	7	8.67
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	7	8.67
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	2	8.66
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	2	8.66
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	11	8.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	11	8.64
(1,875)	1:B:103:LYS:HB3	1:A:4:LYS:H	10	8.64
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	15	8.64
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD2	19	8.63
(1,910)	1:A:4:LYS:HG3	1:B:104:LYS:HD3	19	8.63
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	16	8.61
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	16	8.61
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	11	8.6
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	11	8.6
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	8	8.59
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	8	8.59
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	11	8.59
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	11	8.59
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	18	8.59
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	15	8.55
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	15	8.55
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	1	8.55
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	1	8.55
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	3	8.55
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	3	8.55
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	10	8.54
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	2	8.53
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	2	8.53
(1,881)	1:B:103:LYS:HE3	1:A:4:LYS:H	10	8.52
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	7	8.5
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	7	8.5
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	3	8.49
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	3	8.49
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	12	8.49
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	19	8.48
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	19	8.48
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	8	8.48
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	8	8.48
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	17	8.48
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	20	8.46
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	20	8.46
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	4	8.44
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	2	8.44
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	11	8.43
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	10	8.41
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	10	8.41
(1,854)	1:A:3:LYS:H	1:B:103:LYS:HB2	20	8.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	9	8.38
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	9	8.38
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	16	8.34
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	16	8.34
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	1	8.31
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	1	8.31
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	19	8.31
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	18	8.3
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	18	8.3
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	19	8.29
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	19	8.28
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	6	8.28
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	6	8.28
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	5	8.27
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	5	8.27
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	13	8.27
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	14	8.26
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	14	8.26
(1,889)	1:B:103:LYS:HG2	1:A:4:LYS:HG3	7	8.24
(1,889)	1:B:103:LYS:HG3	1:A:4:LYS:HG3	7	8.24
(1,858)	1:A:3:LYS:H	1:B:103:LYS:HE2	4	8.24
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	13	8.21
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	19	8.21
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	19	8.21
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	15	8.2
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	15	8.2
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	2	8.18
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	17	8.17
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	17	8.17
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	13	8.16
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	13	8.16
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	5	8.09
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	12	8.07
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	12	8.07
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	18	8.06
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	18	8.06
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	3	8.06
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	3	8.06
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	17	8.05
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	6	8.05
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	6	8.05
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	8	8.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	8	8.04
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	1	8.02
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	7	8.01
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	9	8.01
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	16	8.0
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	14	8.0
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	14	8.0
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	16	7.99
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	4	7.97
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	4	7.97
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	10	7.97
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	10	7.97
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	20	7.96
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	20	7.96
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	15	7.95
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	15	7.94
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	15	7.94
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	1	7.93
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	14	7.9
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	9	7.87
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	10	7.87
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	10	7.87
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	10	7.85
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	10	7.85
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	3	7.85
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	17	7.84
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	17	7.84
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG2	4	7.83
(1,861)	1:A:3:LYS:H	1:B:103:LYS:HG3	4	7.83
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	5	7.83
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	7	7.8
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	11	7.8
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	5	7.79
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	3	7.79
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	19	7.78
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	19	7.78
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	15	7.74
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	6	7.74
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	11	7.7
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	8	7.7
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	1	7.69
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	18	7.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	8	7.69
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	12	7.67
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	12	7.67
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	12	7.64
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	3	7.62
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	11	7.62
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	12	7.62
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	16	7.61
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	4	7.61
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	4	7.61
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	20	7.61
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	20	7.61
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	15	7.61
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	20	7.6
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	17	7.6
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	17	7.59
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	7	7.58
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	18	7.58
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	18	7.58
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	6	7.58
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	8	7.57
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	14	7.55
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	9	7.54
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	14	7.54
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD2	19	7.54
(1,860)	1:A:3:LYS:H	1:B:103:LYS:HD3	19	7.54
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	4	7.51
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	19	7.48
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	18	7.46
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	2	7.44
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	13	7.43
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	4	7.4
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	20	7.4
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	6	7.33
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	18	7.3
(1,898)	1:A:4:LYS:H	1:B:107:GLU:H	10	7.29
(1,867)	1:B:103:LYS:HA	1:A:4:LYS:H	10	7.26
(1,859)	1:A:3:LYS:H	1:B:103:LYS:HE3	10	7.25
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	11	7.24
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	10	7.22
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	12	7.21
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	1	7.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	3	7.14
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	20	7.11
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	12	7.1
(1,853)	1:A:3:LYS:H	1:B:103:LYS:HA	4	7.1
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	5	7.09
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	14	7.08
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	18	7.07
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	20	7.07
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	15	7.05
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	16	7.03
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	8	7.03
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	8	7.03
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	9	7.02
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	17	7.02
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	8	7.0
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	20	6.99
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	20	6.99
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	4	6.96
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	10	6.93
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	6	6.9
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	13	6.81
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	2	6.79
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	7	6.79
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	7	6.79
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	17	6.79
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	17	6.79
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	18	6.76
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	18	6.76
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	7	6.74
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	5	6.66
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	17	6.63
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	15	6.61
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	12	6.59
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	20	6.58
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE2	6	6.58
(1,895)	1:A:4:LYS:H	1:B:104:LYS:HE3	6	6.58
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	3	6.52
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	9	6.51
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	19	6.5
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	14	6.49
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	16	6.46
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	11	6.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	18	6.45
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	4	6.42
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	8	6.42
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	13	6.41
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	1	6.39
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	6	6.38
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	10	6.32
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	2	6.28
(1,931)	1:A:5:LEU:H	1:B:107:GLU:H	7	6.28
(1,926)	1:A:5:LEU:H	1:B:105:LEU:HA	19	6.17
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	5	6.0
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	15	5.94
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	1	5.88
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	16	5.84
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	12	5.81
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	5	5.8
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	11	5.8
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	11	5.8
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	11	5.8
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	9	5.79
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	9	5.79
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	18	5.78
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	3	5.77
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	12	5.76
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	15	5.75
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	17	5.75
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	14	5.75
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	17	5.75
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	2	5.75
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	2	5.75
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	3	5.73
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	3	5.73
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	8	5.72
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	7	5.7
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	9	5.7
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	14	5.69
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	20	5.68
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	19	5.67
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	13	5.66
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	16	5.64
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	3	5.63
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	14	5.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	14	5.63
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	19	5.63
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	20	5.62
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	9	5.61
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	13	5.61
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	2	5.61
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	4	5.61
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	19	5.6
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	18	5.6
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	18	5.6
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	4	5.59
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	11	5.59
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	16	5.59
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	16	5.59
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	11	5.58
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	11	5.58
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	6	5.56
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	1	5.56
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	1	5.56
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	1	5.54
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	15	5.54
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	15	5.54
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	6	5.54
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	8	5.53
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	12	5.5
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	12	5.5
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	18	5.49
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	3	5.49
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	3	5.49
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	9	5.49
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	9	5.49
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	3	5.49
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	3	5.49
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	20	5.48
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	20	5.48
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	10	5.47
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	10	5.47
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	5	5.46
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	5	5.46
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	17	5.46
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	17	5.46
(1,897)	1:A:4:LYS:H	1:B:106:TYR:H	10	5.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	10	5.45
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	8	5.45
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	8	5.45
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	14	5.44
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	14	5.44
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	13	5.43
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	7	5.43
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	7	5.43
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	13	5.42
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	13	5.42
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	2	5.4
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	13	5.4
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	13	5.4
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	1	5.37
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	1	5.37
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	9	5.37
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	9	5.37
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	14	5.36
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	14	5.36
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	15	5.36
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	15	5.36
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	18	5.36
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	18	5.36
(1,930)	1:A:5:LEU:H	1:B:106:TYR:H	7	5.35
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	16	5.35
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	16	5.35
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	4	5.35
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	4	5.35
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	17	5.35
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	5	5.34
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	5	5.34
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	11	5.33
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	11	5.33
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	8	5.31
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	8	5.31
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	6	5.29
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	6	5.29
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	11	5.27
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	11	5.27
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	9	5.26
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	9	5.26
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	10	5.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	10	5.26
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	12	5.26
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	12	5.26
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	20	5.25
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	20	5.25
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	3	5.25
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	3	5.25
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	2	5.25
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	2	5.25
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	4	5.22
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	4	5.22
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	2	5.22
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	1	5.22
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	1	5.22
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	16	5.21
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	16	5.21
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	17	5.19
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	17	5.19
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	1	5.19
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	1	5.19
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	14	5.17
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	5	5.15
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	5	5.15
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	2	5.14
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	2	5.14
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	5	5.14
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	14	5.14
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	14	5.14
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	7	5.13
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	7	5.13
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	6	5.12
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	6	5.12
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	13	5.12
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	13	5.12
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	2	5.1
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	2	5.1
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	17	5.1
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	17	5.1
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	2	5.09
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	2	5.09
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	8	5.09
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	8	5.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	16	5.07
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	16	5.07
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	9	5.05
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	15	5.05
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	16	5.05
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	6	5.03
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	15	5.03
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	15	5.03
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	6	4.99
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	6	4.99
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	17	4.95
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	17	4.95
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	3	4.94
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	12	4.94
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	7	4.92
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	7	4.92
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	1	4.85
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	7	4.85
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	7	4.85
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	4	4.8
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	5	4.77
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	5	4.77
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	1	4.75
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	1	4.75
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	8	4.74
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	7	4.72
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	4	4.71
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	4	4.71
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	11	4.7
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	15	4.69
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	15	4.69
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	13	4.67
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	13	4.67
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	10	4.66
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	10	4.66
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	20	4.65
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	20	4.65
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	20	4.63
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	16	4.6
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	16	4.6
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	18	4.59
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	18	4.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	8	4.56
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	8	4.56
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	9	4.55
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	9	4.55
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	14	4.55
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	14	4.55
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	18	4.55
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	18	4.55
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	12	4.55
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	12	4.55
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	20	4.55
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	20	4.55
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	15	4.55
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	15	4.55
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	10	4.54
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	17	4.54
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	17	4.54
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG2	19	4.53
(1,841)	1:A:2:PHE:H	1:B:103:LYS:HG3	19	4.53
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	4	4.5
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	4	4.5
(1,868)	1:B:103:LYS:HA	1:A:5:LEU:H	18	4.46
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	11	4.45
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	11	4.45
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	20	4.4
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	20	4.4
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	18	4.39
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	18	4.39
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	1	4.36
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	1	4.36
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	5	4.32
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	5	4.32
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	2	4.3
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	2	4.3
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	12	4.3
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	12	4.3
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	12	4.3
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	12	4.3
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	7	4.29
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	7	4.29
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	6	4.29
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	6	4.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	10	4.28
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	10	4.28
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	3	4.27
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	3	4.27
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	13	4.24
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	13	4.24
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	8	4.21
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	8	4.21
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	7	4.2
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	7	4.2
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	6	4.19
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	6	4.19
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	18	4.16
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	18	4.16
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	15	4.1
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	15	4.1
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	4	4.07
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	4	4.07
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	8	4.07
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	8	4.07
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	10	4.04
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	10	4.04
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB2	19	4.03
(1,912)	1:A:4:LYS:HG3	1:B:105:LEU:HB3	19	4.03
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB2	19	4.01
(1,908)	1:A:4:LYS:HG2	1:B:105:LEU:HB3	19	4.01
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	19	3.95
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	11	3.94
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	11	3.94
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	9	3.9
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	9	3.9
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	16	3.81
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	16	3.81
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	10	3.8
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	10	3.8
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	6	3.77
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	6	3.77
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	4	3.72
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	4	3.72
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	3	3.69
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	3	3.69
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	12	3.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	12	3.67
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	20	3.67
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	20	3.67
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	14	3.65
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	14	3.65
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	13	3.53
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	13	3.53
