



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:33 PM UTC

PDB ID : 6U4M / pdb_00006u4m
BMRB ID : 30658
Title : Solution structure of paxillin LIM4
Authors : Zhu, L.; Qin, J.
Deposited on : 2019-08-26

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

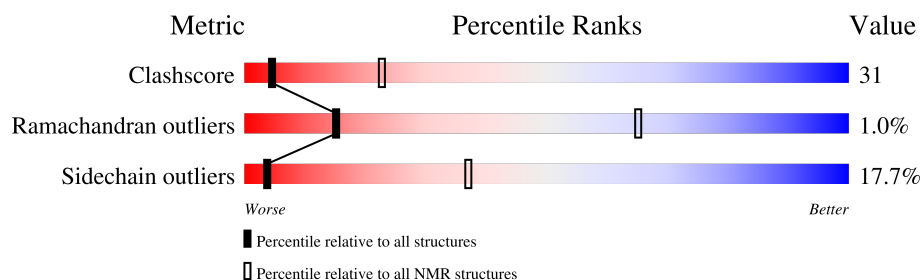
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	72	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:547-A:605 (59)	0.20	17

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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1043 atoms, of which 516 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Paxillin.

Mol	Chain	Residues	Atoms						Trace
1	A	65	Total	C	H	N	O	S	0
			1041	333	516	95	88	9	

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	GLY	-	expression tag	UNP P49023
A	535	ALA	-	expression tag	UNP P49023
A	536	MET	-	expression tag	UNP P49023
A	537	ASP	-	expression tag	UNP P49023
A	538	PRO	-	expression tag	UNP P49023
A	539	GLU	-	expression tag	UNP P49023
A	540	PHE	-	expression tag	UNP P49023

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

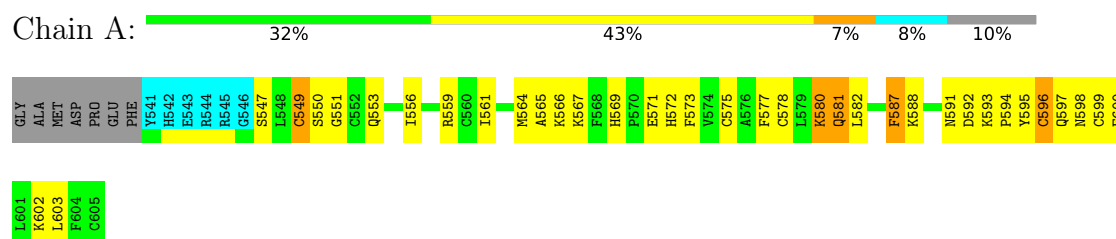
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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: Paxillin

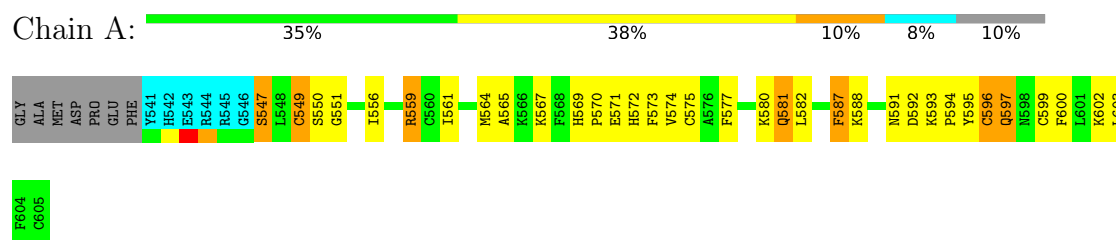


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Paxillin



4.2.2 Score per residue for model 2

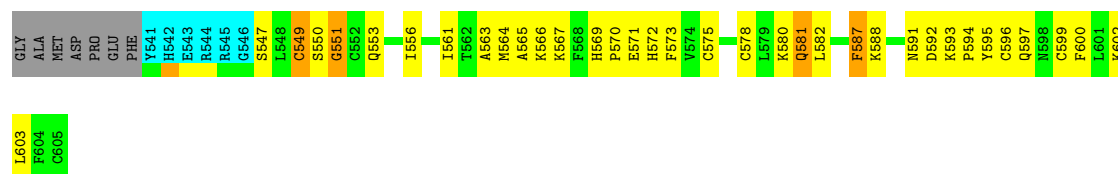
- Molecule 1: Paxillin





4.2.3 Score per residue for model 3

- Molecule 1: Paxillin



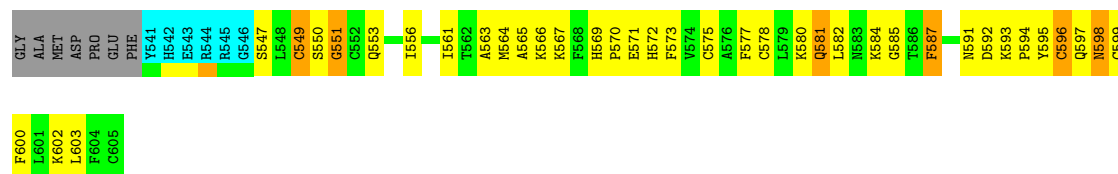
4.2.4 Score per residue for model 4

- Molecule 1: Paxillin



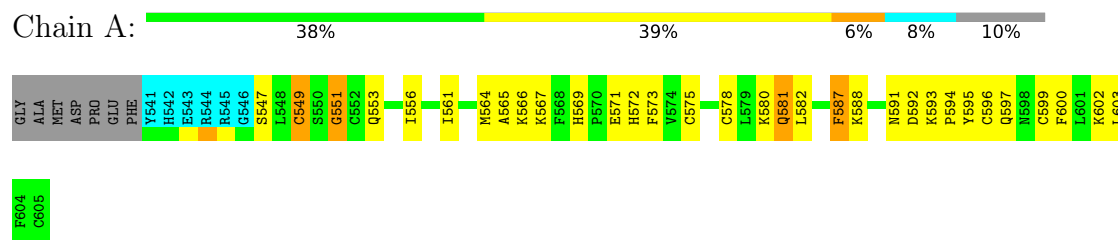
4.2.5 Score per residue for model 5

- Molecule 1: Paxillin



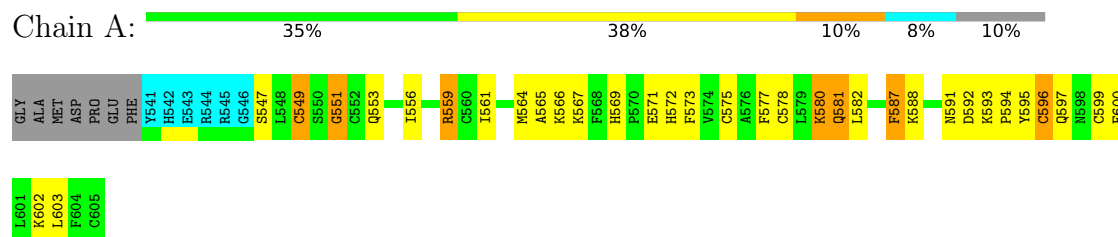
4.2.6 Score per residue for model 6

- Molecule 1: Paxillin



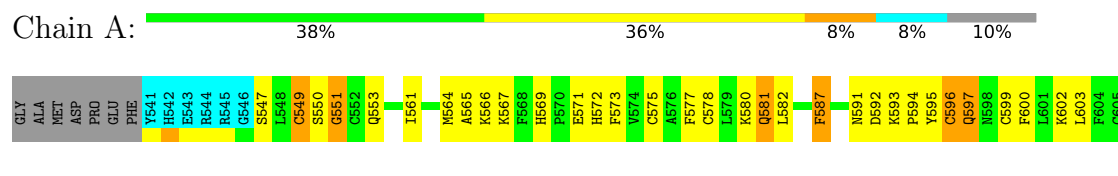
4.2.7 Score per residue for model 7

- Molecule 1: Paxillin



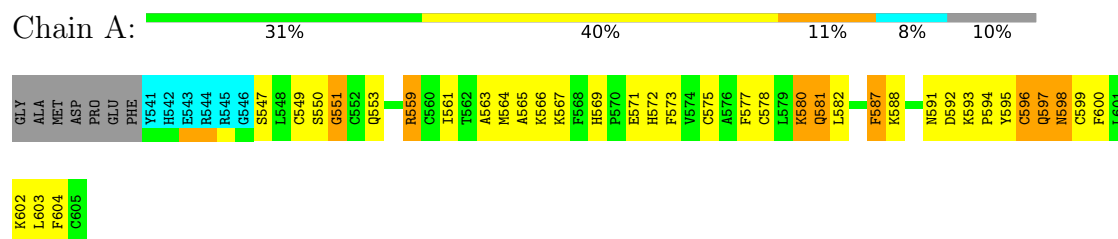
4.2.8 Score per residue for model 8

- Molecule 1: Paxillin



4.2.9 Score per residue for model 9

- Molecule 1: Paxillin



4.2.10 Score per residue for model 10

- Molecule 1: Paxillin





4.2.11 Score per residue for model 11

- Molecule 1: Paxillin

Chain A: 32% 39% 11% 8% 10%



4.2.12 Score per residue for model 12

- Molecule 1: Paxillin

Chain A: 36% 40% 6% 8% 10%



4.2.13 Score per residue for model 13

- Molecule 1: Paxillin

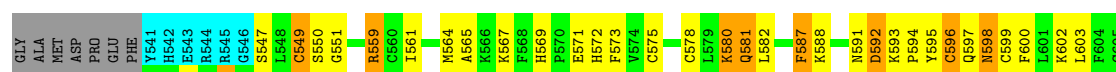
Chain A: 32% 42% 8% 8% 10%



4.2.14 Score per residue for model 14

- Molecule 1: Paxillin

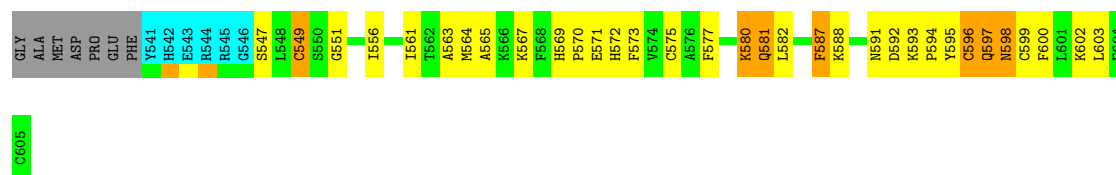
Chain A: 38% 33% 11% 8% 10%



4.2.15 Score per residue for model 15

- Molecule 1: Paxillin

Chain A: 36% 36% 10% 8% 10%



4.2.16 Score per residue for model 16

- Molecule 1: Paxillin

Chain A: 38% 38% 7% 8% 10%



4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Paxillin

Chain A: 33% 42% 7% 8% 10%



4.2.18 Score per residue for model 18

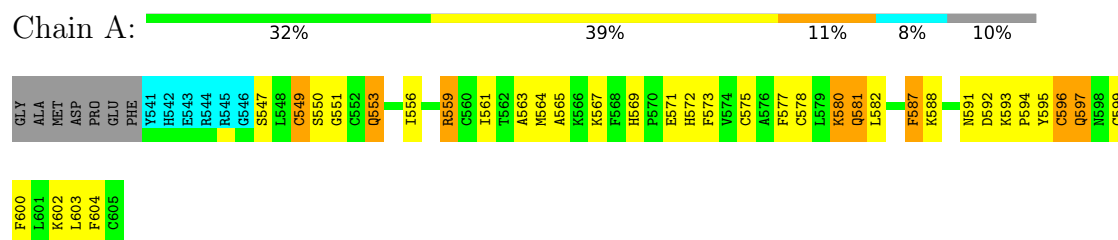
- Molecule 1: Paxillin

Chain A: 35% 35% 12% 8% 10%



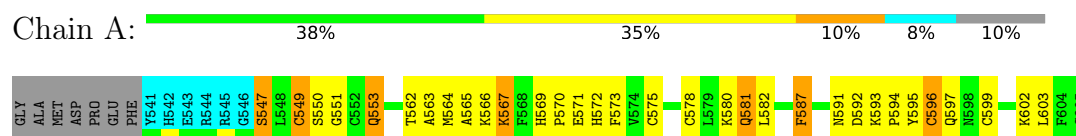
4.2.19 Score per residue for model 19

- Molecule 1: Paxillin



4.2.20 Score per residue for model 20

- Molecule 1: Paxillin



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	769
Number of shifts mapped to atoms	714
Number of unparsed shifts	0
Number of shifts with mapping errors	55
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.38±0.01	0±0/479 (0.0± 0.0%)	1.28±0.01	2±0/638 (0.3± 0.0%)
All	All	1.38	0/9580 (0.0%)	1.28	39/12760 (0.3%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	551	GLY	N-CA-C	-5.94	107.22	113.58	2	19
1	A	572	HIS	CA-CB-CG	-5.66	108.14	113.80	20	20

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	468	465	465	29±2
All	All	9400	9300	9300	578

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:582:LEU:HD11	1:A:596:CYS:HA	0.68	1.65	20	20
1:A:598:ASN:ND2	1:A:598:ASN:H	0.63	1.91	17	2
1:A:561:ILE:HG21	1:A:573:PHE:CD2	0.63	2.28	7	9
1:A:561:ILE:HG21	1:A:573:PHE:CD1	0.61	2.30	4	9
1:A:564:MET:O	1:A:565:ALA:HB3	0.58	1.98	15	20
1:A:575:CYS:HB2	1:A:596:CYS:SG	0.57	2.39	17	20
1:A:575:CYS:SG	1:A:595:TYR:HA	0.57	2.40	6	20
1:A:599:CYS:O	1:A:602:LYS:N	0.56	2.39	7	20
1:A:587:PHE:CD1	1:A:587:PHE:C	0.55	2.85	6	11
1:A:582:LEU:HD11	1:A:596:CYS:CA	0.54	2.33	20	20
1:A:587:PHE:CD2	1:A:587:PHE:C	0.53	2.87	17	3
1:A:575:CYS:HB2	1:A:582:LEU:HD13	0.52	1.82	19	18
1:A:587:PHE:C	1:A:587:PHE:CD2	0.52	2.87	16	6
1:A:598:ASN:ND2	1:A:598:ASN:C	0.52	2.68	5	1
1:A:559:ARG:NH2	1:A:559:ARG:HG2	0.51	2.20	2	4
1:A:598:ASN:C	1:A:598:ASN:ND2	0.51	2.68	14	2
1:A:591:ASN:O	1:A:592:ASP:CB	0.51	2.59	8	20
1:A:562:THR:HG23	1:A:567:LYS:HE2	0.50	1.83	20	1
1:A:580:LYS:CG	1:A:581:GLN:N	0.50	2.75	10	20
1:A:582:LEU:CD1	1:A:596:CYS:SG	0.50	3.00	2	20
1:A:559:ARG:NH2	1:A:559:ARG:CG	0.49	2.74	1	4
1:A:559:ARG:CG	1:A:559:ARG:HH21	0.48	2.22	1	5
1:A:567:LYS:N	1:A:567:LYS:CD	0.48	2.77	16	19
1:A:564:MET:O	1:A:565:ALA:CB	0.47	2.62	18	20
1:A:550:SER:N	1:A:567:LYS:O	0.47	2.46	18	15
1:A:549:CYS:HA	1:A:556:ILE:HD11	0.47	1.85	4	11
1:A:569:HIS:O	1:A:571:GLU:N	0.47	2.48	20	20
1:A:562:THR:OG1	1:A:567:LYS:NZ	0.47	2.47	20	1
1:A:584:LYS:O	1:A:585:GLY:C	0.47	2.58	18	2
1:A:587:PHE:CG	1:A:588:LYS:N	0.46	2.82	15	16
1:A:559:ARG:H	1:A:559:ARG:CD	0.46	2.22	11	1
1:A:559:ARG:CG	1:A:559:ARG:NH2	0.46	2.74	12	1
1:A:553:GLN:N	1:A:553:GLN:CD	0.46	2.74	10	6
1:A:569:HIS:C	1:A:571:GLU:N	0.46	2.74	11	20
1:A:599:CYS:O	1:A:603:LEU:HG	0.46	2.11	18	20
1:A:594:PRO:O	1:A:595:TYR:CG	0.46	2.69	2	20
1:A:569:HIS:C	1:A:571:GLU:H	0.45	2.19	20	8
1:A:584:LYS:O	1:A:586:THR:N	0.45	2.50	18	1
1:A:563:ALA:O	1:A:565:ALA:N	0.45	2.48	11	10
1:A:588:LYS:O	1:A:595:TYR:N	0.45	2.50	2	15
1:A:582:LEU:HD13	1:A:596:CYS:SG	0.45	2.52	18	1
1:A:559:ARG:HG2	1:A:559:ARG:HH21	0.44	1.72	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:575:CYS:C	1:A:577:PHE:H	0.44	2.21	8	16
1:A:551:GLY:H	1:A:553:GLN:NE2	0.44	2.11	6	7
1:A:578:CYS:SG	1:A:580:LYS:HD3	0.43	2.53	20	14
1:A:600:PHE:CD2	1:A:600:PHE:C	0.43	2.96	14	10
1:A:600:PHE:CD1	1:A:600:PHE:C	0.42	2.97	2	8
1:A:596:CYS:O	1:A:597:GLN:C	0.42	2.62	11	9
1:A:599:CYS:O	1:A:603:LEU:N	0.42	2.50	3	6
1:A:559:ARG:HH21	1:A:559:ARG:H	0.42	1.58	7	1
1:A:600:PHE:C	1:A:600:PHE:CD1	0.42	2.97	11	1
1:A:588:LYS:N	1:A:595:TYR:O	0.41	2.53	14	3
1:A:549:CYS:O	1:A:550:SER:C	0.41	2.63	3	9
1:A:580:LYS:HG3	1:A:581:GLN:N	0.41	2.31	10	1
1:A:596:CYS:O	1:A:599:CYS:N	0.41	2.54	18	3
1:A:580:LYS:CG	1:A:581:GLN:H	0.41	2.28	10	11
1:A:584:LYS:C	1:A:586:THR:N	0.41	2.79	18	1
1:A:573:PHE:C	1:A:573:PHE:CD2	0.41	2.99	20	1
1:A:595:TYR:O	1:A:596:CYS:C	0.41	2.64	17	1
1:A:600:PHE:O	1:A:604:PHE:N	0.41	2.53	19	6
1:A:564:MET:C	1:A:566:LYS:H	0.41	2.24	11	1
1:A:574:VAL:HG12	1:A:581:GLN:HA	0.41	1.92	1	1
1:A:599:CYS:O	1:A:600:PHE:C	0.41	2.64	13	2
1:A:582:LEU:HD21	1:A:587:PHE:HB2	0.41	1.93	20	1
1:A:583:ASN:O	1:A:584:LYS:C	0.41	2.64	18	1
1:A:559:ARG:HH21	1:A:559:ARG:HG2	0.40	1.76	12	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	58/72 (81%)	45±1 (78±2%)	12±1 (21±2%)	1±1 (1±1%)	15	65
All	All	1160/1440 (81%)	906 (78%)	242 (21%)	12 (1%)	15	65