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	5	3.47
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	5	3.47
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	17	3.46
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	2	3.38
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	2	3.33
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	17	3.32
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	17	3.32
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	16	3.31
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	11	3.31
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	1	3.3
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	11	3.3
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	16	3.21
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	1	3.18
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	17	3.12
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	3	3.1
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	14	3.1
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	2	3.0
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	2	3.0
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG2	19	2.97
(1,846)	1:A:2:PHE:HA	1:B:104:LYS:HG3	19	2.97
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	13	2.96
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	1	2.95
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	1	2.95
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	7	2.93
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	3	2.91
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	2	2.91
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	11	2.9
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	11	2.9
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	7	2.9
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	16	2.89
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	16	2.89
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	5	2.89
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	9	2.88
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	9	2.87
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	13	2.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	13	2.83
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	2	2.81
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	14	2.8
(1,838)	1:B:101:ASP:HB2	1:A:2:PHE:H	19	2.8
(1,838)	1:B:101:ASP:HB3	1:A:2:PHE:H	19	2.8
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	7	2.79
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	5	2.77
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	9	2.76
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	9	2.76
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	1	2.76
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	13	2.76
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	5	2.73
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	5	2.73
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	13	2.73
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	15	2.7
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	3	2.69
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	3	2.69
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	11	2.69
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	16	2.67
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	7	2.66
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	7	2.66
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	9	2.66
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	8	2.66
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	19	2.65
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	19	2.65
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	1	2.65
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	8	2.61
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	5	2.6
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	8	2.56
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	7	2.54
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	3	2.52
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	15	2.5
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	8	2.48
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	8	2.48
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	17	2.48
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	17	2.48
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	6	2.46
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	20	2.45
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	4	2.44
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	12	2.44
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	14	2.43
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	14	2.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	9	2.43
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	18	2.43
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	18	2.41
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	13	2.39
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	11	2.35
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	10	2.35
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	8	2.34
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	16	2.34
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	15	2.32
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	6	2.31
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	6	2.28
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	6	2.28
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	12	2.26
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	7	2.24
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	15	2.22
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	15	2.22
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	20	2.22
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	2	2.22
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	6	2.21
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	9	2.21
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	14	2.17
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	12	2.16
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	12	2.16
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	18	2.16
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	18	2.16
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	1	2.15
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	10	2.14
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	10	2.14
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	6	2.14
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	17	2.14
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	3	2.14
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	20	2.13
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	20	2.13
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	18	2.13
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	3	2.12
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	11	2.11
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	5	2.1
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	13	2.09
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	10	2.07
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	10	2.06
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	19	2.05
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	18	2.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	15	2.03
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	10	2.02
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	15	2.02
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	12	2.01
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	4	1.99
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	8	1.99
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	20	1.98
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	18	1.98
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	11	1.97
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	10	1.97
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	16	1.97
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	12	1.95
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	14	1.95
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	5	1.95
(1,852)	1:B:102:PHE:HB2	1:A:3:LYS:H	4	1.94
(1,852)	1:B:102:PHE:HB3	1:A:3:LYS:H	4	1.94
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	20	1.93
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	1	1.92
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	4	1.92
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	5	1.91
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	12	1.88
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	3	1.87
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	16	1.87
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	14	1.86
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	17	1.86
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	19	1.86
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	6	1.86
(1,850)	1:B:102:PHE:HB2	1:A:3:LYS:H	4	1.83
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	17	1.83
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	14	1.83
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	15	1.82
(1,851)	1:B:102:PHE:HB3	1:A:3:LYS:H	4	1.82
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	20	1.79
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	9	1.78
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	8	1.73
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	6	1.72
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	8	1.71
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	7	1.7
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	2	1.7
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	6	1.7
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	7	1.7
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	20	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	4	1.69
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	5	1.68
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	4	1.68
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	12	1.68
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	12	1.67
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	18	1.67
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	5	1.67
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	12	1.67
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	18	1.66
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	11	1.66
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	17	1.66
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB2	19	1.66
(1,848)	1:A:2:PHE:HA	1:B:105:LEU:HB3	19	1.66
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	10	1.66
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	18	1.66
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	4	1.65
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	13	1.65
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	3	1.65
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	6	1.65
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	9	1.65
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	14	1.65
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	15	1.65
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	19	1.65
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	5	1.65
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	12	1.64
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	8	1.64
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	11	1.64
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	10	1.64
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	2	1.64
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	1	1.63
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	19	1.63
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	5	1.63
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	13	1.63
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	16	1.63
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	17	1.63
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	20	1.63
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	5	1.62
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	11	1.62
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	14	1.62
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	1	1.62
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	6	1.61
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	7	1.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	17	1.61
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	3	1.6
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	9	1.6
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	14	1.6
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	16	1.6
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	20	1.6
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	16	1.6
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	13	1.6
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	14	1.6
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	10	1.59
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	15	1.59
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	19	1.59
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	1	1.59
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	6	1.59
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	9	1.59
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	2	1.59
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	14	1.59
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	20	1.58
(1,158)	1:A:8:GLN:H	1:A:8:GLN:HE21	7	1.58
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	2	1.57
(1,989)	1:B:108:GLN:H	1:B:108:GLN:HE21	8	1.57
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	8	1.57
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	13	1.57
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	9	1.57
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	9	1.57
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	12	1.57
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	6	1.57
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	10	1.57
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	12	1.57
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	15	1.57
(1,840)	1:A:2:PHE:H	1:B:102:PHE:HB3	17	1.56
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	8	1.56
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	16	1.56
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	14	1.55
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	14	1.55
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	6	1.55
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	9	1.55
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	15	1.53
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	18	1.53
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	10	1.53
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	7	1.53
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	2	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,849)	1:A:2:PHE:HA	1:B:106:TYR:H	19	1.51
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	18	1.5
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	20	1.5
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	9	1.5
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	11	1.5
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	17	1.5
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	2	1.49
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	5	1.49
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	3	1.49
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	13	1.48
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	14	1.48
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	2	1.48
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	7	1.48
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	4	1.47
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	10	1.47
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	7	1.46
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	7	1.46
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	3	1.46
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	18	1.46
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	7	1.46
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	18	1.46
(1,951)	1:B:106:TYR:H	1:B:108:GLN:HE21	3	1.45
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	1	1.45
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	6	1.44
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	8	1.44
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	12	1.44
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	4	1.44
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	20	1.44
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	13	1.43
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	13	1.43
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	20	1.43
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	1	1.43
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	14	1.42
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	16	1.42
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	10	1.42
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	10	1.41
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	11	1.41
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	15	1.41
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	3	1.41
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	5	1.41
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	7	1.4
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	4	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	4	1.4
(1,120)	1:A:6:TYR:H	1:A:8:GLN:HE21	19	1.4
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	6	1.39
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	17	1.39
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	2	1.38
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	17	1.38
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	20	1.38
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	8	1.37
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	1	1.37
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	16	1.36
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	19	1.36
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	13	1.36
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	18	1.36
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	2	1.36
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	12	1.35
(1,839)	1:A:2:PHE:H	1:B:102:PHE:HB2	19	1.34
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	3	1.34
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	7	1.34
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	5	1.33
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	5	1.33
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	5	1.33
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	5	1.33
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	5	1.33
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	5	1.33
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	5	1.33
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	5	1.33
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	5	1.33
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	5	1.33
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	5	1.33
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	5	1.33
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	1	1.31
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	15	1.31
(1,501)	1:A:24:ASN:H	1:A:24:ASN:HD21	4	1.3
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	9	1.29
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	16	1.28
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	19	1.27
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	10	1.27
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	10	1.27
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	10	1.27
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	10	1.27
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	10	1.27
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	10	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	10	1.27
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	10	1.27
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	10	1.27
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	10	1.27
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	10	1.27
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	10	1.27
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	15	1.26
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	19	1.26
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	5	1.26
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	14	1.24
(1,1332)	1:B:124:ASN:H	1:B:124:ASN:HD21	11	1.24
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	18	1.23
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	1	1.22
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	17	1.21
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	2	1.21
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	2	1.21
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	9	1.2
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	19	1.19
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	7	1.19
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	19	1.18
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	2	1.18
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	3	1.18
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	1	1.18
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	17	1.17
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	1	1.17
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	8	1.17
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	16	1.17
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	12	1.16
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	3	1.16
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	4	1.16
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	3	1.16
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	17	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	18	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	18	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	18	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	18	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	18	1.15
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	18	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	18	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	18	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	18	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	18	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	18	1.15
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	18	1.15
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	13	1.15
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	14	1.15
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	13	1.14
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	18	1.14
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	14	1.14
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	2	1.13
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	16	1.13
(1,927)	1:A:5:LEU:H	1:B:105:LEU:HG	19	1.13
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	6	1.12
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	16	1.11
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	18	1.11
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	4	1.11
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	17	1.1
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	17	1.1
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	9	1.09
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	5	1.09
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	5	1.09
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	11	1.08
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	17	1.08
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	17	1.08
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	17	1.08
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	17	1.08
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	17	1.08
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	17	1.08
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	4	1.08
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	2	1.08
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	11	1.08
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	6	1.07
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	15	1.07
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	19	1.07
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	20	1.07
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	8	1.07
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	8	1.07
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	18	1.06
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	4	1.06
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	6	1.06
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	6	1.06
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	9	1.06
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	14	1.06
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	13	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	9	1.05
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	10	1.05
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	1	1.04
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	3	1.04
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	8	1.04
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	17	1.04
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	12	1.04
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	8	1.03
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	16	1.03
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	18	1.03
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	18	1.03
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	20	1.03
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	20	1.03
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	20	1.03
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	20	1.03
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	20	1.03
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	20	1.03
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	20	1.03
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	20	1.03
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	13	1.03
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	5	1.02
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	11	1.02
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	10	1.02
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	15	1.02
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	3	1.02
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	7	1.02
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	12	1.02
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	1	1.02
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	1	1.02
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	20	1.02
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	10	1.02
(1,1310)	1:B:123:THR:H	1:B:124:ASN:HD21	11	1.02
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	6	1.02
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	12	1.01
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	13	1.01
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	1	1.01
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	9	1.01
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	4	1.01
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	9	1.01
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	13	1.01
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	15	1.01
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	14	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	20	1.0
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	10	1.0
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	6	1.0
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	8	1.0
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	6	1.0
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	18	1.0
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	12	1.0
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	2	0.99
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	5	0.99
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	15	0.99
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	10	0.99
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	13	0.99
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	12	0.99
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	18	0.99
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	1	0.99
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	7	0.99
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	11	0.99
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	8	0.98
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	16	0.98
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	3	0.98
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	18	0.98
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	9	0.98
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	16	0.98
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	19	0.97
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	20	0.97
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	9	0.97
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	9	0.97
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	4	0.97
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	4	0.97
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	14	0.97
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	20	0.96
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	4	0.96
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	8	0.96
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	16	0.96
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	2	0.96
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	2	0.96
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	13	0.96
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	1	0.95
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	15	0.95
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	15	0.95
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	15	0.95
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	12	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	19	0.95
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	14	0.95
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	14	0.95
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	1	0.95
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	12	0.95
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	19	0.95
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	8	0.95
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	11	0.94
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	7	0.94
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	15	0.94
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	19	0.94
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	7	0.94
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	9	0.93
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	9	0.93
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	9	0.93
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	2	0.93
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	5	0.93
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	11	0.93
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	1	0.93
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	1	0.93
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	1	0.93
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	16	0.93
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	16	0.93
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	16	0.93
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	16	0.93
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	17	0.93
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	15	0.93
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	20	0.93
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	5	0.92
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	2	0.92
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	2	0.92
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	2	0.92
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	3	0.92
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	3	0.92
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	3	0.92
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	17	0.92
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	17	0.92
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	17	0.92
(1,369)	1:A:17:LYS:H	1:A:19:GLN:HE21	2	0.92
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	11	0.92
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	4	0.92
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	4	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	4	0.92
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	19	0.92
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	18	0.92
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	6	0.91
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	7	0.91
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	16	0.91
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	18	0.91
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	19	0.91
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	14	0.91
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	8	0.91
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	8	0.91
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	8	0.91
(1,1200)	1:B:117:LYS:H	1:B:119:GLN:HE21	4	0.91
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	4	0.91
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	8	0.91
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	12	0.91
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	1	0.9
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	4	0.9
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	11	0.9
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	14	0.9
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	19	0.9
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	19	0.9
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	19	0.9
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	1	0.9
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	4	0.9
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	11	0.9
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	15	0.9
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	17	0.9
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	20	0.9
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	13	0.9
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	20	0.9
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	20	0.9
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	13	0.9
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	18	0.9
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	19	0.9
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	6	0.89
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	17	0.89
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	9	0.89
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	5	0.89
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	8	0.89
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	9	0.89
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	10	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	12	0.89
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	13	0.89
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	20	0.89
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	14	0.89
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	6	0.89
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	8	0.89
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	10	0.89
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	14	0.89
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	2	0.89
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	5	0.89
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	10	0.89
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	14	0.89
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	19	0.88
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	1	0.88
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	1	0.88
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	1	0.88
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	2	0.88
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	3	0.88
(1,173)	1:A:8:GLN:HE21	1:A:9:ILE:H	17	0.88
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	12	0.88
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	12	0.88
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	12	0.88
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	5	0.88
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	16	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	2	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	3	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	4	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	5	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	11	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	12	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	13	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	15	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	16	0.88
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	19	0.88
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	1	0.88
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	11	0.88
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	16	0.88
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	7	0.87
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	15	0.87
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	8	0.87
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	8	0.87
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	8	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	12	0.87
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	12	0.87
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	12	0.87
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	18	0.87
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	18	0.87
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	18	0.87
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	20	0.87
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	20	0.87
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	20	0.87
(1,176)	1:A:8:GLN:HG2	1:A:8:GLN:HE21	14	0.87
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	7	0.87
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	11	0.87
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	1	0.87
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	7	0.87
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	9	0.87
(1,1007)	1:B:108:GLN:HG2	1:B:108:GLN:HE21	17	0.87
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	17	0.87
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	16	0.86
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	10	0.86
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	10	0.86
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	10	0.86
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	3	0.86
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	6	0.86
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	15	0.86
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	10	0.85
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	14	0.85
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	14	0.85
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	14	0.85
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	3	0.84
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	8	0.84
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	15	0.84
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	12	0.84
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	9	0.84
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	5	0.83
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	5	0.83
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	5	0.83
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	11	0.83
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	11	0.83
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	11	0.83
(1,479)	1:A:23:THR:H	1:A:24:ASN:HD21	6	0.83
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	9	0.83
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	9	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	9	0.83
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	9	0.83
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	9	0.83
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	9	0.83
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	9	0.83
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	9	0.83
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	9	0.83
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	9	0.83
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	9	0.83
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	9	0.83
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	7	0.83
(1,1004)	1:B:108:GLN:HE21	1:B:109:ILE:H	20	0.83
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	13	0.82
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	7	0.82
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	7	0.82
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	7	0.82
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	2	0.82
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	6	0.81
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	6	0.81
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	6	0.81
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	14	0.81
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	14	0.81
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	14	0.81
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	12	0.81
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	7	0.81
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	7	0.81
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	7	0.81
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	9	0.81
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	9	0.8
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	4	0.8
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	13	0.8
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	13	0.8
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	13	0.8
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	6	0.8
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	19	0.8
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	8	0.8
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	8	0.8
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	8	0.8
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	8	0.8
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	8	0.8
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	8	0.8
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	16	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	17	0.8
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	10	0.79
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	14	0.79
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	20	0.79
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	8	0.79
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	6	0.79
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	3	0.78
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	15	0.78
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	5	0.78
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	5	0.78
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	13	0.78
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	13	0.78
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	13	0.78
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	13	0.78
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	13	0.78
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	13	0.78
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	8	0.78
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	17	0.78
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	20	0.78
(1,963)	1:B:107:GLU:H	1:B:108:GLN:HE21	2	0.77
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	8	0.77
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	13	0.77
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	17	0.77
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	17	0.77
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	17	0.77
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	7	0.77
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	4	0.76
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	4	0.76
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	4	0.76
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	4	0.76
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	5	0.76
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	10	0.76
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	3	0.76
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	6	0.76
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	11	0.76
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	15	0.76
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	6	0.75
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	6	0.75
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	6	0.75
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	12	0.75
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	5	0.75
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	12	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	3	0.75
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	3	0.74
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD11	17	0.74
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD12	17	0.74
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD13	17	0.74
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD21	17	0.74
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD22	17	0.74
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD23	17	0.74
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	3	0.74
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	4	0.74
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	10	0.74
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	10	0.74
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	10	0.74
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	20	0.74
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	20	0.74
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	20	0.74
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	17	0.74
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	20	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	6	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	6	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	6	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	6	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	6	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	6	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	7	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	7	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	7	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	7	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	7	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	7	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	14	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	14	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	14	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	14	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	14	0.73
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	14	0.73
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	1	0.73
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	14	0.73
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	19	0.73
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	18	0.73
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	3	0.73
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	14	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	18	0.72
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	6	0.72
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	9	0.72
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	9	0.71
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	17	0.71
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	3	0.71
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	3	0.71
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	10	0.71
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	18	0.71
(1,490)	1:A:23:THR:HG21	1:A:24:ASN:HD21	16	0.7
(1,490)	1:A:23:THR:HG22	1:A:24:ASN:HD21	16	0.7
(1,490)	1:A:23:THR:HG23	1:A:24:ASN:HD21	16	0.7
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	7	0.7
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	16	0.7
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	20	0.7
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	5	0.7
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	18	0.7
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	5	0.7
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	5	0.7
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	5	0.7
(1,132)	1:A:7:GLU:H	1:A:8:GLN:HE21	1	0.7
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	2	0.69
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	15	0.69
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	15	0.69
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	10	0.69
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	12	0.69
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	3	0.69
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	3	0.69
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	3	0.69
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	9	0.69
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	13	0.69
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	17	0.68
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	9	0.68
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	10	0.68
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	11	0.68
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	10	0.68
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	4	0.67
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	4	0.67
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	13	0.67
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	5	0.67
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	7	0.67
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	14	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	7	0.67
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	11	0.66
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	14	0.66
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	13	0.66
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	13	0.66
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	13	0.66
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	16	0.66
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	13	0.65
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	13	0.65
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	18	0.65
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	18	0.65
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	18	0.65
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	18	0.65
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	18	0.65
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	18	0.65
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	19	0.65
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	3	0.64
(1,421)	1:A:19:GLN:HE21	1:A:20:LEU:H	1	0.64
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	13	0.64
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	14	0.63
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	1	0.63
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	15	0.63
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	19	0.63
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	13	0.63
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	18	0.63
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	18	0.63
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	10	0.62
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	1	0.62
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	2	0.62
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	6	0.62
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	1	0.62
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	8	0.62
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	1	0.62
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	1	0.62
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	17	0.61
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	2	0.61
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	2	0.61
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	11	0.61
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	20	0.61
(1,979)	1:B:107:GLU:HB2	1:B:108:GLN:HE21	18	0.6
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	12	0.6
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	19	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	11	0.6
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	17	0.6
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	15	0.6
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	15	0.6
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	15	0.6
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	15	0.6
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	19	0.6
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	11	0.59
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	5	0.59
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	15	0.59
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	18	0.59
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	18	0.59
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	18	0.59
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	8	0.58
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	18	0.58
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	4	0.58
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	9	0.58
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	4	0.57
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	6	0.57
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	15	0.57
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	20	0.57
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	10	0.56
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	8	0.56
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	13	0.56
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	16	0.56
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	15	0.56
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	10	0.55
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	6	0.55
(1,1239)	1:B:119:GLN:H	1:B:119:GLN:HE21	4	0.55
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	16	0.55
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	16	0.55
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	7	0.54
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	16	0.54
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	1	0.54
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	5	0.54
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	9	0.54
(1,1736)	1:A:19:GLN:HE22	1:B:120:LEU:HG	2	0.54
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	3	0.53
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	6	0.53
(1,1795)	1:A:2:PHE:H	1:A:2:PHE:HE1	19	0.53
(1,1795)	1:A:2:PHE:H	1:A:2:PHE:HE2	19	0.53
(1,1481)	1:B:132:LEU:H	1:B:133:GLN:HE21	6	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	11	0.53
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	11	0.53
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	11	0.53
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	18	0.53
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	18	0.53
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	18	0.53
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	18	0.53
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	10	0.53
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	10	0.53
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	11	0.52
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	5	0.52
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	7	0.52
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	16	0.52
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	10	0.52
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	2	0.52
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	4	0.52
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	15	0.51
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	15	0.51
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	15	0.51
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	15	0.51
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	15	0.51
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	15	0.51
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	12	0.51
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	5	0.51
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	12	0.51
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	12	0.51
(1,937)	1:B:105:LEU:HA	1:B:108:GLN:HE21	18	0.5
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	10	0.5
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	20	0.5
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	18	0.5
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	8	0.5
(1,1675)	1:A:5:LEU:HD21	1:A:3:LYS:H	19	0.5
(1,1675)	1:A:5:LEU:HD22	1:A:3:LYS:H	19	0.5
(1,1675)	1:A:5:LEU:HD23	1:A:3:LYS:H	19	0.5
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	18	0.5
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	4	0.5
(1,1166)	1:B:116:LEU:H	1:B:119:GLN:HE21	16	0.5
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	7	0.49
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	14	0.49
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	2	0.49
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	11	0.49
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	20	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	9	0.49
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	9	0.49
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	9	0.49
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	16	0.48
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	17	0.48
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	8	0.48
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	2	0.48
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	2	0.48
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	4	0.48
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	4	0.48
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	6	0.48
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	6	0.48
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	7	0.48
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	7	0.48
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	5	0.47
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	5	0.47
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	5	0.47
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	19	0.47
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	19	0.47
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	19	0.47
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	2	0.47
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	3	0.47
(1,741)	1:A:38:THR:H	1:A:38:THR:HG21	8	0.46
(1,741)	1:A:38:THR:H	1:A:38:THR:HG22	8	0.46
(1,741)	1:A:38:THR:H	1:A:38:THR:HG23	8	0.46
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	8	0.46
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	9	0.46
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	13	0.46
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	6	0.46
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	6	0.46
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	4	0.46
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	4	0.46
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	4	0.46
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	4	0.46
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	4	0.46
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	4	0.46
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	4	0.46
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	4	0.46
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	4	0.46
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	4	0.46
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	4	0.46
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	4	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	3	0.46
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	19	0.46
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	19	0.46
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	19	0.46
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	19	0.46
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	19	0.46
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	19	0.46
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	19	0.46
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	19	0.46
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	19	0.46
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	19	0.46
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	19	0.46
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	19	0.46
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	4	0.46
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	7	0.46
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	5	0.46
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	5	0.46
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	15	0.46
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	15	0.46
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	2	0.45
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	9	0.45
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	16	0.45
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	18	0.45
(1,1474)	1:B:131:LYS:HD2	1:B:135:GLU:HG2	16	0.45
(1,1474)	1:B:131:LYS:HD2	1:B:135:GLU:HG3	16	0.45
(1,1474)	1:B:131:LYS:HD3	1:B:135:GLU:HG2	16	0.45
(1,1474)	1:B:131:LYS:HD3	1:B:135:GLU:HG3	16	0.45
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	1	0.45
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	12	0.45
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	20	0.45
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	20	0.45
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	15	0.44
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	12	0.44