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	570	PRO	7
1	A	547	SER	4
1	A	585	GLY	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	53/63 (84%)	44±1 (82±2%)	9±1 (18±2%)	4	37
All	All	1060/1260 (84%)	872 (82%)	188 (18%)	4	37

All 15 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	547	SER	20
1	A	549	CYS	20
1	A	581	GLN	20
1	A	587	PHE	20
1	A	593	LYS	20
1	A	597	GLN	20
1	A	596	CYS	16
1	A	580	LYS	13
1	A	566	LYS	12
1	A	559	ARG	10
1	A	598	ASN	8
1	A	553	GLN	6
1	A	592	ASP	1
1	A	584	LYS	1
1	A	567	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% 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

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	769
Number of shifts mapped to atoms	714
Number of unparsed shifts	0
Number of shifts with mapping errors	55
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. All 55 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	535	ALA	HA	4.112	0.03	1
1	A	535	ALA	HB1	1.265	0.03	1
1	A	535	ALA	HB2	1.265	0.03	1
1	A	535	ALA	HB3	1.265	0.03	1
1	A	535	ALA	C	177.592	0.50	1
1	A	535	ALA	CA	52.788	0.50	1
1	A	535	ALA	CB	18.966	0.50	1
1	A	536	MET	H	8.349	0.03	1
1	A	536	MET	HA	4.37	0.03	1
1	A	536	MET	HB2	1.95	0.03	2
1	A	536	MET	HB3	1.845	0.03	2
1	A	536	MET	HG2	2.427	0.03	2
1	A	536	MET	HG3	2.355	0.03	2
1	A	536	MET	C	175.441	0.50	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	536	MET	CA	54.718	0.50	1
1	A	536	MET	CB	32.15	0.50	1
1	A	536	MET	CG	32.27	0.50	1
1	A	536	MET	N	118.129	0.25	1
1	A	537	ASP	H	8.056	0.03	1
1	A	537	ASP	HA	4.718	0.03	1
1	A	537	ASP	HB2	2.634	0.03	2
1	A	537	ASP	HB3	2.461	0.03	2
1	A	537	ASP	CA	52.519	0.50	1
1	A	537	ASP	CB	40.591	0.50	1
1	A	537	ASP	N	123.081	0.25	1
1	A	538	PRO	HA	4.227	0.03	1
1	A	538	PRO	HB2	2.142	0.03	2
1	A	538	PRO	HD2	3.755	0.03	2
1	A	538	PRO	HD3	3.624	0.03	2
1	A	538	PRO	HG2	1.898	0.03	2
1	A	538	PRO	HG3	1.755	0.03	2
1	A	538	PRO	C	176.991	0.50	1
1	A	538	PRO	CA	63.553	0.50	1
1	A	538	PRO	CB	31.831	0.50	1
1	A	538	PRO	CD	50.515	0.50	1
1	A	538	PRO	CG	27.156	0.50	1
1	A	539	GLU	H	8.415	0.03	1
1	A	539	GLU	HA	3.991	0.03	1
1	A	539	GLU	HB2	1.932	0.03	2
1	A	539	GLU	HB3	1.746	0.03	2
1	A	539	GLU	HG2	2.048	0.03	2
1	A	539	GLU	HG3	1.943	0.03	2
1	A	539	GLU	C	176.251	0.50	1
1	A	539	GLU	CA	56.892	0.50	1
1	A	539	GLU	CB	29.582	0.50	1
1	A	539	GLU	CG	36.09	0.50	1
1	A	539	GLU	N	119.47	0.25	1
1	A	540	PHE	H	7.893	0.03	1
1	A	540	PHE	HA	4.443	0.03	1
1	A	540	PHE	HB2	2.898	0.03	2
1	A	540	PHE	HB3	2.848	0.03	2
1	A	540	PHE	C	175.303	0.50	1
1	A	540	PHE	CA	57.948	0.50	1
1	A	540	PHE	CB	39.638	0.50	1
1	A	540	PHE	N	119.35	0.25	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, <i>ppm</i>	Suggested action
$^{13}\text{C}_\alpha$	71	-0.00 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	67	0.31 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}'$	65	0.43 ± 0.16	None needed (< 0.5 ppm)
^{15}N	65	0.20 ± 0.37	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 660 atoms were assigned a chemical shift out of a possible 801. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	285/292 (98%)	117/118 (99%)	113/118 (96%)	55/56 (98%)
Sidechain	375/426 (88%)	248/275 (90%)	120/133 (90%)	7/18 (39%)
Aromatic	0/83 (0%)	0/42 (0%)	0/39 (0%)	0/2 (0%)
Overall	660/801 (82%)	365/435 (84%)	233/290 (80%)	62/76 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 714 atoms were assigned a chemical shift out of a possible 897. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	315/323 (98%)	129/131 (98%)	125/130 (96%)	61/62 (98%)
Sidechain	399/475 (84%)	262/305 (86%)	130/146 (89%)	7/24 (29%)
Aromatic	0/99 (0%)	0/50 (0%)	0/46 (0%)	0/3 (0%)
Overall	714/897 (80%)	391/486 (80%)	255/322 (79%)	68/89 (76%)