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD11	18	0.44
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD12	18	0.44
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD13	18	0.44
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD21	18	0.44
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD22	18	0.44
(1,1922)	1:B:141:GLN:HE22	1:A:30:LEU:HD23	18	0.44
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	2	0.44
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	18	0.44
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	17	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,408)	1:A:19:GLN:H	1:A:19:GLN:HE21	3	0.43
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	10	0.43
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	20	0.43
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	18	0.43
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	18	0.43
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	20	0.43
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	20	0.43
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	4	0.43
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	9	0.43
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	10	0.43
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	20	0.43
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	6	0.43
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	3	0.43
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	3	0.43
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	9	0.43
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	9	0.43
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	11	0.43
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	11	0.43
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	13	0.43
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	13	0.43
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	10	0.42
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	1	0.42
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	1	0.42
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	19	0.42
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	19	0.42
(1,1865)	1:B:119:GLN:HE22	1:A:19:GLN:HG2	14	0.42
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	11	0.42
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	13	0.42
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	14	0.42
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	1	0.41
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	7	0.41
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	15	0.41
(1,1760)	1:A:24:ASN:HD22	1:B:123:THR:HA	5	0.41
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	9	0.41
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	14	0.41
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	14	0.41
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	17	0.41
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	17	0.41
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	8	0.4
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	8	0.4
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	4	0.4
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	3	0.4
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	13	0.4
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	5	0.4
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	2	0.39
(1,741)	1:A:38:THR:H	1:A:38:THR:HG21	7	0.39
(1,741)	1:A:38:THR:H	1:A:38:THR:HG22	7	0.39
(1,741)	1:A:38:THR:H	1:A:38:THR:HG23	7	0.39
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	7	0.39
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	7	0.39
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	7	0.39
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	7	0.39
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	7	0.39
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	7	0.39
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	7	0.39
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	7	0.39
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	7	0.39
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	7	0.39
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	7	0.39
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	7	0.39
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	17	0.39
(1,148)	1:A:7:GLU:HB2	1:A:8:GLN:HE21	4	0.39
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	11	0.39
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	1	0.38
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	11	0.38
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	16	0.38
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	16	0.38
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	15	0.38
(1,1760)	1:A:24:ASN:HD22	1:B:123:THR:HA	7	0.38
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	1	0.38
(1,1576)	1:B:138:THR:HG21	1:B:139:GLN:H	17	0.38
(1,1576)	1:B:138:THR:HG22	1:B:139:GLN:H	17	0.38
(1,1576)	1:B:138:THR:HG23	1:B:139:GLN:H	17	0.38
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	20	0.38
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	20	0.38
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	8	0.38
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	8	0.38
(1,1153)	1:B:115:LYS:HE2	1:B:119:GLN:HE21	19	0.38
(1,1153)	1:B:115:LYS:HE3	1:B:119:GLN:HE21	19	0.38
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	4	0.37
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	15	0.37
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	15	0.37
(1,521)	1:A:25:MET:H	1:A:25:MET:HG2	17	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	5	0.37
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	13	0.37
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	8	0.37
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	4	0.37
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	4	0.37
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	1	0.37
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	1	0.37
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	1	0.37
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	1	0.37
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	1	0.37
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	1	0.37
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	1	0.37
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	1	0.37
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	1	0.37
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	1	0.37
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	1	0.37
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	1	0.37
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	16	0.37
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	18	0.37
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	1	0.37
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	1	0.37
(1,1547)	1:B:135:GLU:HG2	1:B:136:LYS:H	16	0.37
(1,1547)	1:B:135:GLU:HG3	1:B:136:LYS:H	16	0.37
(1,1475)	1:B:131:LYS:HG2	1:B:132:LEU:H	16	0.37
(1,1475)	1:B:131:LYS:HG3	1:B:132:LEU:H	16	0.37
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	6	0.37
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	15	0.37
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	3	0.36
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	10	0.36
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	3	0.36
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	14	0.36
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	3	0.36
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	14	0.36
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	12	0.36
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	12	0.36
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	11	0.36
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	19	0.36
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	2	0.36
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	10	0.36
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	10	0.36
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	12	0.36
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	12	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	7	0.35
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	8	0.35
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	9	0.35
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	12	0.35
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	19	0.35
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	20	0.35
(1,918)	1:B:104:LYS:HD2	1:B:108:GLN:HG2	8	0.35
(1,918)	1:B:104:LYS:HD3	1:B:108:GLN:HG2	8	0.35
(1,741)	1:A:38:THR:H	1:A:38:THR:HG21	16	0.35
(1,741)	1:A:38:THR:H	1:A:38:THR:HG22	16	0.35
(1,741)	1:A:38:THR:H	1:A:38:THR:HG23	16	0.35
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	6	0.35
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	12	0.35
(1,1930)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	12	0.35
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	7	0.35
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	3	0.35
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	9	0.35
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	3	0.35
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	5	0.35
(1,1252)	1:B:119:GLN:HE21	1:B:120:LEU:H	19	0.35
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	2	0.34
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	3	0.34
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	7	0.34
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	19	0.34
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	19	0.34
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	7	0.34
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	8	0.34
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	13	0.34
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	13	0.34
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	19	0.34
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	19	0.34
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	20	0.34
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	20	0.34
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	15	0.34
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	9	0.34
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	9	0.34
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	9	0.34
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	9	0.34
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	7	0.33
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	16	0.33
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	18	0.33
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	4	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	4	0.33
(1,650)	1:A:32:LEU:H	1:A:33:GLN:HE21	12	0.33
(1,521)	1:A:25:MET:H	1:A:25:MET:HG2	18	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	9	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	9	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	9	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	9	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	9	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	9	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	9	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	9	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	9	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	9	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	9	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	9	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	17	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	17	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	17	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	17	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	17	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	17	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	17	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	17	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	17	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	17	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	17	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	17	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	19	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	19	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	19	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	19	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	19	0.33
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	19	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	19	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	19	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	19	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	19	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	19	0.33
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	19	0.33
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	12	0.33
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	14	0.33
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	10	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	6	0.33
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	6	0.33
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	15	0.33
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	15	0.33
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	16	0.33
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	16	0.33
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	13	0.33
(1,106)	1:A:5:LEU:HA	1:A:8:GLN:HE21	19	0.33
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	16	0.32
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	10	0.32
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	13	0.32
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	9	0.32
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	17	0.32
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	1	0.32
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	18	0.32
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	1	0.32
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	18	0.32
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD21	1	0.32
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD22	1	0.32
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD23	1	0.32
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	20	0.32
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	20	0.32
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	2	0.32
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	19	0.32
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	19	0.32
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	19	0.32
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	19	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	2	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	2	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	2	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	2	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	2	0.32
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	2	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	2	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	2	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	2	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	2	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	2	0.32
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	2	0.32
(1,1866)	1:B:119:GLN:HE22	1:A:20:LEU:HG	6	0.32
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	4	0.32
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	4	0.32
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	4	0.32
(1,1576)	1:B:138:THR:HG21	1:B:139:GLN:H	2	0.32
(1,1576)	1:B:138:THR:HG22	1:B:139:GLN:H	2	0.32
(1,1576)	1:B:138:THR:HG23	1:B:139:GLN:H	2	0.32
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	1	0.31
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	7	0.31
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	14	0.31
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	18	0.31
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	13	0.31
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	13	0.31
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	13	0.31
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	13	0.31
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	13	0.31
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	13	0.31
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	13	0.31
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	13	0.31
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	13	0.31
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	13	0.31
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	13	0.31
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	13	0.31
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	11	0.31
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	9	0.31
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	20	0.31
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	19	0.31
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	19	0.31
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	19	0.31
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	4	0.3
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	18	0.3
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	19	0.3
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	11	0.3
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	6	0.3
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	6	0.3
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	15	0.3
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	18	0.3
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	7	0.3
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	11	0.3
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	12	0.3
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	20	0.3
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	7	0.3
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	11	0.3
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	20	0.3
(1,521)	1:A:25:MET:H	1:A:25:MET:HG2	1	0.3
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	1	0.3
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	17	0.3
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	2	0.3
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	2	0.3
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	7	0.3
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	7	0.3
(1,286)	1:A:14:GLU:HG2	1:A:15:LYS:HA	9	0.3
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	5	0.3
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	17	0.3
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	1	0.3
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	17	0.3
(1,1352)	1:B:125:MET:H	1:B:125:MET:HG2	19	0.3
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	18	0.3
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	18	0.3
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	18	0.3
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	18	0.3
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	16	0.29
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	2	0.29
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	13	0.29
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	2	0.29
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	13	0.29
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD21	11	0.29
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD22	11	0.29
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD23	11	0.29
(1,87)	1:A:4:LYS:HD2	1:A:8:GLN:HG2	2	0.29
(1,87)	1:A:4:LYS:HD3	1:A:8:GLN:HG2	2	0.29
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	5	0.29
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	5	0.29
(1,1769)	1:A:30:LEU:HB3	1:B:130:LEU:HG	5	0.29
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	13	0.29
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	20	0.29
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	7	0.29
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	7	0.29
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	11	0.29
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	11	0.29
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	2	0.29
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	2	0.29
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	3	0.29
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	10	0.29
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	15	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	6	0.28
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	6	0.28
(1,799)	1:A:41:GLN:HG2	1:A:42:GLU:H	8	0.28
(1,799)	1:A:41:GLN:HG3	1:A:42:GLU:H	8	0.28
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	9	0.28
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	11	0.28
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	11	0.28
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	13	0.28
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	13	0.28
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	15	0.28
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	15	0.28
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	19	0.28
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	19	0.28
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	18	0.28
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	18	0.28
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	18	0.28
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	18	0.28
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	18	0.28
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	18	0.28
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	18	0.28
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	18	0.28
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	18	0.28
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	18	0.28
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	18	0.28
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	18	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	14	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	14	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	14	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	14	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	14	0.28
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	14	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	14	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	14	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	14	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	14	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	14	0.28
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	14	0.28
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	19	0.28
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	8	0.28
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	8	0.28
(1,1675)	1:A:5:LEU:HD21	1:A:3:LYS:H	7	0.28
(1,1675)	1:A:5:LEU:HD22	1:A:3:LYS:H	7	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1675)	1:A:5:LEU:HD23	1:A:3:LYS:H	7	0.28
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG2	15	0.28
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG3	15	0.28
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	7	0.28
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	2	0.28
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	15	0.28
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	15	0.28
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	15	0.28
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	15	0.28
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	20	0.28
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	20	0.28
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	20	0.28
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	20	0.28
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	3	0.27
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	13	0.27
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	2	0.27
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	9	0.27
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	17	0.27
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	3	0.27
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	9	0.27
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	17	0.27
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	3	0.27
(1,45)	1:A:3:LYS:HD2	1:A:4:LYS:H	14	0.27
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	6	0.27
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	6	0.27
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	18	0.27
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	5	0.27
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	5	0.27
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	5	0.27
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	5	0.27
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	5	0.27
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	5	0.27
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	5	0.27
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	5	0.27
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	5	0.27
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	5	0.27
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	5	0.27
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	5	0.27
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	2	0.27
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	2	0.27
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG2	7	0.27
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1602)	1:B:140:ARG:HA	1:B:141:GLN:H	15	0.27
(1,1547)	1:B:135:GLU:HG2	1:B:136:LYS:H	2	0.27
(1,1547)	1:B:135:GLU:HG3	1:B:136:LYS:H	2	0.27
(1,1474)	1:B:131:LYS:HD2	1:B:135:GLU:HG2	5	0.27
(1,1474)	1:B:131:LYS:HD2	1:B:135:GLU:HG3	5	0.27
(1,1474)	1:B:131:LYS:HD3	1:B:135:GLU:HG2	5	0.27
(1,1474)	1:B:131:LYS:HD3	1:B:135:GLU:HG3	5	0.27
(2,75)	1:A:6:TYR:O	1:A:10:LEU:H	19	0.26
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	3	0.26
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	4	0.26
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	4	0.26
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	1	0.26
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	2	0.26
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	9	0.26
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	9	0.26
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	2	0.26
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	11	0.26
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	5	0.26
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	5	0.26
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	5	0.26
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	5	0.26
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	5	0.26
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	5	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	1	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	1	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	1	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	1	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	1	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	1	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	11	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	11	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	11	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	11	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	11	0.26
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	11	0.26
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	9	0.26
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	9	0.26
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	14	0.26
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	14	0.26
(1,1646)	1:B:142:GLU:HG2	1:B:143:ARG:H	8	0.26
(1,1646)	1:B:142:GLU:HG3	1:B:143:ARG:H	8	0.26
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG2	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG3	19	0.26
(1,1630)	1:B:141:GLN:HG2	1:B:142:GLU:H	1	0.26
(1,1630)	1:B:141:GLN:HG3	1:B:142:GLU:H	1	0.26
(1,1624)	1:B:141:GLN:HB2	1:B:142:GLU:H	10	0.26
(1,1624)	1:B:141:GLN:HB3	1:B:142:GLU:H	10	0.26
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	20	0.26
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	7	0.25
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	7	0.25
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	8	0.25
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	9	0.25
(1,760)	1:A:39:GLN:HE21	1:A:40:ARG:HG2	14	0.25
(1,760)	1:A:39:GLN:HE21	1:A:40:ARG:HG3	14	0.25
(1,760)	1:A:39:GLN:HE22	1:A:40:ARG:HG2	14	0.25
(1,760)	1:A:39:GLN:HE22	1:A:40:ARG:HG3	14	0.25
(1,594)	1:A:29:ASP:H	1:A:31:LYS:HG2	5	0.25
(1,594)	1:A:29:ASP:H	1:A:31:LYS:HG3	5	0.25
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	5	0.25
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	8	0.25
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	13	0.25
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	19	0.25
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	7	0.25
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	19	0.25
(1,286)	1:A:14:GLU:HG2	1:A:15:LYS:HA	12	0.25
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	5	0.25
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	15	0.25
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	17	0.25
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	17	0.25
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	17	0.25
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	17	0.25
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	18	0.25
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	18	0.25
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	18	0.25
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	18	0.25
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	18	0.25
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	18	0.25
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	18	0.25
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	18	0.25
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	1	0.25
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	18	0.25
(1,1425)	1:B:129:ASP:H	1:B:131:LYS:HG2	9	0.25
(1,1425)	1:B:129:ASP:H	1:B:131:LYS:HG3	9	0.25
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	19	0.25
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	5	0.25
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	16	0.24
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	8	0.24
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	17	0.24
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	16	0.24
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	18	0.24
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	10	0.24
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	7	0.24
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	4	0.24
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	10	0.24
(1,797)	1:A:41:GLN:HE21	1:A:43:ARG:H	7	0.24
(1,797)	1:A:41:GLN:HE22	1:A:43:ARG:H	7	0.24
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG2	10	0.24
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG3	10	0.24
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG2	10	0.24
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG3	10	0.24
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG2	10	0.24
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG3	10	0.24
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	3	0.24
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	9	0.24
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	19	0.24
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	6	0.24
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	20	0.24
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	1	0.24
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	17	0.24
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	10	0.24
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	10	0.24
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	17	0.24
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	17	0.24
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	19	0.24
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	9	0.24
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	9	0.24
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	9	0.24
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	9	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	3	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	3	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	3	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	3	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	3	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	3	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	9	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	9	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	9	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	9	0.24
(1,1904)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	9	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	3	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	3	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	3	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	3	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	3	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	3	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD11	9	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD12	9	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD13	9	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD21	9	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD22	9	0.24
(1,1903)	1:B:133:GLN:HE21	1:A:34:LEU:HD23	9	0.24
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	5	0.24
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	5	0.24
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	3	0.24
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	13	0.24
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	7	0.24
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	14	0.24
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	16	0.24
(1,1039)	1:B:109:ILE:HG21	1:B:113:ASN:HD21	17	0.24
(1,1039)	1:B:109:ILE:HG22	1:B:113:ASN:HD21	17	0.24
(1,1039)	1:B:109:ILE:HG23	1:B:113:ASN:HD21	17	0.24
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	2	0.23
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	6	0.23
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	9	0.23
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	14	0.23
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	3	0.23
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	20	0.23
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	3	0.23
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	10	0.23
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	10	0.23
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	18	0.23
(1,797)	1:A:41:GLN:HE21	1:A:43:ARG:H	6	0.23
(1,797)	1:A:41:GLN:HE22	1:A:43:ARG:H	6	0.23
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	7	0.23
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	18	0.23
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	9	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	18	0.23
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	9	0.23
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	3	0.23
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	3	0.23
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	8	0.23
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	8	0.23
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	20	0.23
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	20	0.23
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	12	0.23
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	12	0.23
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	12	0.23
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	12	0.23
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	5	0.23
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	1	0.23
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	1	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	5	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	5	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	5	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	5	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	5	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	5	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	20	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	20	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	20	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	20	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	20	0.23
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	20	0.23
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD11	11	0.23
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD12	11	0.23
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD13	11	0.23
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD21	11	0.23
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD22	11	0.23
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD23	11	0.23
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD11	11	0.23
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD12	11	0.23
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD13	11	0.23
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD21	11	0.23
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD22	11	0.23
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD23	11	0.23
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	12	0.23
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	12	0.23
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	12	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	12	0.23
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	12	0.23
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	12	0.23
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	12	0.23
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	12	0.23
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	12	0.23
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	12	0.23
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	12	0.23
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	12	0.23
(1,1760)	1:A:24:ASN:HD22	1:B:123:THR:HA	4	0.23
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	12	0.23
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	2	0.23
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	2	0.23
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	3	0.23
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	3	0.23
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	6	0.23
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	1	0.23
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	4	0.23
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	14	0.23
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	19	0.23
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	11	0.23
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	11	0.23
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	11	0.23
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	11	0.23
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	14	0.23
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	14	0.23
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	14	0.23
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	19	0.22
(2,75)	1:A:6:TYR:O	1:A:10:LEU:H	12	0.22
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	8	0.22
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	9	0.22
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	3	0.22
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	9	0.22
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	9	0.22
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	18	0.22
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	18	0.22
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	10	0.22
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	1	0.22
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	7	0.22
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE1	17	0.22
(1,1689)	1:A:9:ILE:H	1:B:106:TYR:HE2	17	0.22
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	2	0.22
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	5	0.22
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	4	0.22
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	1	0.22
(1,1321)	1:B:123:THR:HG21	1:B:124:ASN:HD21	2	0.22
(1,1321)	1:B:123:THR:HG22	1:B:124:ASN:HD21	2	0.22
(1,1321)	1:B:123:THR:HG23	1:B:124:ASN:HD21	2	0.22
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	13	0.22
(1,1195)	1:B:117:LYS:H	1:B:117:LYS:HE3	17	0.22
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	8	0.22
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	2	0.22
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	2	0.22
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	2	0.22
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	2	0.22
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	20	0.22
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	20	0.22
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	20	0.22
(2,75)	1:A:6:TYR:O	1:A:10:LEU:H	14	0.21
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	10	0.21
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	13	0.21
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	12	0.21
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	18	0.21
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	8	0.21
(2,65)	1:A:34:LEU:O	1:A:38:THR:H	5	0.21
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	8	0.21
(2,131)	1:A:34:LEU:O	1:A:38:THR:H	5	0.21
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	8	0.21
(1,968)	1:B:107:GLU:HA	1:B:110:LEU:HB3	19	0.21
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG2	5	0.21
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG3	5	0.21
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG2	5	0.21
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG3	5	0.21
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG2	5	0.21
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG3	5	0.21
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	9	0.21
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	3	0.21
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	8	0.21
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	12	0.21
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	16	0.21
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	20	0.21
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	17	0.21
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	17	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	17	0.21
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	17	0.21
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	17	0.21
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	17	0.21
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	9	0.21
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	10	0.21
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	7	0.21
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	7	0.21
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	11	0.21
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	11	0.21
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	18	0.21
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	18	0.21
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	5	0.21
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	5	0.21
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	5	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	14	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	14	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	14	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	14	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	14	0.21
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	14	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	1	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	3	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	4	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	6	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	7	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	11	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	13	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	18	0.21
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	19	0.21
(1,1681)	1:A:5:LEU:HD21	1:B:105:LEU:HD11	19	0.21
(1,1681)	1:A:5:LEU:HD21	1:B:105:LEU:HD12	19	0.21
(1,1681)	1:A:5:LEU:HD21	1:B:105:LEU:HD13	19	0.21
(1,1681)	1:A:5:LEU:HD22	1:B:105:LEU:HD11	19	0.21
(1,1681)	1:A:5:LEU:HD22	1:B:105:LEU:HD12	19	0.21
(1,1681)	1:A:5:LEU:HD22	1:B:105:LEU:HD13	19	0.21
(1,1681)	1:A:5:LEU:HD23	1:B:105:LEU:HD11	19	0.21
(1,1681)	1:A:5:LEU:HD23	1:B:105:LEU:HD12	19	0.21
(1,1681)	1:A:5:LEU:HD23	1:B:105:LEU:HD13	19	0.21
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	12	0.21
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	20	0.21
(1,1659)	1:B:144:PHE:H	1:B:144:PHE:HB2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	1:B:141:GLN:HG2	1:B:142:GLU:H	5	0.21
(1,1630)	1:B:141:GLN:HG3	1:B:142:GLU:H	5	0.21
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG2	11	0.21
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG3	11	0.21
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG2	11	0.21
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG3	11	0.21
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	20	0.21
(1,148)	1:A:7:GLU:HB2	1:A:8:GLN:HE21	3	0.21
(1,1425)	1:B:129:ASP:H	1:B:131:LYS:HG2	11	0.21
(1,1425)	1:B:129:ASP:H	1:B:131:LYS:HG3	11	0.21
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	16	0.21
(1,1194)	1:B:117:LYS:H	1:B:117:LYS:HE2	6	0.21
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	7	0.21
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	18	0.21
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	1	0.21
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	1	0.21
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	1	0.21
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	1	0.21
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	18	0.21
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	15	0.21
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	15	0.21
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	15	0.21
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	4	0.2
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	18	0.2
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	5	0.2
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	17	0.2
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	18	0.2
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	15	0.2
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	15	0.2
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	17	0.2
(1,920)	1:B:104:LYS:HE2	1:B:108:GLN:HG2	18	0.2
(1,920)	1:B:104:LYS:HE3	1:B:108:GLN:HG2	18	0.2
(1,918)	1:B:104:LYS:HD2	1:B:108:GLN:HG2	6	0.2
(1,918)	1:B:104:LYS:HD3	1:B:108:GLN:HG2	6	0.2
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	15	0.2
(1,834)	1:A:1:ASP:HA	1:A:4:LYS:H	12	0.2
(1,745)	1:A:38:THR:HG21	1:A:39:GLN:H	5	0.2
(1,745)	1:A:38:THR:HG22	1:A:39:GLN:H	5	0.2
(1,745)	1:A:38:THR:HG23	1:A:39:GLN:H	5	0.2
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	5	0.2
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	15	0.2
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:A:1:ASP:HA	1:A:4:LYS:H	12	0.2
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	1	0.2
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	2	0.2
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	2	0.2
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	2	0.2
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	2	0.2
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	14	0.2
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	14	0.2
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	14	0.2
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	14	0.2
(1,1897)	1:B:130:LEU:H	1:A:30:LEU:HG	9	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	3	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	3	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	3	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	3	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	3	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	3	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	3	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	3	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	3	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	3	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	3	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	3	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	11	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	11	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	11	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	11	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	11	0.2
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	11	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	11	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	11	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	11	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	11	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	11	0.2
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	11	0.2
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	12	0.2
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	15	0.2
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	20	0.2
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	18	0.2
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	18	0.2
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	18	0.2
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	18	0.2
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	18	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	2	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	5	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	8	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	9	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	10	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	12	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	15	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	16	0.2
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	20	0.2
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	20	0.2
(1,1760)	1:A:24:ASN:HD22	1:B:123:THR:HA	8	0.2
(1,1675)	1:A:5:LEU:HD21	1:A:3:LYS:H	2	0.2
(1,1675)	1:A:5:LEU:HD22	1:A:3:LYS:H	2	0.2
(1,1675)	1:A:5:LEU:HD23	1:A:3:LYS:H	2	0.2
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	9	0.2
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	11	0.2
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	17	0.2
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	6	0.2
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	19	0.2
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	10	0.2
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	9	0.2
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	6	0.2
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	13	0.2
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	4	0.2
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	4	0.2
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	4	0.2
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	4	0.2
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	14	0.2
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	14	0.2
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	14	0.2
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	14	0.2
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	3	0.2
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	10	0.2
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	14	0.2
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	20	0.2
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	5	0.2
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	5	0.2
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	5	0.2
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	1	0.19
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	7	0.19
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	2	0.19
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	11	0.19
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	15	0.19
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	16	0.19
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	4	0.19
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	10	0.19
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	15	0.19
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	16	0.19
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	4	0.19
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	10	0.19
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	1	0.19
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	4	0.19
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	7	0.19
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	9	0.19
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	14	0.19
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	16	0.19
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	19	0.19
(1,776)	1:A:40:ARG:HG2	1:A:41:GLN:H	17	0.19
(1,776)	1:A:40:ARG:HG3	1:A:41:GLN:H	17	0.19
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	19	0.19
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	19	0.19
(1,745)	1:A:38:THR:HG21	1:A:39:GLN:H	9	0.19
(1,745)	1:A:38:THR:HG22	1:A:39:GLN:H	9	0.19
(1,745)	1:A:38:THR:HG23	1:A:39:GLN:H	9	0.19
(1,745)	1:A:38:THR:HG21	1:A:39:GLN:H	12	0.19
(1,745)	1:A:38:THR:HG22	1:A:39:GLN:H	12	0.19
(1,745)	1:A:38:THR:HG23	1:A:39:GLN:H	12	0.19
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	19	0.19
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	2	0.19
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	10	0.19
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	16	0.19
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	20	0.19
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	8	0.19
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	11	0.19
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	14	0.19
(1,286)	1:A:14:GLU:HG2	1:A:15:LYS:HA	17	0.19
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	14	0.19
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	1	0.19
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	1	0.19
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	1	0.19
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	3	0.19
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	3	0.19
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	3	0.19
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	3	0.19
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD11	3	0.19
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD12	3	0.19
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD13	3	0.19
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD21	3	0.19
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD22	3	0.19
(1,1923)	1:A:41:GLN:HE22	1:B:130:LEU:HD23	3	0.19
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	20	0.19
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	20	0.19
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	20	0.19
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	20	0.19
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	20	0.19
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	20	0.19
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	3	0.19
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	4	0.19
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	13	0.19
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	17	0.19
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	8	0.19
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	8	0.19
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	8	0.19
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	8	0.19
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	8	0.19
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	8	0.19
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	8	0.19
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	8	0.19
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	8	0.19
(1,1793)	1:B:139:GLN:HE22	1:A:39:GLN:HE21	11	0.19
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	14	0.19
(1,178)	1:A:8:GLN:HG3	1:A:8:GLN:HE21	17	0.19
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	6	0.19
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	8	0.19
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	8	0.19
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	7	0.19
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	10	0.19
(1,1635)	1:B:141:GLN:HG2	1:B:143:ARG:HD2	15	0.19
(1,1635)	1:B:141:GLN:HG2	1:B:143:ARG:HD3	15	0.19
(1,1635)	1:B:141:GLN:HG3	1:B:143:ARG:HD2	15	0.19
(1,1635)	1:B:141:GLN:HG3	1:B:143:ARG:HD3	15	0.19
(1,1630)	1:B:141:GLN:HG2	1:B:142:GLU:H	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	1:B:141:GLN:HG3	1:B:142:GLU:H	9	0.19
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG2	6	0.19
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG3	6	0.19
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG2	6	0.19
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG3	6	0.19
(1,1549)	1:B:135:GLU:HG2	1:B:136:LYS:HD2	2	0.19
(1,1549)	1:B:135:GLU:HG2	1:B:136:LYS:HD3	2	0.19
(1,1549)	1:B:135:GLU:HG3	1:B:136:LYS:HD2	2	0.19
(1,1549)	1:B:135:GLU:HG3	1:B:136:LYS:HD3	2	0.19
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	7	0.19
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	17	0.19
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	12	0.19
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	19	0.19
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	19	0.19
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	19	0.19
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	19	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	4	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	5	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	6	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	7	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	8	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	11	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	12	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	13	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	15	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	16	0.19
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	19	0.19
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	1	0.19
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	1	0.19
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	1	0.19
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	9	0.18
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	15	0.18
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	1	0.18
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	16	0.18
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	1	0.18
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	16	0.18
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	2	0.18
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	10	0.18
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	11	0.18
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	15	0.18
(1,87)	1:A:4:LYS:HD2	1:A:8:GLN:HG2	8	0.18
(1,87)	1:A:4:LYS:HD3	1:A:8:GLN:HG2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	11	0.18
(1,825)	1:A:43:ARG:HB2	1:A:44:PHE:H	11	0.18
(1,825)	1:A:43:ARG:HB3	1:A:44:PHE:H	11	0.18
(1,811)	1:A:42:GLU:H	1:A:43:ARG:HG2	20	0.18
(1,811)	1:A:42:GLU:H	1:A:43:ARG:HG3	20	0.18
(1,800)	1:A:41:GLN:HG2	1:A:42:GLU:HA	8	0.18
(1,800)	1:A:41:GLN:HG3	1:A:42:GLU:HA	8	0.18
(1,774)	1:A:40:ARG:HD2	1:A:41:GLN:HG2	11	0.18
(1,774)	1:A:40:ARG:HD2	1:A:41:GLN:HG3	11	0.18
(1,774)	1:A:40:ARG:HD3	1:A:41:GLN:HG2	11	0.18
(1,774)	1:A:40:ARG:HD3	1:A:41:GLN:HG3	11	0.18
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	17	0.18
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	11	0.18
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	10	0.18
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	10	0.18
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	19	0.18
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	5	0.18
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	18	0.18
(1,335)	1:A:16:LEU:H	1:A:19:GLN:HE21	2	0.18
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	14	0.18
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	14	0.18
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	3	0.18
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	4	0.18
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	7	0.18
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	20	0.18
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	6	0.18
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	5	0.18
(1,1933)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	5	0.18
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	10	0.18
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	10	0.18
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	10	0.18
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	10	0.18
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	10	0.18
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	10	0.18
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	18	0.18
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	8	0.18
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	8	0.18
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	6	0.18
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	6	0.18
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	6	0.18
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	6	0.18
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	6	0.18
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	6	0.18
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	6	0.18
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	6	0.18
(1,1775)	1:A:33:GLN:HB2	1:B:134:LEU:HA	19	0.18
(1,1775)	1:A:33:GLN:HB3	1:B:134:LEU:HA	19	0.18
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	11	0.18
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	11	0.18
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	11	0.18
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	11	0.18
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	11	0.18
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	11	0.18
(1,1735)	1:A:19:GLN:HE22	1:B:119:GLN:HG2	14	0.18
(1,1700)	1:A:9:ILE:HD11	1:B:110:LEU:HA	17	0.18
(1,1700)	1:A:9:ILE:HD12	1:B:110:LEU:HA	17	0.18
(1,1700)	1:A:9:ILE:HD13	1:B:110:LEU:HA	17	0.18