7.1.4 Statistically unusual chemical shifts [i](#)

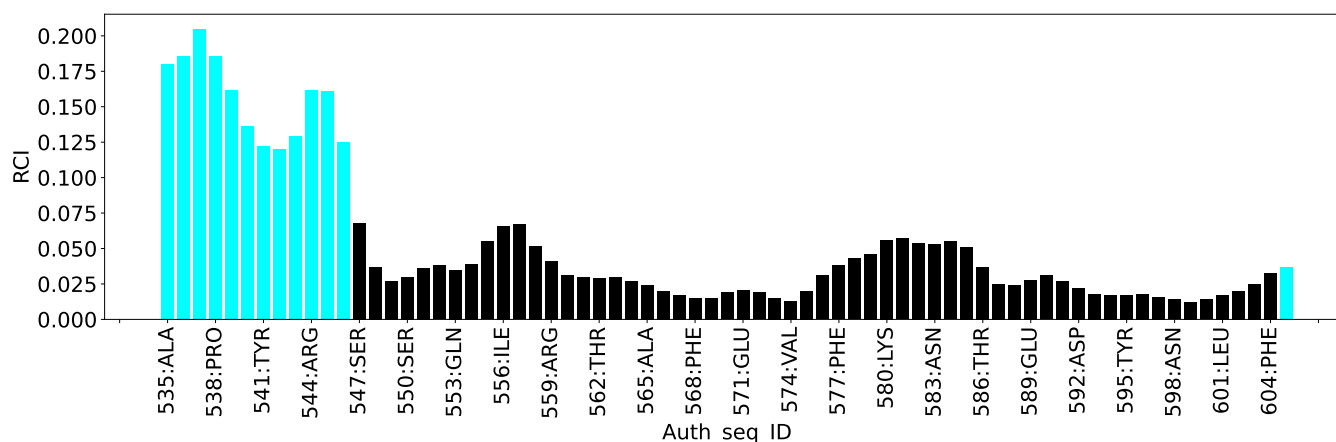
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	603	LEU	HB3	-0.48	-0.26 – 3.31	-5.6
1	A	590	GLN	HB3	0.57	0.71 – 3.33	-5.5

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	3149
Intra-residue ($ i-j =0$)	754
Sequential ($ i-j =1$)	1006
Medium range ($ i-j >1$ and $ i-j <5$)	541
Long range ($ i-j \geq 5$)	848
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	120
Number of restraints per residue	42.6
Number of long range restraints per residue ¹	11.5

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	108.7	0.2
0.2-0.5 (Medium)	156.7	0.5
>0.5 (Large)	35.4	1.87

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

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

9 Distance violation analysis ⓘ

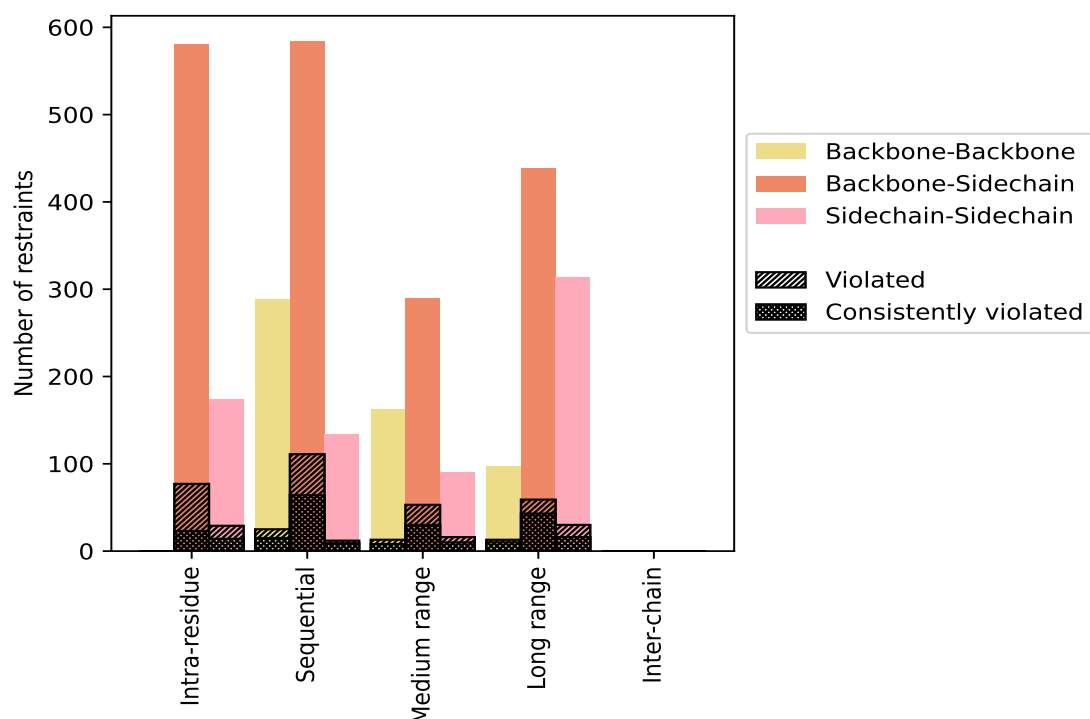
9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	754	23.9	106	14.1	3.4	37	4.9	1.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	580	18.4	77	13.3	2.4	23	4.0	0.7
Sidechain-Sidechain	174	5.5	29	16.7	0.9	14	8.0	0.4
Sequential (i-j =1)	1006	31.9	148	14.7	4.7	88	8.7	2.8
Backbone-Backbone	288	9.1	25	8.7	0.8	15	5.2	0.5
Backbone-Sidechain	584	18.5	111	19.0	3.5	64	11.0	2.0
Sidechain-Sidechain	134	4.3	12	9.0	0.4	9	6.7	0.3
Medium range (i-j >1 & i-j <5)	541	17.2	82	15.2	2.6	48	8.9	1.5
Backbone-Backbone	162	5.1	13	8.0	0.4	8	4.9	0.3
Backbone-Sidechain	289	9.2	53	18.3	1.7	30	10.4	1.0
Sidechain-Sidechain	90	2.9	16	17.8	0.5	10	11.1	0.3
Long range (i-j ≥5)	848	26.9	102	12.0	3.2	69	8.1	2.2
Backbone-Backbone	97	3.1	13	13.4	0.4	10	10.3	0.3
Backbone-Sidechain	438	13.9	59	13.5	1.9	43	9.8	1.4
Sidechain-Sidechain	313	9.9	30	9.6	1.0	16	5.1	0.5
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3149	100.0	438	13.9	13.9	242	7.7	7.7
Backbone-Backbone	547	17.4	51	9.3	1.6	33	6.0	1.0
Backbone-Sidechain	1891	60.1	300	15.9	9.5	160	8.5	5.1
Sidechain-Sidechain	711	22.6	87	12.2	2.8	49	6.9	1.6

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	54	102	58	83	0	297	0.31	1.83	0.23	0.25
2	50	111	63	83	0	307	0.32	1.8	0.27	0.26
3	51	113	58	82	0	304	0.31	1.81	0.23	0.26
4	62	113	60	83	0	318	0.29	1.58	0.2	0.24
5	52	115	63	81	0	311	0.3	1.83	0.23	0.24
6	50	113	58	84	0	305	0.3	1.8	0.23	0.25
7	60	109	63	81	0	313	0.3	1.81	0.23	0.25
8	54	103	59	82	0	298	0.31	1.8	0.23	0.25
9	56	106	62	80	0	304	0.31	1.82	0.23	0.25
10	60	105	62	85	0	312	0.32	1.8	0.26	0.25