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	1	0.18
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	1	0.18
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	10	0.18
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	10	0.18
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	16	0.18
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	16	0.18
(1,1679)	1:A:5:LEU:HD21	1:B:105:LEU:HA	12	0.18
(1,1679)	1:A:5:LEU:HD22	1:B:105:LEU:HA	12	0.18
(1,1679)	1:A:5:LEU:HD23	1:B:105:LEU:HA	12	0.18
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	2	0.18
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	14	0.18
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	19	0.18
(1,1660)	1:B:144:PHE:H	1:B:144:PHE:HB3	9	0.18
(1,1630)	1:B:141:GLN:HG2	1:B:142:GLU:H	16	0.18
(1,1630)	1:B:141:GLN:HG3	1:B:142:GLU:H	16	0.18
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	1	0.18
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	15	0.18
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	18	0.18
(1,126)	1:A:6:TYR:HA	1:A:9:ILE:HB	9	0.18
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	14	0.18
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	17	0.18
(1,1116)	1:B:114:GLU:HG2	1:B:115:LYS:H	9	0.18
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	1	0.18
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	2	0.18
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	9	0.18
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	11	0.18
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	11	0.18
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	6	0.17
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	19	0.17
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	15	0.17
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	14	0.17
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	19	0.17
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	14	0.17
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	19	0.17
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	12	0.17
(1,815)	1:A:42:GLU:HG2	1:A:43:ARG:H	13	0.17
(1,815)	1:A:42:GLU:HG3	1:A:43:ARG:H	13	0.17
(1,799)	1:A:41:GLN:HG2	1:A:42:GLU:H	10	0.17
(1,799)	1:A:41:GLN:HG3	1:A:42:GLU:H	10	0.17
(1,742)	1:A:38:THR:H	1:A:39:GLN:HG2	15	0.17
(1,742)	1:A:38:THR:H	1:A:39:GLN:HG3	15	0.17
(1,54)	1:A:3:LYS:HG2	1:A:3:LYS:HE3	18	0.17
(1,54)	1:A:3:LYS:HG3	1:A:3:LYS:HE3	18	0.17
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	2	0.17
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	14	0.17
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	5	0.17
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	10	0.17
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	14	0.17
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	10	0.17
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	13	0.17
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	14	0.17
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	6	0.17
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	4	0.17
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	4	0.17
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	6	0.17
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	10	0.17
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	5	0.17
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	5	0.17
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	5	0.17
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	5	0.17
(1,20)	1:A:2:PHE:HB3	1:A:3:LYS:H	13	0.17
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	8	0.17
(1,1842)	1:B:109:ILE:HG21	1:A:6:TYR:HE1	12	0.17
(1,1842)	1:B:109:ILE:HG21	1:A:6:TYR:HE2	12	0.17
(1,1842)	1:B:109:ILE:HG22	1:A:6:TYR:HE1	12	0.17
(1,1842)	1:B:109:ILE:HG22	1:A:6:TYR:HE2	12	0.17
(1,1842)	1:B:109:ILE:HG23	1:A:6:TYR:HE1	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1842)	1:B:109:ILE:HG23	1:A:6:TYR:HE2	12	0.17
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	19	0.17
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	19	0.17
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	9	0.17
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	9	0.17
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	20	0.17
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	20	0.17
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	1	0.17
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	1	0.17
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	1	0.17
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	1	0.17
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	1	0.17
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	1	0.17
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	1	0.17
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	1	0.17
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	1	0.17
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	16	0.17
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	16	0.17
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	16	0.17
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD11	14	0.17
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD12	14	0.17
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD13	14	0.17
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD21	14	0.17
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD22	14	0.17
(1,1776)	1:A:33:GLN:HB2	1:B:134:LEU:HD23	14	0.17
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD11	14	0.17
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD12	14	0.17
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD13	14	0.17
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD21	14	0.17
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD22	14	0.17
(1,1776)	1:A:33:GLN:HB3	1:B:134:LEU:HD23	14	0.17
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	9	0.17
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	13	0.17
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	13	0.17
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	13	0.17
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	13	0.17
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	13	0.17
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	13	0.17
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	15	0.17
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	15	0.17
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	4	0.17
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	13	0.17
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	15	0.17
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	18	0.17
(1,1593)	1:B:139:GLN:HG2	1:B:140:ARG:H	16	0.17
(1,1593)	1:B:139:GLN:HG3	1:B:140:ARG:H	16	0.17
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	13	0.17
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	5	0.17
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	18	0.17
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	20	0.17
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	16	0.17
(1,1256)	1:B:119:GLN:HG2	1:B:120:LEU:H	16	0.17
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	6	0.17
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	9	0.17
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	12	0.17
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	15	0.17
(1,1009)	1:B:108:GLN:HG3	1:B:108:GLN:HE21	17	0.17
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	3	0.16
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	14	0.16
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	16	0.16
(2,69)	1:A:3:LYS:O	1:A:7:GLU:H	5	0.16
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	1	0.16
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	3	0.16
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	18	0.16
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	19	0.16
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	5	0.16
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	7	0.16
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	11	0.16
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	17	0.16
(2,61)	1:A:32:LEU:O	1:A:36:LYS:H	16	0.16
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	3	0.16
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	18	0.16
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	19	0.16
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	5	0.16
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	7	0.16
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	11	0.16
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	17	0.16
(2,127)	1:A:32:LEU:O	1:A:36:LYS:H	16	0.16
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD21	3	0.16
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD22	3	0.16
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD23	3	0.16
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD21	16	0.16
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD22	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD23	16	0.16
(1,89)	1:A:4:LYS:HE2	1:A:8:GLN:HG2	7	0.16
(1,89)	1:A:4:LYS:HE3	1:A:8:GLN:HG2	7	0.16
(1,89)	1:A:4:LYS:HE2	1:A:8:GLN:HG2	19	0.16
(1,89)	1:A:4:LYS:HE3	1:A:8:GLN:HG2	19	0.16
(1,87)	1:A:4:LYS:HD2	1:A:8:GLN:HG2	5	0.16
(1,87)	1:A:4:LYS:HD3	1:A:8:GLN:HG2	5	0.16
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	16	0.16
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	16	0.16
(1,658)	1:A:32:LEU:HA	1:A:35:GLU:HG2	17	0.16
(1,658)	1:A:32:LEU:HA	1:A:35:GLU:HG3	17	0.16
(1,628)	1:A:31:LYS:H	1:A:31:LYS:HG2	5	0.16
(1,628)	1:A:31:LYS:H	1:A:31:LYS:HG3	5	0.16
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	11	0.16
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	15	0.16
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	16	0.16
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	20	0.16
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	8	0.16
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	20	0.16
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	4	0.16
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	7	0.16
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	13	0.16
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	18	0.16
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	4	0.16
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	8	0.16
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	5	0.16
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	16	0.16
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	13	0.16
(1,20)	1:A:2:PHE:HB3	1:A:3:LYS:H	2	0.16
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	9	0.16
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	9	0.16
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	9	0.16
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	9	0.16
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	9	0.16
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	9	0.16
(1,1890)	1:B:124:ASN:HD22	1:A:23:THR:HA	6	0.16
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	2	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	4	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	4	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	4	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	4	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	4	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	4	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	4	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	4	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	14	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	14	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	14	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	14	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	14	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	14	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	14	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	14	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	14	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	18	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	18	0.16
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	18	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	18	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	18	0.16
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	18	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	18	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	18	0.16
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	18	0.16
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE1	19	0.16
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE2	19	0.16
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE1	19	0.16
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE2	19	0.16
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	18	0.16
(1,1760)	1:A:24:ASN:HD22	1:B:123:THR:HA	6	0.16
(1,1717)	1:A:10:LEU:H	1:B:109:ILE:HG12	19	0.16
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	5	0.16
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	5	0.16
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	16	0.16
(1,1656)	1:B:143:ARG:HB2	1:B:144:PHE:H	17	0.16
(1,1656)	1:B:143:ARG:HB3	1:B:144:PHE:H	17	0.16
(1,1628)	1:B:141:GLN:HE21	1:B:143:ARG:H	16	0.16
(1,1628)	1:B:141:GLN:HE22	1:B:143:ARG:H	16	0.16
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG2	4	0.16
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG3	4	0.16
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG2	4	0.16
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG3	4	0.16
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG2	7	0.16
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG2	7	0.16
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG3	7	0.16
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	5	0.16
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	11	0.16
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	2	0.16
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	12	0.16
(1,148)	1:A:7:GLU:HB2	1:A:8:GLN:HE21	8	0.16
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	12	0.16
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	8	0.16
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	8	0.16
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	8	0.16
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	10	0.16
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	10	0.16
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	10	0.16
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	2	0.15
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	8	0.15
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	9	0.15
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	14	0.15
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	17	0.15
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	4	0.15
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	1	0.15
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	11	0.15
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	12	0.15
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	8	0.15
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	12	0.15
(2,61)	1:A:32:LEU:O	1:A:36:LYS:H	4	0.15
(2,59)	1:A:31:LYS:O	1:A:35:GLU:H	7	0.15
(2,59)	1:A:31:LYS:O	1:A:35:GLU:H	12	0.15
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	11	0.15
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	12	0.15
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	8	0.15
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	12	0.15
(2,127)	1:A:32:LEU:O	1:A:36:LYS:H	4	0.15
(2,125)	1:A:31:LYS:O	1:A:35:GLU:H	7	0.15
(2,125)	1:A:31:LYS:O	1:A:35:GLU:H	12	0.15
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	6	0.15
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	13	0.15
(1,984)	1:B:107:GLU:HB3	1:B:108:GLN:HE21	3	0.15
(1,892)	1:A:4:LYS:H	1:A:4:LYS:HG2	18	0.15
(1,89)	1:A:4:LYS:HE2	1:A:8:GLN:HG2	6	0.15
(1,89)	1:A:4:LYS:HE3	1:A:8:GLN:HG2	6	0.15
(1,89)	1:A:4:LYS:HE2	1:A:8:GLN:HG2	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,89)	1:A:4:LYS:HE3	1:A:8:GLN:HG2	16	0.15
(1,776)	1:A:40:ARG:HG2	1:A:41:GLN:H	15	0.15
(1,776)	1:A:40:ARG:HG3	1:A:41:GLN:H	15	0.15
(1,774)	1:A:40:ARG:HD2	1:A:41:GLN:HG2	9	0.15
(1,774)	1:A:40:ARG:HD2	1:A:41:GLN:HG3	9	0.15
(1,774)	1:A:40:ARG:HD3	1:A:41:GLN:HG2	9	0.15
(1,774)	1:A:40:ARG:HD3	1:A:41:GLN:HG3	9	0.15
(1,759)	1:A:39:GLN:HE21	1:A:40:ARG:HB2	14	0.15
(1,759)	1:A:39:GLN:HE21	1:A:40:ARG:HB3	14	0.15
(1,759)	1:A:39:GLN:HE22	1:A:40:ARG:HB2	14	0.15
(1,759)	1:A:39:GLN:HE22	1:A:40:ARG:HB3	14	0.15
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	3	0.15
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	3	0.15
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	5	0.15
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	5	0.15
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE21	16	0.15
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE22	16	0.15
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE21	20	0.15
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE22	20	0.15
(1,61)	1:A:4:LYS:H	1:A:4:LYS:HG2	18	0.15
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	18	0.15
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	17	0.15
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	11	0.15
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	15	0.15
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	12	0.15
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	2	0.15
(1,286)	1:A:14:GLU:HG2	1:A:15:LYS:HA	15	0.15
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	2	0.15
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	11	0.15
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	11	0.15
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	11	0.15
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	11	0.15
(1,201)	1:A:9:ILE:HG21	1:A:10:LEU:H	20	0.15
(1,201)	1:A:9:ILE:HG22	1:A:10:LEU:H	20	0.15
(1,201)	1:A:9:ILE:HG23	1:A:10:LEU:H	20	0.15
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB2	7	0.15
(1,1931)	1:B:141:GLN:HE22	1:A:40:ARG:HB3	7	0.15
(1,1925)	1:B:141:GLN:HE21	1:A:41:GLN:HE22	19	0.15
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD11	12	0.15
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD12	12	0.15
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD13	12	0.15
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD21	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD22	12	0.15
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD23	12	0.15
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD11	12	0.15
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD12	12	0.15
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD13	12	0.15
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD21	12	0.15
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD22	12	0.15
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD23	12	0.15
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	11	0.15
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	16	0.15
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	19	0.15
(1,1842)	1:B:109:ILE:HG21	1:A:6:TYR:HE1	19	0.15
(1,1842)	1:B:109:ILE:HG21	1:A:6:TYR:HE2	19	0.15
(1,1842)	1:B:109:ILE:HG22	1:A:6:TYR:HE1	19	0.15
(1,1842)	1:B:109:ILE:HG22	1:A:6:TYR:HE2	19	0.15
(1,1842)	1:B:109:ILE:HG23	1:A:6:TYR:HE1	19	0.15
(1,1842)	1:B:109:ILE:HG23	1:A:6:TYR:HE2	19	0.15
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	7	0.15
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	7	0.15
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	13	0.15
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	13	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	2	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	2	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	2	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	2	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	2	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	2	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	2	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	2	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	2	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	16	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	16	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	16	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	16	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	16	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	16	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	16	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	16	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	16	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	20	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	20	0.15
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	20	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	20	0.15
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	20	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	20	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	20	0.15
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	20	0.15
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	1	0.15
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	1	0.15
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	1	0.15
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	10	0.15
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	10	0.15
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	10	0.15
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	9	0.15
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	9	0.15
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	9	0.15
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	9	0.15
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	9	0.15
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	9	0.15
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG21	10	0.15
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG22	10	0.15
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG23	10	0.15
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG21	13	0.15
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG22	13	0.15
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG23	13	0.15
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	2	0.15
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	2	0.15
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	2	0.15
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	2	0.15
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	2	0.15
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	2	0.15
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	7	0.15
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	7	0.15
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	7	0.15
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	7	0.15
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	7	0.15
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	7	0.15
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB1	7	0.15
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB2	7	0.15
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB3	7	0.15
(1,1679)	1:A:5:LEU:HD21	1:B:105:LEU:HA	20	0.15
(1,1679)	1:A:5:LEU:HD22	1:B:105:LEU:HA	20	0.15
(1,1679)	1:A:5:LEU:HD23	1:B:105:LEU:HA	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	3	0.15
(1,167)	1:A:8:GLN:HA	1:A:8:GLN:HE21	8	0.15
(1,1593)	1:B:139:GLN:HG2	1:B:140:ARG:H	14	0.15
(1,1593)	1:B:139:GLN:HG3	1:B:140:ARG:H	14	0.15
(1,1536)	1:B:134:LEU:HD11	1:B:135:GLU:HA	2	0.15
(1,1536)	1:B:134:LEU:HD12	1:B:135:GLU:HA	2	0.15
(1,1536)	1:B:134:LEU:HD13	1:B:135:GLU:HA	2	0.15
(1,1536)	1:B:134:LEU:HD21	1:B:135:GLU:HA	2	0.15
(1,1536)	1:B:134:LEU:HD22	1:B:135:GLU:HA	2	0.15
(1,1536)	1:B:134:LEU:HD23	1:B:135:GLU:HA	2	0.15
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	7	0.15
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	15	0.15
(1,1168)	1:B:116:LEU:HA	1:B:116:LEU:HG	19	0.15
(1,1120)	1:B:114:GLU:HG3	1:B:115:LYS:HA	9	0.15
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	17	0.15
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	17	0.15
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	17	0.15
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	17	0.15
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	17	0.15
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	17	0.15
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	17	0.15
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	20	0.15
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	20	0.15
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	20	0.15
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	18	0.15
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	18	0.15
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	18	0.15
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	10	0.14
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	15	0.14
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	20	0.14
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	20	0.14
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	3	0.14
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	10	0.14
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	4	0.14
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	7	0.14
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	20	0.14
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	6	0.14
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	18	0.14
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	4	0.14
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	7	0.14
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	20	0.14
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	18	0.14
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	5	0.14
(1,984)	1:B:107:GLU:HB3	1:B:108:GLN:HE21	20	0.14
(1,970)	1:B:107:GLU:HA	1:B:111:ALA:H	9	0.14
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD21	14	0.14
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD22	14	0.14
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD23	14	0.14
(1,920)	1:B:104:LYS:HE2	1:B:108:GLN:HG2	20	0.14
(1,920)	1:B:104:LYS:HE3	1:B:108:GLN:HG2	20	0.14
(1,918)	1:B:104:LYS:HD2	1:B:108:GLN:HG2	7	0.14
(1,918)	1:B:104:LYS:HD3	1:B:108:GLN:HG2	7	0.14
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	8	0.14
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	17	0.14
(1,828)	1:A:44:PHE:H	1:A:44:PHE:HB2	19	0.14
(1,811)	1:A:42:GLU:H	1:A:43:ARG:HG2	15	0.14
(1,811)	1:A:42:GLU:H	1:A:43:ARG:HG3	15	0.14
(1,776)	1:A:40:ARG:HG2	1:A:41:GLN:H	11	0.14
(1,776)	1:A:40:ARG:HG3	1:A:41:GLN:H	11	0.14
(1,762)	1:A:39:GLN:HG2	1:A:40:ARG:H	6	0.14
(1,762)	1:A:39:GLN:HG3	1:A:40:ARG:H	6	0.14
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	1	0.14
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	1	0.14
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	12	0.14
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	12	0.14
(1,699)	1:A:34:LEU:HG	1:A:35:GLU:H	9	0.14
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	3	0.14
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	19	0.14
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	8	0.14
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	17	0.14
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	6	0.14
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	17	0.14
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	1	0.14
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	16	0.14
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	17	0.14
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	15	0.14
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	9	0.14
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	15	0.14
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	1	0.14
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	14	0.14
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	10	0.14
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	10	0.14
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	10	0.14
(1,1924)	1:A:41:GLN:HE21	1:B:141:GLN:HE22	19	0.14
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	11	0.14
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	11	0.14
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	11	0.14
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	11	0.14
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	11	0.14
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	11	0.14
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD11	16	0.14
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD12	16	0.14
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD13	16	0.14
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD21	16	0.14
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD22	16	0.14
(1,1892)	1:B:126:GLU:HG2	1:A:27:LEU:HD23	16	0.14
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD11	16	0.14
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD12	16	0.14
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD13	16	0.14
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD21	16	0.14
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD22	16	0.14
(1,1892)	1:B:126:GLU:HG3	1:A:27:LEU:HD23	16	0.14
(1,1883)	1:B:123:THR:HG21	1:A:24:ASN:HB3	2	0.14
(1,1883)	1:B:123:THR:HG22	1:A:24:ASN:HB3	2	0.14
(1,1883)	1:B:123:THR:HG23	1:A:24:ASN:HB3	2	0.14
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	1	0.14
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	1	0.14
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	12	0.14
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	12	0.14
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	12	0.14
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	12	0.14
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	12	0.14
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	12	0.14
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	12	0.14
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	12	0.14
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	12	0.14
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	15	0.14
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	15	0.14
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	15	0.14
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	15	0.14
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	15	0.14
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	15	0.14
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	15	0.14
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	15	0.14
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	12	0.14
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	12	0.14
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	12	0.14
(1,1789)	1:A:37:ALA:HB1	1:B:134:LEU:HA	5	0.14
(1,1789)	1:A:37:ALA:HB2	1:B:134:LEU:HA	5	0.14
(1,1789)	1:A:37:ALA:HB3	1:B:134:LEU:HA	5	0.14
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	9	0.14
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	9	0.14
(1,1679)	1:A:5:LEU:HD21	1:B:105:LEU:HA	4	0.14
(1,1679)	1:A:5:LEU:HD22	1:B:105:LEU:HA	4	0.14
(1,1679)	1:A:5:LEU:HD23	1:B:105:LEU:HA	4	0.14
(1,1679)	1:A:5:LEU:HD21	1:B:105:LEU:HA	17	0.14
(1,1679)	1:A:5:LEU:HD22	1:B:105:LEU:HA	17	0.14
(1,1679)	1:A:5:LEU:HD23	1:B:105:LEU:HA	17	0.14
(1,1659)	1:B:144:PHE:H	1:B:144:PHE:HB2	1	0.14
(1,1656)	1:B:143:ARG:HB2	1:B:144:PHE:H	1	0.14
(1,1656)	1:B:143:ARG:HB3	1:B:144:PHE:H	1	0.14
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG2	6	0.14
(1,1642)	1:B:142:GLU:H	1:B:143:ARG:HG3	6	0.14