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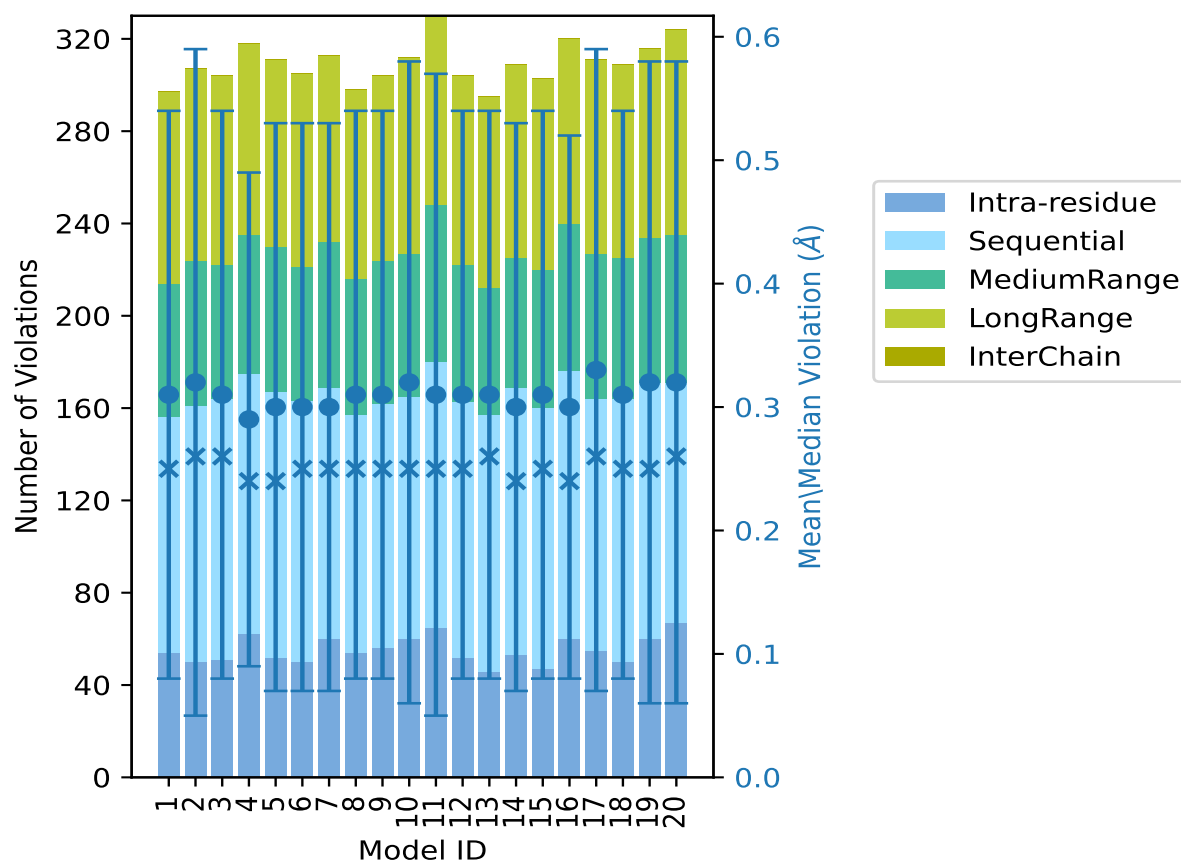
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	65	115	68	82	0	330	0.31	1.79	0.26	0.25
12	52	111	59	82	0	304	0.31	1.87	0.23	0.25
13	46	111	55	83	0	295	0.31	1.78	0.23	0.26
14	53	116	56	84	0	309	0.3	1.82	0.23	0.24
15	47	113	60	83	0	303	0.31	1.87	0.23	0.25
16	60	116	64	80	0	320	0.3	1.84	0.22	0.24
17	55	109	63	84	0	311	0.33	1.79	0.26	0.26
18	50	114	61	84	0	309	0.31	1.87	0.23	0.25
19	60	111	63	82	0	316	0.32	1.79	0.26	0.25
20	67	104	64	89	0	324	0.32	1.79	0.26	0.26

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble

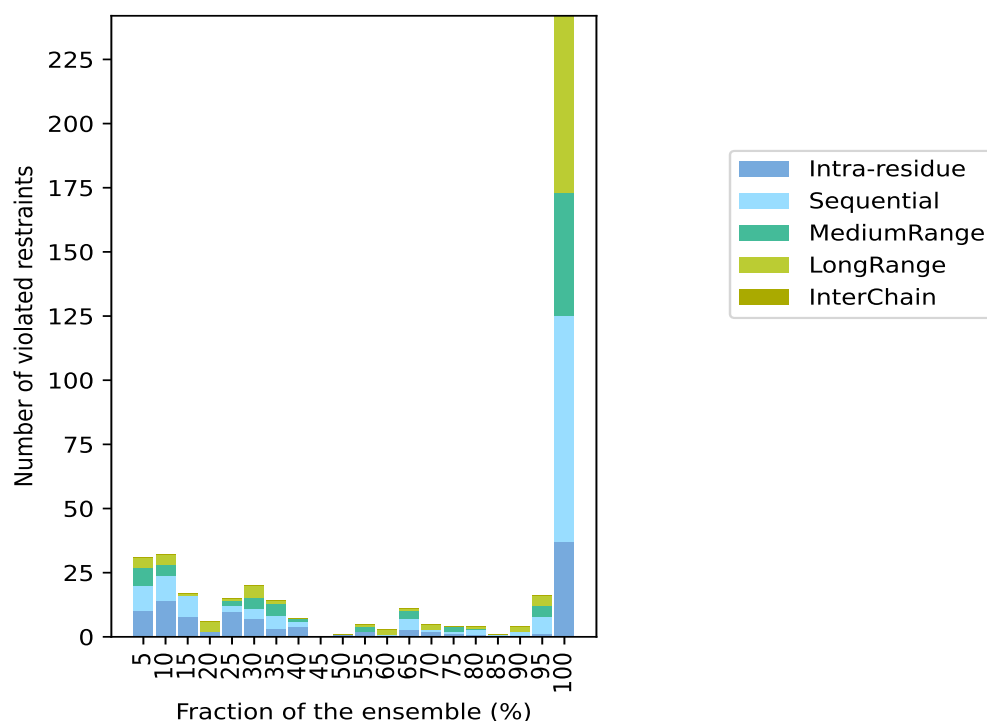
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2711(IR:648, SQ:858, MR:459, LR:746, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
10	10	7	4	0	31	1	5.0
14	10	4	4	0	32	2	10.0
8	8	0	1	0	17	3	15.0
2	0	0	4	0	6	4	20.0
10	2	2	1	0	15	5	25.0
7	4	4	5	0	20	6	30.0
3	5	5	1	0	14	7	35.0
4	2	1	0	0	7	8	40.0
0	0	0	0	0	0	9	45.0
1	0	0	0	0	1	10	50.0
2	0	2	1	0	5	11	55.0
0	1	0	2	0	3	12	60.0
3	4	3	1	0	11	13	65.0
2	1	0	2	0	5	14	70.0
1	1	2	0	0	4	15	75.0
1	2	0	1	0	4	16	80.0
0	1	0	0	0	1	17	85.0
0	2	0	2	0	4	18	90.0
1	7	4	4	0	16	19	95.0
37	88	48	69	0	242	20	100.0

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

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

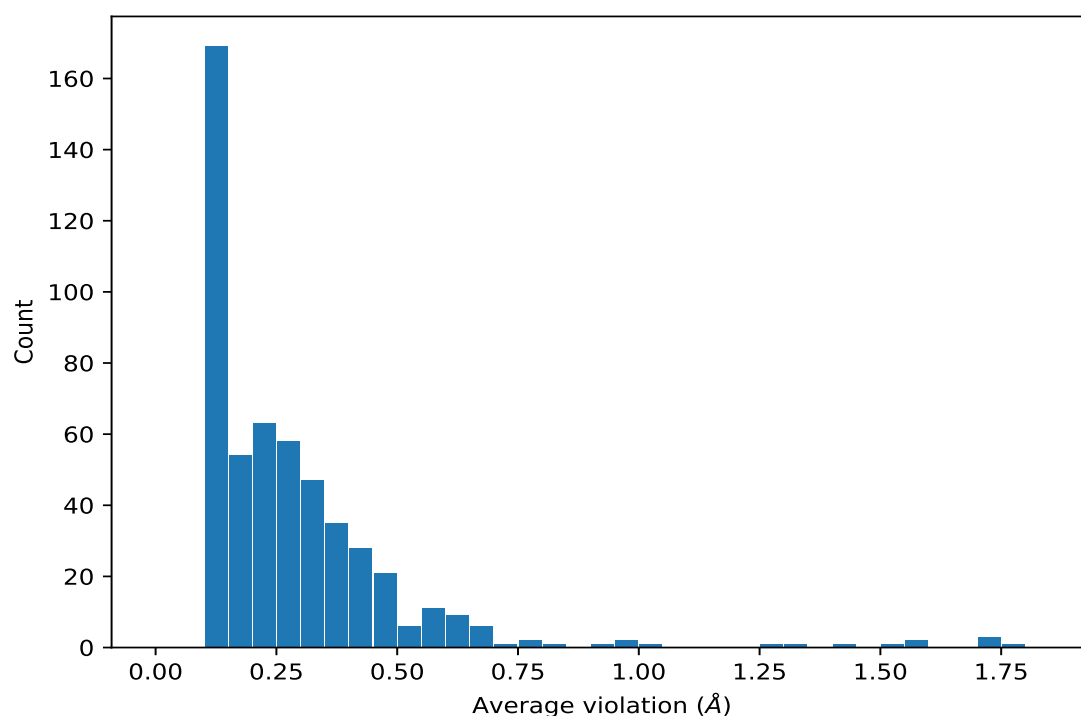
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	20	1.72	0.25	1.81
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	20	1.72	0.25	1.81
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	20	1.72	0.25	1.81
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	20	1.58	0.01	1.58
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	20	1.44	0.02	1.44
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	20	1.26	0.02	1.26
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	20	1.0	0.03	1.0
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	20	0.98	0.01	0.98
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	20	0.96	0.03	0.95
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	20	0.92	0.01	0.92
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	20	0.81	0.01	0.81
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	20	0.79	0.02	0.78
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	20	0.76	0.03	0.76
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	20	0.68	0.01	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	20	0.68	0.01	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	20	0.68	0.01	0.68

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	20	0.68	0.06	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	20	0.68	0.06	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	20	0.68	0.06	0.69
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	20	0.64	0.08	0.65
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	20	0.64	0.0	0.64
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	20	0.63	0.01	0.63
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	20	0.62	0.03	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	20	0.62	0.01	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	20	0.61	0.03	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	20	0.61	0.03	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	20	0.61	0.03	0.62
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	20	0.6	0.06	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	20	0.6	0.06	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	20	0.6	0.06	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	20	0.58	0.02	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	20	0.58	0.02	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	20	0.58	0.02	0.58
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	20	0.57	0.04	0.57
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	20	0.57	0.02	0.56
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	20	0.56	0.01	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	20	0.56	0.01	0.56
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	20	0.56	0.01	0.56
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	20	0.53	0.01	0.53
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	20	0.53	0.01	0.53
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	20	0.52	0.01	0.52
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	20	0.52	0.02	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	20	0.51	0.01	0.51
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	20	0.5	0.02	0.5
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	20	0.49	0.02	0.49
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	20	0.49	0.02	0.5
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	20	0.49	0.02	0.49
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	20	0.49	0.01	0.49
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	20	0.48	0.04	0.48
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	20	0.48	0.04	0.48
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	20	0.48	0.04	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	20	0.48	0.01	0.48
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	20	0.47	0.02	0.47
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	20	0.47	0.01	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	20	0.46	0.01	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	20	0.46	0.01	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	20	0.45	0.0	0.45
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	20	0.44	0.01	0.44

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	20	0.43	0.01	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	20	0.43	0.01	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	20	0.43	0.01	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	20	0.43	0.01	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	20	0.42	0.0	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	20	0.42	0.0	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	20	0.42	0.0	0.42
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	20	0.42	0.02	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	20	0.41	0.01	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	20	0.41	0.01	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	20	0.41	0.01	0.41
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	20	0.41	0.01	0.4
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	20	0.4	0.02	0.41
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	20	0.4	0.01	0.4
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	20	0.4	0.01	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	20	0.4	0.01	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	20	0.4	0.01	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	20	0.4	0.01	0.4
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	20	0.4	0.04	0.41
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	20	0.4	0.04	0.41
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	20	0.4	0.04	0.41
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	20	0.39	0.02	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	20	0.39	0.01	0.39
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	20	0.39	0.09	0.42
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	20	0.39	0.09	0.42
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	20	0.39	0.09	0.42
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	20	0.39	0.02	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	20	0.38	0.01	0.39
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	20	0.38	0.04	0.37
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	20	0.38	0.01	0.38
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	20	0.38	0.02	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	20	0.38	0.01	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	20	0.37	0.01	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	20	0.37	0.01	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	20	0.37	0.01	0.37
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	20	0.37	0.01	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	20	0.37	0.01	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	20	0.37	0.0	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	20	0.37	0.0	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	20	0.37	0.0	0.37
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	20	0.37	0.02	0.36
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	20	0.37	0.02	0.37

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	20	0.37	0.01	0.36
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	20	0.36	0.02	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	20	0.36	0.01	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	20	0.36	0.01	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	20	0.36	0.01	0.36
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	20	0.36	0.05	0.33
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	20	0.36	0.02	0.35
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	20	0.36	0.02	0.36
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	20	0.36	0.02	0.36
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	20	0.36	0.08	0.39
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	20	0.36	0.02	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	20	0.36	0.02	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	20	0.36	0.02	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	20	0.35	0.02	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	20	0.35	0.01	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	20	0.35	0.01	0.35
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	20	0.35	0.03	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	20	0.34	0.01	0.34
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	20	0.34	0.02	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	20	0.34	0.04	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	20	0.34	0.04	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	20	0.34	0.04	0.34
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	20	0.34	0.03	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	20	0.34	0.01	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	20	0.34	0.01	0.34
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	20	0.34	0.02	0.34
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	20	0.34	0.02	0.34
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	20	0.34	0.02	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	20	0.34	0.01	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	20	0.34	0.01	0.34
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	20	0.34	0.03	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	20	0.33	0.02	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	20	0.33	0.02	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	20	0.33	0.02	0.33
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	20	0.33	0.02	0.32
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	20	0.33	0.01	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	20	0.33	0.01	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	20	0.33	0.01	0.33
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	20	0.33	0.04	0.34
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	20	0.33	0.04	0.34
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	20	0.33	0.04	0.34
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	20	0.32	0.01	0.32

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	20	0.32	0.02	0.32
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	20	0.32	0.06	0.32
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	20	0.32	0.02	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	20	0.31	0.01	0.31
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	20	0.31	0.01	0.32
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	20	0.31	0.01	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	20	0.31	0.01	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	20	0.31	0.01	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	20	0.31	0.0	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	20	0.31	0.02	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	20	0.31	0.02	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	20	0.31	0.02	0.31
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	20	0.31	0.04	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	20	0.3	0.01	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	20	0.3	0.0	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	20	0.3	0.01	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	20	0.3	0.01	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	20	0.3	0.01	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	20	0.3	0.01	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	20	0.3	0.01	0.3
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	20	0.3	0.02	0.3
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	20	0.3	0.02	0.3
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	20	0.3	0.02	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	20	0.3	0.01	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	20	0.3	0.01	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	20	0.3	0.01	0.3
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	20	0.3	0.03	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	20	0.3	0.03	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	20	0.3	0.03	0.29
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	20	0.3	0.1	0.34
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	20	0.3	0.03	0.3
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	20	0.29	0.01	0.28
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	20	0.29	0.01	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	20	0.29	0.01	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	20	0.29	0.0	0.29
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	20	0.29	0.02	0.3
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	20	0.28	0.01	0.29
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	20	0.28	0.01	0.29
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	20	0.28	0.01	0.29
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	20	0.28	0.0	0.28
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	20	0.28	0.03	0.29
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	20	0.27	0.01	0.28