(1,1635)	1:B:141:GLN:HG2	1:B:143:ARG:HD2	19	0.14
(1,1635)	1:B:141:GLN:HG2	1:B:143:ARG:HD3	19	0.14
(1,1635)	1:B:141:GLN:HG3	1:B:143:ARG:HD2	19	0.14
(1,1635)	1:B:141:GLN:HG3	1:B:143:ARG:HD3	19	0.14
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	11	0.14
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	16	0.14
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	11	0.14
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	13	0.14
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	14	0.14
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	8	0.14
(1,126)	1:A:6:TYR:HA	1:A:9:ILE:HB	13	0.14
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	5	0.14
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	20	0.14
(1,1168)	1:B:116:LEU:HA	1:B:116:LEU:HG	18	0.14
(1,1116)	1:B:114:GLU:HG2	1:B:115:LYS:H	15	0.14
(1,1116)	1:B:114:GLU:HG2	1:B:115:LYS:H	18	0.14
(1,1116)	1:B:114:GLU:HG2	1:B:115:LYS:H	19	0.14
(2,74)	1:A:5:LEU:O	1:A:9:ILE:N	5	0.13
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	15	0.13
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	2	0.13
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	13	0.13
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	2	0.13
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	9	0.13
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	13	0.13
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	14	0.13
(2,59)	1:A:31:LYS:O	1:A:35:GLU:H	6	0.13
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	2	0.13
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	13	0.13
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	17	0.13
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	2	0.13
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	9	0.13
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	13	0.13
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	14	0.13
(2,125)	1:A:31:LYS:O	1:A:35:GLU:H	6	0.13
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	3	0.13
(1,983)	1:B:107:GLU:HB3	1:B:108:GLN:H	20	0.13
(1,970)	1:B:107:GLU:HA	1:B:111:ALA:H	13	0.13
(1,959)	1:B:107:GLU:H	1:B:107:GLU:HB2	20	0.13
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD21	5	0.13
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD22	5	0.13
(1,929)	1:A:5:LEU:H	1:B:105:LEU:HD23	5	0.13
(1,804)	1:A:41:GLN:HG2	1:A:43:ARG:HD2	3	0.13
(1,804)	1:A:41:GLN:HG2	1:A:43:ARG:HD3	3	0.13
(1,804)	1:A:41:GLN:HG3	1:A:43:ARG:HD2	3	0.13
(1,804)	1:A:41:GLN:HG3	1:A:43:ARG:HD3	3	0.13
(1,758)	1:A:39:GLN:HE21	1:A:40:ARG:H	4	0.13
(1,758)	1:A:39:GLN:HE22	1:A:40:ARG:H	4	0.13
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE21	2	0.13
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE22	2	0.13
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE21	7	0.13
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE22	7	0.13
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE21	18	0.13
(1,670)	1:A:33:GLN:H	1:A:33:GLN:HE22	18	0.13
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	6	0.13
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	7	0.13
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	16	0.13
(1,522)	1:A:25:MET:H	1:A:25:MET:HG3	10	0.13
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	12	0.13
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	13	0.13
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	3	0.13
(1,410)	1:A:19:GLN:H	1:A:19:GLN:HG2	6	0.13
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	2	0.13
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	2	0.13
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	5	0.13
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	2	0.13
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	17	0.13
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	2	0.13
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	18	0.13
(1,201)	1:A:9:ILE:HG21	1:A:10:LEU:H	15	0.13
(1,201)	1:A:9:ILE:HG22	1:A:10:LEU:H	15	0.13
(1,201)	1:A:9:ILE:HG23	1:A:10:LEU:H	15	0.13
(1,1915)	1:B:134:LEU:HD11	1:A:37:ALA:HA	2	0.13
(1,1915)	1:B:134:LEU:HD12	1:A:37:ALA:HA	2	0.13
(1,1915)	1:B:134:LEU:HD13	1:A:37:ALA:HA	2	0.13
(1,1915)	1:B:134:LEU:HD21	1:A:37:ALA:HA	2	0.13
(1,1915)	1:B:134:LEU:HD22	1:A:37:ALA:HA	2	0.13
(1,1915)	1:B:134:LEU:HD23	1:A:37:ALA:HA	2	0.13
(1,1883)	1:B:123:THR:HG21	1:A:24:ASN:HB3	7	0.13
(1,1883)	1:B:123:THR:HG22	1:A:24:ASN:HB3	7	0.13
(1,1883)	1:B:123:THR:HG23	1:A:24:ASN:HB3	7	0.13
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	6	0.13
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	2	0.13
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	2	0.13
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	14	0.13
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	14	0.13
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE1	15	0.13
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE2	15	0.13
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE1	15	0.13
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE2	15	0.13
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	7	0.13
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	7	0.13
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	7	0.13
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	8	0.13
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	8	0.13
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	8	0.13
(1,1789)	1:A:37:ALA:HB1	1:B:134:LEU:HA	9	0.13
(1,1789)	1:A:37:ALA:HB2	1:B:134:LEU:HA	9	0.13
(1,1789)	1:A:37:ALA:HB3	1:B:134:LEU:HA	9	0.13
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	2	0.13
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	2	0.13
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	2	0.13
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	2	0.13
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	2	0.13
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	3	0.13
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	3	0.13
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	3	0.13
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	3	0.13
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	3	0.13
(1,1774)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	3	0.13
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD11	3	0.13
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD12	3	0.13
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD13	3	0.13
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD21	3	0.13
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD22	3	0.13
(1,1773)	1:A:33:GLN:HE21	1:B:134:LEU:HD23	3	0.13
(1,1770)	1:A:30:LEU:HB3	1:B:130:LEU:HD11	9	0.13
(1,1770)	1:A:30:LEU:HB3	1:B:130:LEU:HD12	9	0.13
(1,1770)	1:A:30:LEU:HB3	1:B:130:LEU:HD13	9	0.13
(1,1770)	1:A:30:LEU:HB3	1:B:130:LEU:HD21	9	0.13
(1,1770)	1:A:30:LEU:HB3	1:B:130:LEU:HD22	9	0.13
(1,1770)	1:A:30:LEU:HB3	1:B:130:LEU:HD23	9	0.13
(1,1768)	1:A:30:LEU:HB2	1:B:130:LEU:HG	3	0.13
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	11	0.13
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG21	7	0.13
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG22	7	0.13
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG23	7	0.13
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	19	0.13
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	19	0.13
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	19	0.13
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	19	0.13
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	19	0.13
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	19	0.13
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB1	10	0.13
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB2	10	0.13
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB3	10	0.13
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	6	0.13
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	6	0.13
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	12	0.13
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	12	0.13
(1,1666)	1:A:2:PHE:HA	1:B:102:PHE:HB3	19	0.13
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE1	12	0.13
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE2	12	0.13
(1,1653)	1:B:143:ARG:HA	1:B:143:ARG:HG2	11	0.13
(1,1653)	1:B:143:ARG:HA	1:B:143:ARG:HG3	11	0.13
(1,1602)	1:B:140:ARG:HA	1:B:141:GLN:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG2	19	0.13
(1,1591)	1:B:139:GLN:HE21	1:B:140:ARG:HG3	19	0.13
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG2	19	0.13
(1,1591)	1:B:139:GLN:HE22	1:B:140:ARG:HG3	19	0.13
(1,1530)	1:B:134:LEU:HG	1:B:135:GLU:H	12	0.13
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	10	0.13
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	14	0.13
(1,139)	1:A:7:GLU:HA	1:A:11:ALA:H	17	0.13
(1,128)	1:A:7:GLU:H	1:A:7:GLU:HB2	10	0.13
(1,1256)	1:B:119:GLN:HG2	1:B:120:LEU:H	4	0.13
(1,1256)	1:B:119:GLN:HG2	1:B:120:LEU:H	19	0.13
(1,1256)	1:B:119:GLN:HG2	1:B:120:LEU:H	20	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	3	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	3	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	3	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	3	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	7	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	7	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	7	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	7	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	8	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	8	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	8	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	8	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	13	0.13
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	13	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	13	0.13
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	13	0.13
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	8	0.13
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	8	0.13
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	8	0.13
(1,1029)	1:B:109:ILE:HB	1:B:110:LEU:H	19	0.13
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	2	0.13
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	2	0.13
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	2	0.13
(2,80)	1:A:8:GLN:O	1:A:12:GLU:N	6	0.12
(2,73)	1:A:5:LEU:O	1:A:9:ILE:H	12	0.12
(2,70)	1:A:3:LYS:O	1:A:7:GLU:N	2	0.12
(2,67)	1:A:2:PHE:O	1:A:6:TYR:H	9	0.12
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	6	0.12
(2,61)	1:A:32:LEU:O	1:A:36:LYS:H	7	0.12
(2,61)	1:A:32:LEU:O	1:A:36:LYS:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,61)	1:A:32:LEU:O	1:A:36:LYS:H	14	0.12
(2,59)	1:A:31:LYS:O	1:A:35:GLU:H	13	0.12
(2,55)	1:A:29:ASP:O	1:A:33:GLN:H	17	0.12
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	6	0.12
(2,127)	1:A:32:LEU:O	1:A:36:LYS:H	7	0.12
(2,127)	1:A:32:LEU:O	1:A:36:LYS:H	12	0.12
(2,127)	1:A:32:LEU:O	1:A:36:LYS:H	14	0.12
(2,125)	1:A:31:LYS:O	1:A:35:GLU:H	13	0.12
(2,121)	1:A:29:ASP:O	1:A:33:GLN:H	17	0.12
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	18	0.12
(1,998)	1:B:108:GLN:HA	1:B:108:GLN:HE21	19	0.12
(1,984)	1:B:107:GLU:HB3	1:B:108:GLN:HE21	4	0.12
(1,983)	1:B:107:GLU:HB3	1:B:108:GLN:H	3	0.12
(1,89)	1:A:4:LYS:HE2	1:A:8:GLN:HG2	15	0.12
(1,89)	1:A:4:LYS:HE3	1:A:8:GLN:HG2	15	0.12
(1,845)	1:A:2:PHE:HA	1:A:4:LYS:HG3	19	0.12
(1,833)	1:A:1:ASP:HA	1:A:3:LYS:H	14	0.12
(1,822)	1:A:43:ARG:HA	1:A:43:ARG:HG2	18	0.12
(1,822)	1:A:43:ARG:HA	1:A:43:ARG:HG3	18	0.12
(1,797)	1:A:41:GLN:HE21	1:A:43:ARG:H	14	0.12
(1,797)	1:A:41:GLN:HE22	1:A:43:ARG:H	14	0.12
(1,797)	1:A:41:GLN:HE21	1:A:43:ARG:H	19	0.12
(1,797)	1:A:41:GLN:HE22	1:A:43:ARG:H	19	0.12
(1,770)	1:A:40:ARG:HA	1:A:40:ARG:HG2	13	0.12
(1,770)	1:A:40:ARG:HA	1:A:40:ARG:HG3	13	0.12
(1,760)	1:A:39:GLN:HE21	1:A:40:ARG:HG2	2	0.12
(1,760)	1:A:39:GLN:HE21	1:A:40:ARG:HG3	2	0.12
(1,760)	1:A:39:GLN:HE22	1:A:40:ARG:HG2	2	0.12
(1,760)	1:A:39:GLN:HE22	1:A:40:ARG:HG3	2	0.12
(1,751)	1:A:39:GLN:H	1:A:40:ARG:H	14	0.12
(1,699)	1:A:34:LEU:HG	1:A:35:GLU:H	12	0.12
(1,667)	1:A:32:LEU:HD11	1:A:33:GLN:HE21	13	0.12
(1,667)	1:A:32:LEU:HD11	1:A:33:GLN:HE22	13	0.12
(1,667)	1:A:32:LEU:HD12	1:A:33:GLN:HE21	13	0.12
(1,667)	1:A:32:LEU:HD12	1:A:33:GLN:HE22	13	0.12
(1,667)	1:A:32:LEU:HD13	1:A:33:GLN:HE21	13	0.12
(1,667)	1:A:32:LEU:HD13	1:A:33:GLN:HE22	13	0.12
(1,667)	1:A:32:LEU:HD21	1:A:33:GLN:HE21	13	0.12
(1,667)	1:A:32:LEU:HD21	1:A:33:GLN:HE22	13	0.12
(1,667)	1:A:32:LEU:HD22	1:A:33:GLN:HE21	13	0.12
(1,667)	1:A:32:LEU:HD22	1:A:33:GLN:HE22	13	0.12
(1,667)	1:A:32:LEU:HD23	1:A:33:GLN:HE21	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:A:32:LEU:HD23	1:A:33:GLN:HE22	13	0.12
(1,658)	1:A:32:LEU:HA	1:A:35:GLU:HG2	9	0.12
(1,658)	1:A:32:LEU:HA	1:A:35:GLU:HG3	9	0.12
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	13	0.12
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	7	0.12
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	13	0.12
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	18	0.12
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	1	0.12
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	4	0.12
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	7	0.12
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	18	0.12
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	19	0.12
(1,370)	1:A:17:LYS:H	1:A:19:GLN:HG2	7	0.12
(1,370)	1:A:17:LYS:H	1:A:19:GLN:HG2	13	0.12
(1,370)	1:A:17:LYS:H	1:A:19:GLN:HG2	14	0.12
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	7	0.12
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	8	0.12
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	9	0.12
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	15	0.12
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	16	0.12
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	3	0.12
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	19	0.12
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	16	0.12
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	16	0.12
(1,289)	1:A:14:GLU:HG3	1:A:15:LYS:HA	13	0.12
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	13	0.12
(1,28)	1:A:3:LYS:H	1:A:3:LYS:HE3	8	0.12
(1,20)	1:A:2:PHE:HB3	1:A:3:LYS:H	5	0.12
(1,20)	1:A:2:PHE:HB3	1:A:3:LYS:H	8	0.12
(1,20)	1:A:2:PHE:HB3	1:A:3:LYS:H	10	0.12
(1,2)	1:A:1:ASP:HA	1:A:3:LYS:H	14	0.12
(1,1874)	1:B:120:LEU:HD11	1:A:20:LEU:HG	20	0.12
(1,1874)	1:B:120:LEU:HD12	1:A:20:LEU:HG	20	0.12
(1,1874)	1:B:120:LEU:HD13	1:A:20:LEU:HG	20	0.12
(1,1874)	1:B:120:LEU:HD21	1:A:20:LEU:HG	20	0.12
(1,1874)	1:B:120:LEU:HD22	1:A:20:LEU:HG	20	0.12
(1,1874)	1:B:120:LEU:HD23	1:A:20:LEU:HG	20	0.12
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	9	0.12
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	9	0.12
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	13	0.12
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	13	0.12
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE1	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:B:109:ILE:H	1:A:6:TYR:HE2	16	0.12
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	3	0.12
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	3	0.12
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	6	0.12
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	6	0.12
(1,1816)	1:B:105:LEU:HD21	1:A:6:TYR:HE1	19	0.12
(1,1816)	1:B:105:LEU:HD21	1:A:6:TYR:HE2	19	0.12
(1,1816)	1:B:105:LEU:HD22	1:A:6:TYR:HE1	19	0.12
(1,1816)	1:B:105:LEU:HD22	1:A:6:TYR:HE2	19	0.12
(1,1816)	1:B:105:LEU:HD23	1:A:6:TYR:HE1	19	0.12
(1,1816)	1:B:105:LEU:HD23	1:A:6:TYR:HE2	19	0.12
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD11	10	0.12
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD12	10	0.12
(1,1812)	1:B:105:LEU:HD21	1:A:5:LEU:HD13	10	0.12
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD11	10	0.12
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD12	10	0.12
(1,1812)	1:B:105:LEU:HD22	1:A:5:LEU:HD13	10	0.12
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD11	10	0.12
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD12	10	0.12
(1,1812)	1:B:105:LEU:HD23	1:A:5:LEU:HD13	10	0.12
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE1	10	0.12
(1,1800)	1:B:102:PHE:HD1	1:A:2:PHE:HE2	10	0.12
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE1	10	0.12
(1,1800)	1:B:102:PHE:HD2	1:A:2:PHE:HE2	10	0.12
(1,1768)	1:A:30:LEU:HB2	1:B:130:LEU:HG	19	0.12
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	10	0.12
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	15	0.12
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	1	0.12
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	1	0.12
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	1	0.12
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	1	0.12
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	1	0.12
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	1	0.12
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	5	0.12
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	5	0.12
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	5	0.12
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	5	0.12
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	5	0.12
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	5	0.12
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	12	0.12
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	12	0.12
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	12	0.12
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	12	0.12
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	12	0.12
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	11	0.12
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	11	0.12
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE1	3	0.12
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE2	3	0.12
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE1	11	0.12
(1,1664)	1:A:2:PHE:H	1:B:102:PHE:HE2	11	0.12
(1,1659)	1:B:144:PHE:H	1:B:144:PHE:HB2	16	0.12
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	7	0.12
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	14	0.12
(1,1573)	1:B:138:THR:H	1:B:139:GLN:HG2	15	0.12
(1,1573)	1:B:138:THR:H	1:B:139:GLN:HG3	15	0.12
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	8	0.12
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	6	0.12
(1,148)	1:A:7:GLU:HB2	1:A:8:GLN:HE21	18	0.12
(1,14)	1:A:2:PHE:HA	1:A:4:LYS:HG3	19	0.12
(1,1353)	1:B:125:MET:H	1:B:125:MET:HG3	11	0.12
(1,128)	1:A:7:GLU:H	1:A:7:GLU:HB2	7	0.12
(1,128)	1:A:7:GLU:H	1:A:7:GLU:HB2	17	0.12
(1,126)	1:A:6:TYR:HA	1:A:9:ILE:HB	11	0.12
(1,126)	1:A:6:TYR:HA	1:A:9:ILE:HB	18	0.12
(1,1256)	1:B:119:GLN:HG2	1:B:120:LEU:H	11	0.12
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	1	0.12
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	19	0.12
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG2	5	0.12
(1,1088)	1:B:112:GLU:HG2	1:B:115:LYS:HG3	5	0.12
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG2	5	0.12
(1,1088)	1:B:112:GLU:HG3	1:B:115:LYS:HG3	5	0.12
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	15	0.12
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	15	0.12
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	15	0.12
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	18	0.12
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	18	0.12
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	18	0.12
(2,97)	1:A:17:LYS:O	1:A:21:HIS:H	1	0.11
(2,79)	1:A:8:GLN:O	1:A:12:GLU:H	13	0.11
(2,7)	1:A:5:LEU:O	1:A:9:ILE:H	2	0.11
(2,68)	1:A:2:PHE:O	1:A:6:TYR:N	4	0.11
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	9	0.11
(2,66)	1:A:34:LEU:O	1:A:38:THR:N	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	1	0.11
(2,63)	1:A:33:GLN:O	1:A:37:ALA:H	20	0.11
(2,59)	1:A:31:LYS:O	1:A:35:GLU:H	1	0.11
(2,31)	1:A:17:LYS:O	1:A:21:HIS:H	1	0.11
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	9	0.11
(2,132)	1:A:34:LEU:O	1:A:38:THR:N	10	0.11
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	1	0.11
(2,129)	1:A:33:GLN:O	1:A:37:ALA:H	20	0.11
(2,125)	1:A:31:LYS:O	1:A:35:GLU:H	1	0.11
(1,984)	1:B:107:GLU:HB3	1:B:108:GLN:HE21	18	0.11
(1,983)	1:B:107:GLU:HB3	1:B:108:GLN:H	13	0.11
(1,968)	1:B:107:GLU:HA	1:B:110:LEU:HB3	15	0.11
(1,907)	1:A:4:LYS:HG2	1:A:5:LEU:H	3	0.11
(1,892)	1:A:4:LYS:H	1:A:4:LYS:HG2	10	0.11
(1,892)	1:A:4:LYS:H	1:A:4:LYS:HG2	11	0.11
(1,836)	1:A:1:ASP:HB2	1:A:2:PHE:H	7	0.11
(1,828)	1:A:44:PHE:H	1:A:44:PHE:HB2	15	0.11
(1,819)	1:A:43:ARG:H	1:A:43:ARG:HG2	15	0.11
(1,819)	1:A:43:ARG:H	1:A:43:ARG:HG3	15	0.11
(1,805)	1:A:41:GLN:HG2	1:A:43:ARG:HG2	20	0.11
(1,805)	1:A:41:GLN:HG2	1:A:43:ARG:HG3	20	0.11
(1,805)	1:A:41:GLN:HG3	1:A:43:ARG:HG2	20	0.11
(1,805)	1:A:41:GLN:HG3	1:A:43:ARG:HG3	20	0.11
(1,804)	1:A:41:GLN:HG2	1:A:43:ARG:HD2	14	0.11
(1,804)	1:A:41:GLN:HG2	1:A:43:ARG:HD3	14	0.11
(1,804)	1:A:41:GLN:HG3	1:A:43:ARG:HD2	14	0.11
(1,804)	1:A:41:GLN:HG3	1:A:43:ARG:HD3	14	0.11
(1,799)	1:A:41:GLN:HG2	1:A:42:GLU:H	13	0.11
(1,799)	1:A:41:GLN:HG3	1:A:42:GLU:H	13	0.11
(1,776)	1:A:40:ARG:HG2	1:A:41:GLN:H	20	0.11
(1,776)	1:A:40:ARG:HG3	1:A:41:GLN:H	20	0.11
(1,76)	1:A:4:LYS:HG2	1:A:5:LEU:H	3	0.11
(1,751)	1:A:39:GLN:H	1:A:40:ARG:H	5	0.11
(1,751)	1:A:39:GLN:H	1:A:40:ARG:H	10	0.11
(1,751)	1:A:39:GLN:H	1:A:40:ARG:H	16	0.11
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG2	9	0.11
(1,746)	1:A:38:THR:HG21	1:A:39:GLN:HG3	9	0.11
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG2	9	0.11
(1,746)	1:A:38:THR:HG22	1:A:39:GLN:HG3	9	0.11
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG2	9	0.11
(1,746)	1:A:38:THR:HG23	1:A:39:GLN:HG3	9	0.11
(1,699)	1:A:34:LEU:HG	1:A:35:GLU:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:A:4:LYS:H	1:A:4:LYS:HG2	10	0.11
(1,61)	1:A:4:LYS:H	1:A:4:LYS:HG2	11	0.11
(1,560)	1:A:27:LEU:HB2	1:A:27:LEU:HG	1	0.11
(1,560)	1:A:27:LEU:HB2	1:A:27:LEU:HG	15	0.11
(1,560)	1:A:27:LEU:HB2	1:A:27:LEU:HG	20	0.11
(1,551)	1:A:27:LEU:H	1:A:27:LEU:HB3	11	0.11
(1,5)	1:A:1:ASP:HB2	1:A:2:PHE:H	7	0.11
(1,48)	1:A:3:LYS:HD3	1:A:4:LYS:H	15	0.11
(1,46)	1:A:3:LYS:HD2	1:A:4:LYS:HG2	11	0.11
(1,459)	1:A:21:HIS:H	1:A:24:ASN:HD21	14	0.11
(1,425)	1:A:19:GLN:HG2	1:A:20:LEU:H	2	0.11
(1,394)	1:A:18:ALA:H	1:A:19:GLN:HG2	9	0.11
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	1	0.11
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	3	0.11
(1,363)	1:A:17:LYS:H	1:A:17:LYS:HE2	20	0.11
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	12	0.11
(1,337)	1:A:16:LEU:HA	1:A:16:LEU:HG	20	0.11
(1,322)	1:A:15:LYS:HE2	1:A:19:GLN:HE21	1	0.11
(1,322)	1:A:15:LYS:HE3	1:A:19:GLN:HE21	1	0.11
(1,288)	1:A:14:GLU:HG3	1:A:15:LYS:H	3	0.11
(1,288)	1:A:14:GLU:HG3	1:A:15:LYS:H	8	0.11
(1,288)	1:A:14:GLU:HG3	1:A:15:LYS:H	11	0.11
(1,286)	1:A:14:GLU:HG2	1:A:15:LYS:HA	5	0.11
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	10	0.11
(1,285)	1:A:14:GLU:HG2	1:A:15:LYS:H	20	0.11
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG2	20	0.11
(1,257)	1:A:12:GLU:HG2	1:A:15:LYS:HG3	20	0.11
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG2	20	0.11
(1,257)	1:A:12:GLU:HG3	1:A:15:LYS:HG3	20	0.11
(1,20)	1:A:2:PHE:HB3	1:A:3:LYS:H	11	0.11
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB2	3	0.11
(1,1932)	1:A:41:GLN:HE22	1:B:140:ARG:HB3	3	0.11
(1,1924)	1:A:41:GLN:HE21	1:B:141:GLN:HE22	5	0.11
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD11	9	0.11
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD12	9	0.11
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD13	9	0.11
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD21	9	0.11
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD22	9	0.11
(1,1906)	1:B:133:GLN:HB2	1:A:34:LEU:HD23	9	0.11
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD11	9	0.11
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD12	9	0.11
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD13	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD21	9	0.11
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD22	9	0.11
(1,1906)	1:B:133:GLN:HB3	1:A:34:LEU:HD23	9	0.11
(1,1895)	1:B:127:LEU:H	1:A:27:LEU:HD11	6	0.11
(1,1895)	1:B:127:LEU:H	1:A:27:LEU:HD12	6	0.11
(1,1895)	1:B:127:LEU:H	1:A:27:LEU:HD13	6	0.11
(1,1895)	1:B:127:LEU:H	1:A:27:LEU:HD21	6	0.11
(1,1895)	1:B:127:LEU:H	1:A:27:LEU:HD22	6	0.11
(1,1895)	1:B:127:LEU:H	1:A:27:LEU:HD23	6	0.11
(1,1883)	1:B:123:THR:HG21	1:A:24:ASN:HB3	17	0.11
(1,1883)	1:B:123:THR:HG22	1:A:24:ASN:HB3	17	0.11
(1,1883)	1:B:123:THR:HG23	1:A:24:ASN:HB3	17	0.11
(1,1883)	1:B:123:THR:HG21	1:A:24:ASN:HB3	18	0.11
(1,1883)	1:B:123:THR:HG22	1:A:24:ASN:HB3	18	0.11
(1,1883)	1:B:123:THR:HG23	1:A:24:ASN:HB3	18	0.11
(1,1873)	1:B:120:LEU:HD11	1:A:19:GLN:HB2	11	0.11
(1,1873)	1:B:120:LEU:HD11	1:A:19:GLN:HB3	11	0.11
(1,1873)	1:B:120:LEU:HD12	1:A:19:GLN:HB2	11	0.11
(1,1873)	1:B:120:LEU:HD12	1:A:19:GLN:HB3	11	0.11
(1,1873)	1:B:120:LEU:HD13	1:A:19:GLN:HB2	11	0.11
(1,1873)	1:B:120:LEU:HD13	1:A:19:GLN:HB3	11	0.11
(1,1873)	1:B:120:LEU:HD21	1:A:19:GLN:HB2	11	0.11
(1,1873)	1:B:120:LEU:HD21	1:A:19:GLN:HB3	11	0.11
(1,1873)	1:B:120:LEU:HD22	1:A:19:GLN:HB2	11	0.11
(1,1873)	1:B:120:LEU:HD22	1:A:19:GLN:HB3	11	0.11
(1,1873)	1:B:120:LEU:HD23	1:A:19:GLN:HB2	11	0.11
(1,1873)	1:B:120:LEU:HD23	1:A:19:GLN:HB3	11	0.11
(1,1873)	1:B:120:LEU:HD11	1:A:19:GLN:HB2	12	0.11
(1,1873)	1:B:120:LEU:HD11	1:A:19:GLN:HB3	12	0.11
(1,1873)	1:B:120:LEU:HD12	1:A:19:GLN:HB2	12	0.11
(1,1873)	1:B:120:LEU:HD12	1:A:19:GLN:HB3	12	0.11
(1,1873)	1:B:120:LEU:HD13	1:A:19:GLN:HB2	12	0.11
(1,1873)	1:B:120:LEU:HD13	1:A:19:GLN:HB3	12	0.11
(1,1873)	1:B:120:LEU:HD21	1:A:19:GLN:HB2	12	0.11
(1,1873)	1:B:120:LEU:HD21	1:A:19:GLN:HB3	12	0.11
(1,1873)	1:B:120:LEU:HD22	1:A:19:GLN:HB2	12	0.11
(1,1873)	1:B:120:LEU:HD22	1:A:19:GLN:HB3	12	0.11
(1,1873)	1:B:120:LEU:HD23	1:A:19:GLN:HB2	12	0.11
(1,1873)	1:B:120:LEU:HD23	1:A:19:GLN:HB3	12	0.11
(1,1864)	1:B:119:GLN:HE22	1:A:19:GLN:HE21	14	0.11
(1,185)	1:A:9:ILE:H	1:A:9:ILE:HB	5	0.11
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE1	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1818)	1:B:106:TYR:H	1:A:2:PHE:HE2	16	0.11
(1,1791)	1:A:37:ALA:HB1	1:B:137:ALA:HA	6	0.11
(1,1791)	1:A:37:ALA:HB2	1:B:137:ALA:HA	6	0.11
(1,1791)	1:A:37:ALA:HB3	1:B:137:ALA:HA	6	0.11
(1,1789)	1:A:37:ALA:HB1	1:B:134:LEU:HA	17	0.11
(1,1789)	1:A:37:ALA:HB2	1:B:134:LEU:HA	17	0.11
(1,1789)	1:A:37:ALA:HB3	1:B:134:LEU:HA	17	0.11
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD11	8	0.11
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD12	8	0.11
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD13	8	0.11
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD21	8	0.11
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD22	8	0.11
(1,1787)	1:A:37:ALA:H	1:B:134:LEU:HD23	8	0.11
(1,1786)	1:A:34:LEU:HD11	1:B:138:THR:HG21	9	0.11
(1,1786)	1:A:34:LEU:HD11	1:B:138:THR:HG22	9	0.11
(1,1786)	1:A:34:LEU:HD11	1:B:138:THR:HG23	9	0.11
(1,1786)	1:A:34:LEU:HD12	1:B:138:THR:HG21	9	0.11
(1,1786)	1:A:34:LEU:HD12	1:B:138:THR:HG22	9	0.11
(1,1786)	1:A:34:LEU:HD12	1:B:138:THR:HG23	9	0.11
(1,1786)	1:A:34:LEU:HD13	1:B:138:THR:HG21	9	0.11
(1,1786)	1:A:34:LEU:HD13	1:B:138:THR:HG22	9	0.11
(1,1786)	1:A:34:LEU:HD13	1:B:138:THR:HG23	9	0.11
(1,1786)	1:A:34:LEU:HD21	1:B:138:THR:HG21	9	0.11
(1,1786)	1:A:34:LEU:HD21	1:B:138:THR:HG22	9	0.11
(1,1786)	1:A:34:LEU:HD21	1:B:138:THR:HG23	9	0.11
(1,1786)	1:A:34:LEU:HD22	1:B:138:THR:HG21	9	0.11
(1,1786)	1:A:34:LEU:HD22	1:B:138:THR:HG22	9	0.11
(1,1786)	1:A:34:LEU:HD22	1:B:138:THR:HG23	9	0.11
(1,1786)	1:A:34:LEU:HD23	1:B:138:THR:HG21	9	0.11
(1,1786)	1:A:34:LEU:HD23	1:B:138:THR:HG22	9	0.11
(1,1786)	1:A:34:LEU:HD23	1:B:138:THR:HG23	9	0.11
(1,1769)	1:A:30:LEU:HB3	1:B:130:LEU:HG	2	0.11
(1,1768)	1:A:30:LEU:HB2	1:B:130:LEU:HG	8	0.11
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	17	0.11
(1,1764)	1:A:27:LEU:H	1:B:127:LEU:HB2	19	0.11
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG21	9	0.11
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG22	9	0.11
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG23	9	0.11
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG21	17	0.11
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG22	17	0.11
(1,1763)	1:A:27:LEU:H	1:B:123:THR:HG23	17	0.11
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	4	0.11
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	4	0.11
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	4	0.11
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	4	0.11
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	4	0.11
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG2	9	0.11
(1,1755)	1:A:23:THR:HG21	1:B:126:GLU:HG3	9	0.11
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG2	9	0.11
(1,1755)	1:A:23:THR:HG22	1:B:126:GLU:HG3	9	0.11
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG2	9	0.11
(1,1755)	1:A:23:THR:HG23	1:B:126:GLU:HG3	9	0.11
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB1	1	0.11
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB2	1	0.11
(1,174)	1:A:8:GLN:HE22	1:A:11:ALA:HB3	1	0.11
(1,1688)	1:A:9:ILE:H	1:B:106:TYR:HD1	13	0.11
(1,1688)	1:A:9:ILE:H	1:B:106:TYR:HD2	13	0.11
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	7	0.11
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	7	0.11
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE1	14	0.11
(1,1687)	1:A:6:TYR:H	1:B:102:PHE:HE2	14	0.11
(1,1679)	1:A:5:LEU:HD21	1:B:105:LEU:HA	5	0.11
(1,1679)	1:A:5:LEU:HD22	1:B:105:LEU:HA	5	0.11
(1,1679)	1:A:5:LEU:HD23	1:B:105:LEU:HA	5	0.11
(1,1679)	1:A:5:LEU:HD21	1:B:105:LEU:HA	6	0.11
(1,1679)	1:A:5:LEU:HD22	1:B:105:LEU:HA	6	0.11
(1,1679)	1:A:5:LEU:HD23	1:B:105:LEU:HA	6	0.11
(1,1659)	1:B:144:PHE:H	1:B:144:PHE:HB2	13	0.11
(1,1631)	1:B:141:GLN:HG2	1:B:142:GLU:HA	4	0.11
(1,1631)	1:B:141:GLN:HG3	1:B:142:GLU:HA	4	0.11
(1,1593)	1:B:139:GLN:HG2	1:B:140:ARG:H	9	0.11
(1,1593)	1:B:139:GLN:HG3	1:B:140:ARG:H	9	0.11
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	10	0.11
(1,1582)	1:B:139:GLN:H	1:B:140:ARG:H	12	0.11
(1,153)	1:A:7:GLU:HB3	1:A:8:GLN:HE21	9	0.11
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	3	0.11
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	15	0.11
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	16	0.11
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	17	0.11
(1,152)	1:A:7:GLU:HB3	1:A:8:GLN:H	19	0.11
(1,1459)	1:B:131:LYS:H	1:B:131:LYS:HG2	11	0.11
(1,1459)	1:B:131:LYS:H	1:B:131:LYS:HG3	11	0.11
(1,131)	1:A:7:GLU:H	1:A:8:GLN:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,131)	1:A:7:GLU:H	1:A:8:GLN:H	10	0.11
(1,1290)	1:B:121:HIS:H	1:B:124:ASN:HD21	4	0.11
(1,126)	1:A:6:TYR:HA	1:A:9:ILE:HB	1	0.11
(1,1256)	1:B:119:GLN:HG2	1:B:120:LEU:H	1	0.11
(1,1201)	1:B:117:LYS:H	1:B:119:GLN:HG2	17	0.11
(1,1168)	1:B:116:LEU:HA	1:B:116:LEU:HG	16	0.11
(1,1119)	1:B:114:GLU:HG3	1:B:115:LYS:H	20	0.11
(1,1116)	1:B:114:GLU:HG2	1:B:115:LYS:H	1	0.11
(1,1116)	1:B:114:GLU:HG2	1:B:115:LYS:H	3	0.11
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	5	0.11
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	5	0.11
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	5	0.11
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	6	0.11
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	6	0.11
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	6	0.11
(1,1032)	1:B:109:ILE:HG21	1:B:110:LEU:H	12	0.11
(1,1032)	1:B:109:ILE:HG22	1:B:110:LEU:H	12	0.11
(1,1032)	1:B:109:ILE:HG23	1:B:110:LEU:H	12	0.11
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	12	0.11
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	12	0.11
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	12	0.11
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB1	16	0.11
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB2	16	0.11
(1,1005)	1:B:108:GLN:HE22	1:B:111:ALA:HB3	16	0.11