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	20	0.27	0.03	0.26
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	20	0.27	0.02	0.27
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	20	0.27	0.02	0.27
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	20	0.27	0.02	0.27
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	20	0.27	0.02	0.26
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	20	0.27	0.02	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	20	0.26	0.01	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	20	0.26	0.02	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	20	0.26	0.01	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	20	0.26	0.01	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	20	0.25	0.01	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	20	0.25	0.01	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	20	0.25	0.01	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	20	0.25	0.0	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	20	0.25	0.0	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	20	0.25	0.0	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	20	0.25	0.01	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	20	0.25	0.01	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	20	0.25	0.01	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	20	0.25	0.01	0.25
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	20	0.25	0.01	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	20	0.25	0.01	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	20	0.24	0.0	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	20	0.24	0.01	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	20	0.24	0.0	0.24
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	20	0.24	0.02	0.24
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	20	0.24	0.03	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	20	0.24	0.03	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	20	0.24	0.03	0.23
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	20	0.24	0.01	0.24
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	20	0.23	0.04	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	20	0.23	0.02	0.23
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	20	0.23	0.02	0.23
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	20	0.23	0.02	0.23
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	20	0.23	0.01	0.24
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	20	0.23	0.01	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	20	0.23	0.01	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	20	0.23	0.02	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	20	0.23	0.01	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	20	0.23	0.0	0.23
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	20	0.23	0.02	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	20	0.23	0.01	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	20	0.23	0.01	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	20	0.23	0.01	0.23
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	20	0.22	0.05	0.22
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	20	0.22	0.05	0.22
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	20	0.22	0.05	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	20	0.22	0.01	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	20	0.22	0.0	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	20	0.22	0.02	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	20	0.22	0.02	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	20	0.22	0.02	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	20	0.22	0.0	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	20	0.22	0.02	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	20	0.22	0.0	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	20	0.22	0.01	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	20	0.22	0.0	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	20	0.21	0.01	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	20	0.21	0.01	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	20	0.21	0.01	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	20	0.21	0.01	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	20	0.21	0.01	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	20	0.21	0.0	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	20	0.21	0.01	0.21
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	20	0.21	0.03	0.2
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	20	0.21	0.03	0.2
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	20	0.2	0.04	0.19
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	20	0.2	0.0	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	20	0.2	0.01	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	20	0.2	0.01	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	20	0.2	0.01	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	20	0.2	0.01	0.2
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	20	0.2	0.02	0.2
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	20	0.2	0.03	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	20	0.2	0.03	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	20	0.2	0.03	0.19
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	20	0.2	0.02	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	20	0.19	0.01	0.19
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	20	0.19	0.04	0.2
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	20	0.19	0.02	0.19
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	20	0.19	0.02	0.2
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	20	0.19	0.01	0.19
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	20	0.19	0.02	0.18
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	20	0.18	0.02	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	20	0.18	0.0	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	20	0.18	0.0	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	20	0.18	0.0	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	20	0.18	0.01	0.18
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	20	0.18	0.01	0.18
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	20	0.18	0.02	0.18
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	20	0.17	0.0	0.17
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	20	0.17	0.02	0.16
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	20	0.17	0.02	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	20	0.17	0.01	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	20	0.17	0.01	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	20	0.16	0.01	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	20	0.16	0.01	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	20	0.16	0.01	0.16
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	20	0.16	0.02	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	20	0.16	0.03	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	20	0.16	0.03	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	20	0.16	0.03	0.16
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	20	0.15	0.03	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	20	0.15	0.01	0.15
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	20	0.15	0.02	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	20	0.15	0.0	0.15
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	20	0.15	0.02	0.15
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	20	0.15	0.02	0.15
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	20	0.14	0.02	0.15
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	20	0.14	0.01	0.14
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	20	0.14	0.01	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	20	0.14	0.01	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	20	0.14	0.0	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	20	0.14	0.0	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	20	0.14	0.0	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	20	0.14	0.0	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	20	0.14	0.0	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	20	0.14	0.01	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	20	0.14	0.01	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	20	0.14	0.0	0.14
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	20	0.13	0.01	0.14
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	20	0.13	0.01	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	20	0.13	0.01	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	20	0.13	0.01	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	20	0.13	0.01	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	20	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	20	0.13	0.01	0.13
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	20	0.12	0.02	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	20	0.12	0.0	0.12
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	20	0.12	0.01	0.12
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	20	0.12	0.01	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	20	0.12	0.01	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	20	0.12	0.01	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	20	0.12	0.0	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	20	0.12	0.0	0.12
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	20	0.11	0.01	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	20	0.11	0.0	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	20	0.11	0.0	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	20	0.11	0.01	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	20	0.11	0.01	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	20	0.11	0.01	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	20	0.11	0.01	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	20	0.11	0.01	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	20	0.11	0.01	0.11
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	19	1.3	0.1	1.34
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	19	0.71	0.58	0.33
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	19	0.63	0.13	0.68
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	19	0.39	0.06	0.39
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	19	0.29	0.08	0.31
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	19	0.25	0.06	0.25
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	19	0.17	0.02	0.16
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	19	0.16	0.02	0.16
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	19	0.16	0.02	0.16
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	19	0.16	0.02	0.16
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	19	0.14	0.01	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	19	0.14	0.01	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	19	0.13	0.0	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	19	0.13	0.0	0.13
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	19	0.12	0.01	0.12
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	19	0.12	0.01	0.12
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	18	0.14	0.03	0.14
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	18	0.14	0.03	0.14
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	18	0.14	0.03	0.14