10 Dihedral-angle violation analysis (i)

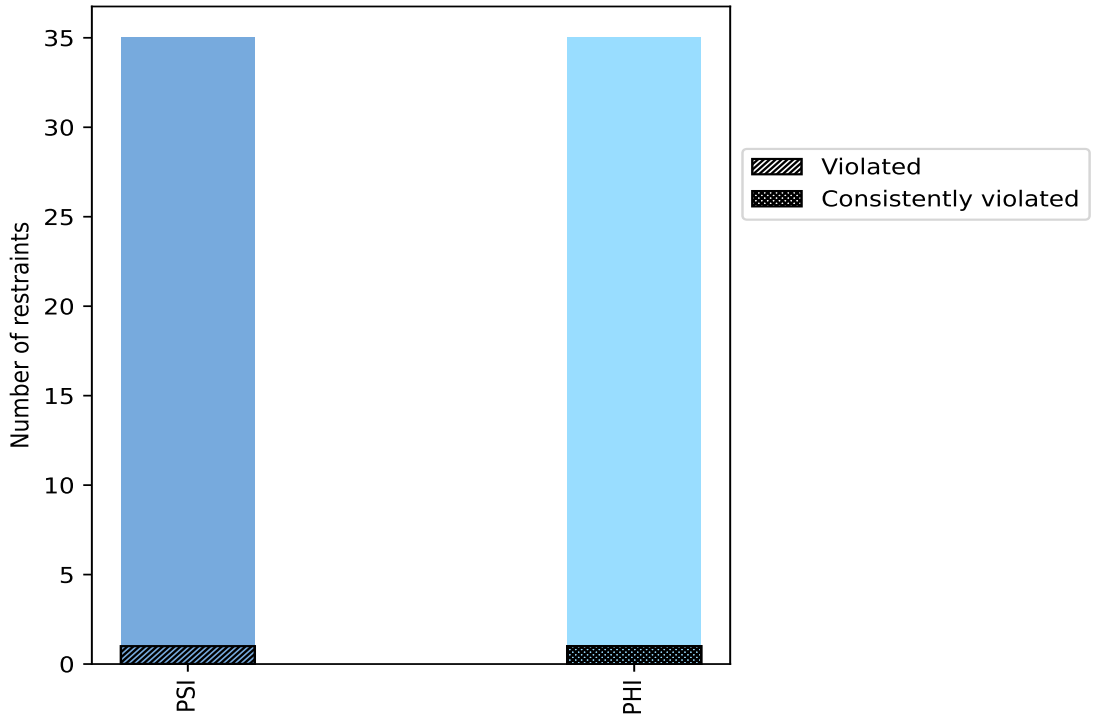
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	35	50.0	1	2.9	1.4	0	0.0	0.0
PHI	35	50.0	1	2.9	1.4	1	2.9	1.4
Total	70	100.0	2	2.9	2.9	1	1.4	1.4

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

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



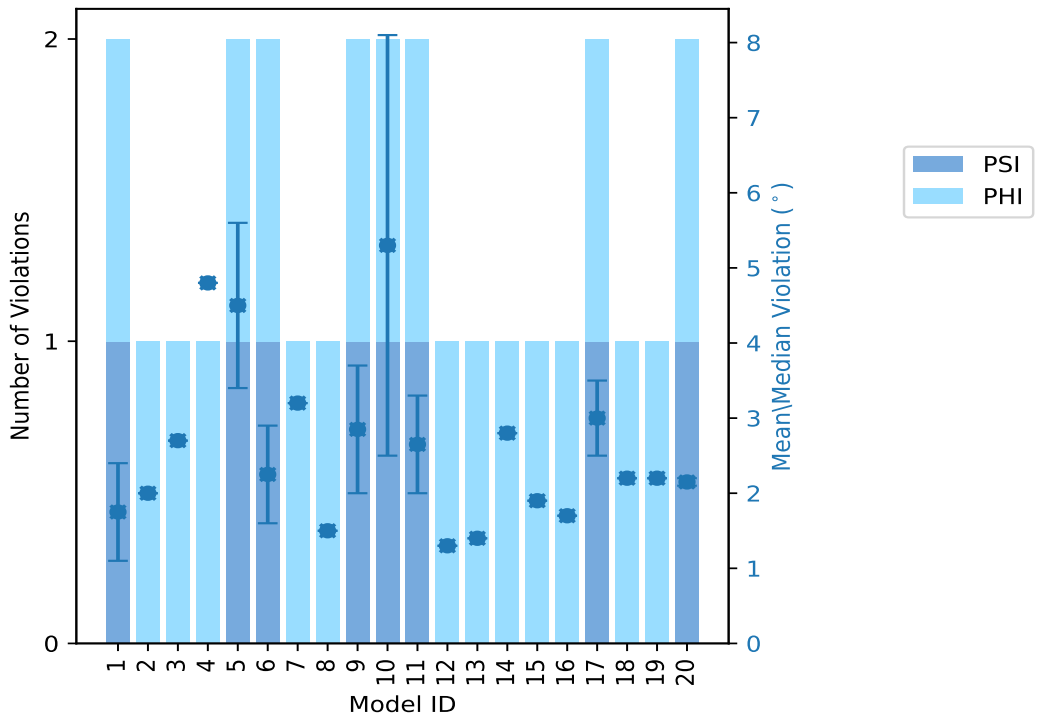
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (i)

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	1	2	1.75	2.4	0.65	1.75
2	0	1	1	2.0	2.0	0.0	2.0
3	0	1	1	2.7	2.7	0.0	2.7
4	0	1	1	4.8	4.8	0.0	4.8
5	1	1	2	4.5	5.6	1.1	4.5
6	1	1	2	2.25	2.9	0.65	2.25
7	0	1	1	3.2	3.2	0.0	3.2
8	0	1	1	1.5	1.5	0.0	1.5
9	1	1	2	2.85	3.7	0.85	2.85
10	1	1	2	5.3	8.1	2.8	5.3
11	1	1	2	2.65	3.3	0.65	2.65
12	0	1	1	1.3	1.3	0.0	1.3
13	0	1	1	1.4	1.4	0.0	1.4
14	0	1	1	2.8	2.8	0.0	2.8
15	0	1	1	1.9	1.9	0.0	1.9
16	0	1	1	1.7	1.7	0.0	1.7
17	1	1	2	3.0	3.5	0.5	3.0
18	0	1	1	2.2	2.2	0.0	2.2
19	0	1	1	2.2	2.2	0.0	2.2
20	1	1	2	2.15	2.2	0.05	2.15

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	1	5.0
0	0	0	2	10.0
0	0	0	3	15.0
0	0	0	4	20.0
0	0	0	5	25.0
0	0	0	6	30.0
0	0	0	7	35.0
1	0	1	8	40.0
0	0	0	9	45.0
0	0	0	10	50.0
0	0	0	11	55.0

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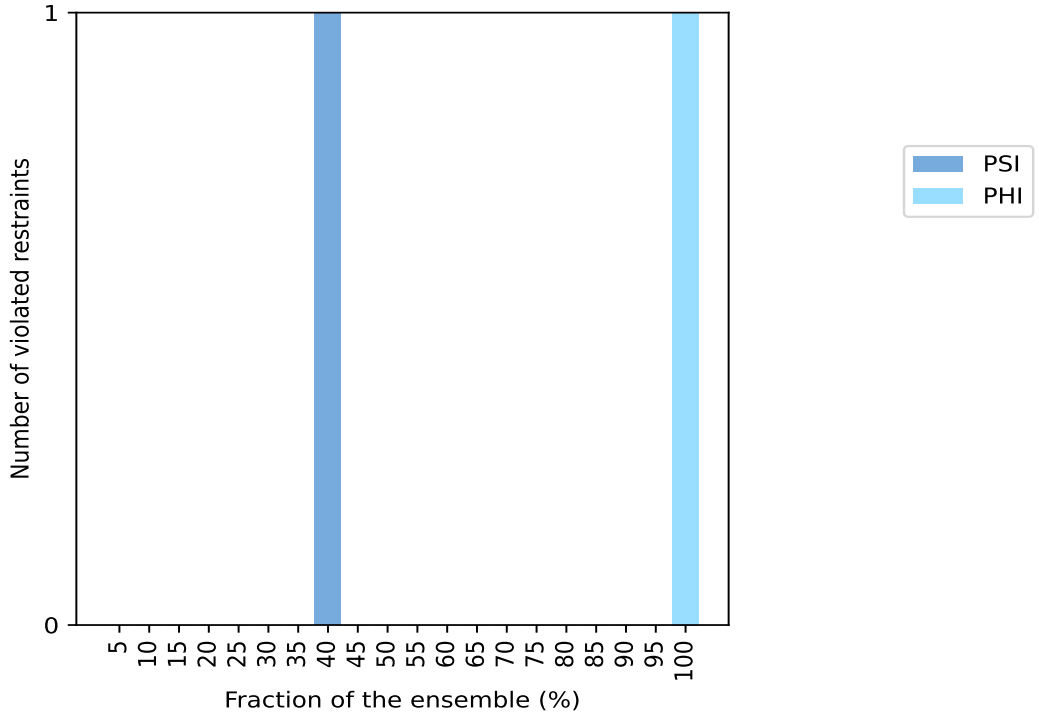
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	1	1	20	100.0

[1] Number of models with violations

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

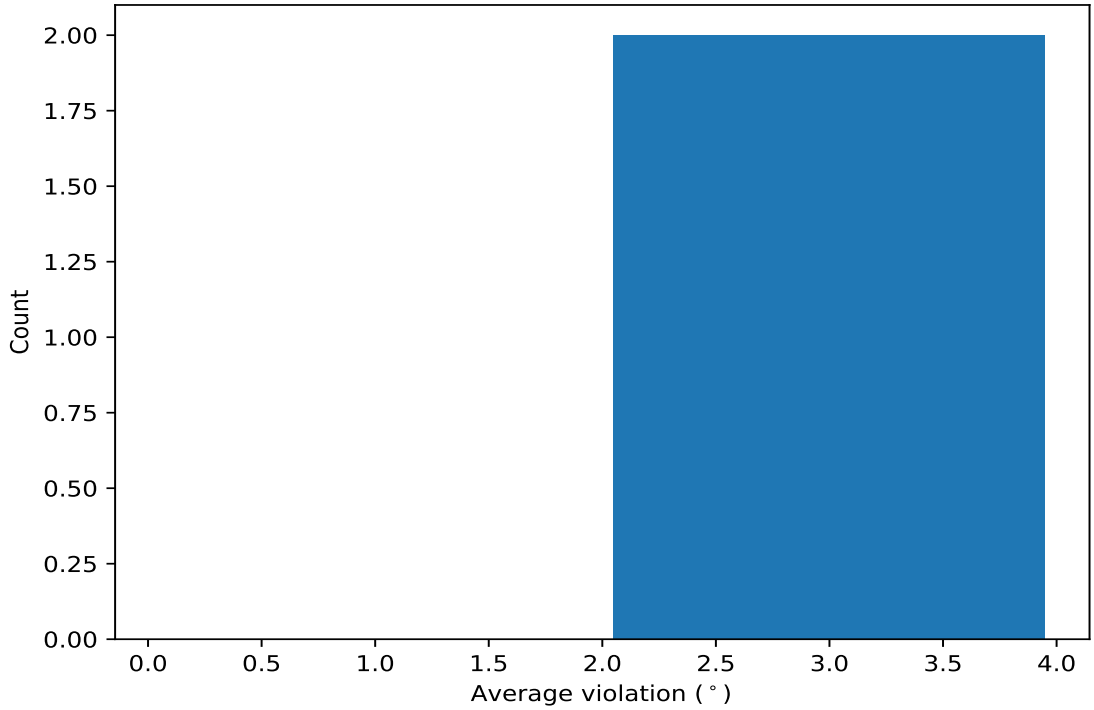


10.4 Most violated dihedral-angle restraints in the ensemble (i)

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

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

in the ensemble



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

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

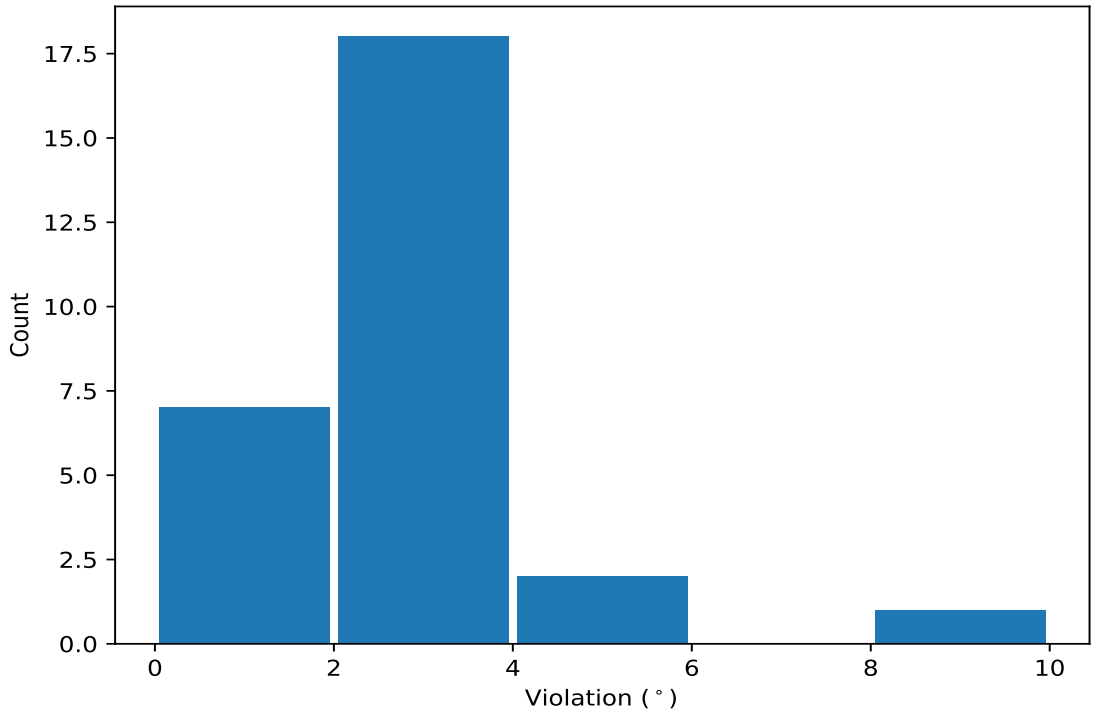
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	20	2.32	0.79	2.2
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	8	3.79	2.03	3.4

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	10	8.1
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	5	5.6
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	4	4.8
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	9	3.7
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	17	3.5
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	5	3.4
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	11	3.3
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	7	3.2
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	6	2.9
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	14	2.8
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	3	2.7
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	10	2.5
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	17	2.5
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1	2.4
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	18	2.2
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	19	2.2
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	20	2.2
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	20	2.1
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	2	2.0
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	9	2.0
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	11	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	15	1.9
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	16	1.7
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	6	1.6
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	8	1.5
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	13	1.4
(1,69)	1:A:36:LYS:C	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	12	1.3
(1,70)	1:A:37:ALA:N	1:A:37:ALA:CA	1:A:37:ALA:C	1:A:38:THR:N	1	1.1