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	18	0.11	0.01	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	18	0.11	0.01	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	18	0.11	0.01	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	18	0.11	0.01	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	18	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	17	0.35	0.02	0.35
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	16	0.16	0.04	0.16
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	16	0.12	0.02	0.12
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	16	0.12	0.01	0.11
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	16	0.11	0.01	0.11
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	16	0.11	0.01	0.11
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	16	0.11	0.01	0.11
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	15	0.28	0.03	0.3
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	15	0.15	0.02	0.15
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	15	0.13	0.02	0.13
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	15	0.11	0.0	0.11
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	14	0.15	0.0	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	14	0.15	0.0	0.15
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	14	0.13	0.01	0.13
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	14	0.13	0.01	0.13
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	14	0.11	0.01	0.11
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	13	0.41	0.25	0.31
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	13	0.41	0.25	0.31
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	13	0.22	0.11	0.17
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	13	0.2	0.06	0.17
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	13	0.15	0.03	0.15
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	13	0.15	0.03	0.15
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	13	0.11	0.0	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	13	0.11	0.0	0.11
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	13	0.11	0.01	0.11
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	13	0.11	0.01	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	13	0.11	0.0	0.11
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	12	0.13	0.02	0.12
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	12	0.12	0.01	0.12
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	12	0.12	0.01	0.12
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	12	0.12	0.01	0.12
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	12	0.12	0.01	0.12
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	12	0.12	0.01	0.12
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	12	0.12	0.01	0.12
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	11	0.16	0.04	0.16
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	11	0.12	0.02	0.11
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	11	0.11	0.01	0.11
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	11	0.1	0.0	0.1
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	11	0.1	0.0	0.1
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	10	0.41	0.02	0.42
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	8	0.18	0.01	0.18
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	8	0.18	0.01	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	8	0.16	0.05	0.14
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	8	0.16	0.05	0.14
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	8	0.1	0.0	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	8	0.1	0.0	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	8	0.1	0.0	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	8	0.1	0.0	0.1
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	8	0.1	0.0	0.1
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	7	0.41	0.04	0.39
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	7	0.19	0.08	0.16
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	7	0.19	0.08	0.16
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	7	0.18	0.06	0.18
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	7	0.18	0.06	0.18
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	7	0.15	0.06	0.13
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	7	0.14	0.02	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	7	0.14	0.02	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	7	0.14	0.02	0.14
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	7	0.12	0.01	0.12
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	7	0.12	0.01	0.12
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	7	0.12	0.01	0.12
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	7	0.11	0.0	0.11
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	7	0.11	0.01	0.1
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	7	0.11	0.0	0.11
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	7	0.11	0.0	0.11
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	7	0.1	0.01	0.1
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	7	0.1	0.01	0.1
(2,244)	1:550:A:SER:HA	1:553:A:GLN:HE21	6	1.79	0.0	1.79
(2,246)	1:550:A:SER:HB2	1:553:A:GLN:HE21	6	1.58	0.02	1.58
(2,245)	1:550:A:SER:HB3	1:553:A:GLN:HE21	6	1.52	0.01	1.52
(2,165)	1:548:A:LEU:HD21	1:553:A:GLN:HE21	6	0.49	0.02	0.49
(2,165)	1:548:A:LEU:HD22	1:553:A:GLN:HE21	6	0.49	0.02	0.49
(2,165)	1:548:A:LEU:HD23	1:553:A:GLN:HE21	6	0.49	0.02	0.49
(2,1209)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	6	0.46	0.01	0.46
(1,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	6	0.34	0.25	0.18
(2,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	6	0.34	0.25	0.18
(1,297)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	6	0.18	0.0	0.18
(2,311)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	6	0.18	0.0	0.18
(1,1396)	1:598:A:ASN:HA	1:598:A:ASN:HD21	6	0.17	0.05	0.16
(2,1411)	1:598:A:ASN:HA	1:598:A:ASN:HD21	6	0.17	0.05	0.16
(1,1194)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	6	0.16	0.01	0.16
(1,67)	1:542:A:HIS:HA	1:543:A:GLU:H	6	0.15	0.02	0.16
(2,67)	1:542:A:HIS:HA	1:543:A:GLU:H	6	0.15	0.02	0.16
(1,1391)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	6	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	6	0.12	0.01	0.12
(2,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	6	0.12	0.01	0.12
(1,1072)	1:583:A:ASN:HB2	1:583:A:ASN:H	6	0.12	0.0	0.12
(1,254)	1:550:A:SER:HB2	1:567:A:LYS:H	6	0.11	0.01	0.1
(2,264)	1:550:A:SER:HB2	1:567:A:LYS:H	6	0.11	0.01	0.1
(1,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	5	0.21	0.03	0.22
(2,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	5	0.21	0.03	0.22
(1,419)	1:559:A:ARG:HA	1:559:A:ARG:HG2	5	0.19	0.01	0.19
(2,433)	1:559:A:ARG:HA	1:559:A:ARG:HG2	5	0.19	0.01	0.19
(1,430)	1:559:A:ARG:HD3	1:560:A:CYS:H	5	0.19	0.05	0.17
(2,444)	1:559:A:ARG:HD3	1:560:A:CYS:H	5	0.19	0.05	0.17
(1,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	5	0.19	0.04	0.19
(2,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	5	0.19	0.04	0.19
(1,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	5	0.16	0.02	0.16
(2,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	5	0.16	0.02	0.16
(1,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	5	0.14	0.02	0.13
(1,474)	1:561:A:ILE:HG21	1:563:A:ALA:H	5	0.11	0.0	0.11
(1,474)	1:561:A:ILE:HG22	1:563:A:ALA:H	5	0.11	0.0	0.11
(1,474)	1:561:A:ILE:HG23	1:563:A:ALA:H	5	0.11	0.0	0.11
(2,488)	1:561:A:ILE:HG21	1:563:A:ALA:H	5	0.11	0.0	0.11
(2,488)	1:561:A:ILE:HG22	1:563:A:ALA:H	5	0.11	0.0	0.11
(2,488)	1:561:A:ILE:HG23	1:563:A:ALA:H	5	0.11	0.0	0.11
(1,982)	1:581:A:GLN:HB3	1:581:A:GLN:H	5	0.1	0.0	0.1
(2,997)	1:581:A:GLN:HB3	1:581:A:GLN:H	5	0.1	0.0	0.1
(1,104)	1:547:A:SER:HB3	1:547:A:SER:H	4	0.19	0.0	0.19
(2,104)	1:547:A:SER:HB3	1:547:A:SER:H	4	0.19	0.0	0.19
(1,123)	1:547:A:SER:H	1:556:A:ILE:HB	4	0.13	0.01	0.13
(2,123)	1:547:A:SER:H	1:556:A:ILE:HB	4	0.13	0.01	0.13
(1,1188)	1:588:A:LYS:H	1:597:A:GLN:HB3	4	0.12	0.01	0.12
(1,877)	1:576:A:ALA:H	1:582:A:LEU:HB3	4	0.11	0.0	0.11
(1,424)	1:559:A:ARG:HG2	1:559:A:ARG:H	3	0.44	0.0	0.44
(2,438)	1:559:A:ARG:HG2	1:559:A:ARG:H	3	0.44	0.0	0.44
(1,420)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	3	0.15	0.0	0.15
(2,434)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	3	0.15	0.0	0.15
(1,1406)	1:598:A:ASN:HB2	1:599:A:CYS:H	3	0.14	0.0	0.14
(2,1421)	1:598:A:ASN:HB2	1:599:A:CYS:H	3	0.14	0.0	0.14
(1,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	3	0.13	0.02	0.13
(2,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	3	0.13	0.02	0.13
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG21	3	0.12	0.0	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG22	3	0.12	0.0	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG23	3	0.12	0.0	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG21	3	0.12	0.0	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG22	3	0.12	0.0	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG23	3	0.12	0.0	0.12
(2,460)	1:560:A:CYS:HA	1:570:A:PRO:HD2	3	0.12	0.01	0.11
(1,1507)	1:602:A:LYS:HG3	1:602:A:LYS:H	3	0.11	0.0	0.11
(2,1522)	1:602:A:LYS:HG3	1:602:A:LYS:H	3	0.11	0.0	0.11
(1,1132)	1:587:A:PHE:H	1:588:A:LYS:H	3	0.1	0.0	0.1
(2,1147)	1:587:A:PHE:H	1:588:A:LYS:H	3	0.1	0.0	0.1
(1,1247)	1:590:A:GLN:H	1:591:A:ASN:HB3	3	0.1	0.0	0.1
(2,1544)	1:602:A:LYS:H	1:603:A:LEU:HG	3	0.1	0.0	0.1
(1,422)	1:559:A:ARG:HG3	1:559:A:ARG:HA	2	0.49	0.0	0.49
(2,436)	1:559:A:ARG:HG3	1:559:A:ARG:HA	2	0.49	0.0	0.49
(1,1405)	1:598:A:ASN:HB3	1:599:A:CYS:H	2	0.46	0.01	0.46
(2,1420)	1:598:A:ASN:HB3	1:599:A:CYS:H	2	0.46	0.01	0.46
(1,91)	1:545:A:ARG:HB3	1:546:A:GLY:HA3	2	0.35	0.2	0.35
(2,91)	1:545:A:ARG:HB3	1:546:A:GLY:HA3	2	0.35	0.2	0.35
(1,609)	1:566:A:LYS:HA	1:566:A:LYS:HG3	2	0.3	0.0	0.3
(2,623)	1:566:A:LYS:HA	1:566:A:LYS:HG3	2	0.3	0.0	0.3
(1,90)	1:545:A:ARG:H	1:546:A:GLY:HA3	2	0.29	0.06	0.29
(2,90)	1:545:A:ARG:H	1:546:A:GLY:HA3	2	0.29	0.06	0.29
(1,82)	1:545:A:ARG:HA	1:545:A:ARG:HG3	2	0.24	0.1	0.24
(2,82)	1:545:A:ARG:HA	1:545:A:ARG:HG3	2	0.24	0.1	0.24
(1,68)	1:542:A:HIS:HB3	1:543:A:GLU:H	2	0.22	0.02	0.22
(2,68)	1:542:A:HIS:HB3	1:543:A:GLU:H	2	0.22	0.02	0.22
(1,69)	1:542:A:HIS:HB2	1:543:A:GLU:H	2	0.15	0.02	0.15
(2,69)	1:542:A:HIS:HB2	1:543:A:GLU:H	2	0.15	0.02	0.15
(1,566)	1:563:A:ALA:HA	1:566:A:LYS:HB3	2	0.15	0.0	0.15
(2,580)	1:563:A:ALA:HA	1:566:A:LYS:HB3	2	0.15	0.0	0.15
(1,83)	1:545:A:ARG:HB3	1:545:A:ARG:HD3	2	0.13	0.01	0.13
(2,83)	1:545:A:ARG:HB3	1:545:A:ARG:HD3	2	0.13	0.01	0.13
(1,418)	1:559:A:ARG:HA	1:559:A:ARG:HD3	2	0.12	0.02	0.12
(2,432)	1:559:A:ARG:HA	1:559:A:ARG:HD3	2	0.12	0.02	0.12
(1,618)	1:566:A:LYS:H	1:566:A:LYS:HE3	2	0.11	0.01	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	2	0.11	0.0	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	2	0.11	0.0	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	2	0.11	0.0	0.11
(2,632)	1:566:A:LYS:H	1:566:A:LYS:HE3	2	0.11	0.01	0.11
(2,926)	1:577:A:PHE:H	1:595:A:TYR:HA	2	0.11	0.0	0.11
(1,806)	1:574:A:VAL:HA	1:582:A:LEU:HG	2	0.11	0.0	0.11
(1,1099)	1:584:A:LYS:HB3	1:586:A:THR:H	2	0.11	0.0	0.11
(1,220)	1:549:A:CYS:H	1:568:A:PHE:HA	2	0.1	0.0	0.1
(1,1472)	1:601:A:LEU:HD21	1:601:A:LEU:HA	2	0.1	0.0	0.1
(1,1472)	1:601:A:LEU:HD22	1:601:A:LEU:HA	2	0.1	0.0	0.1

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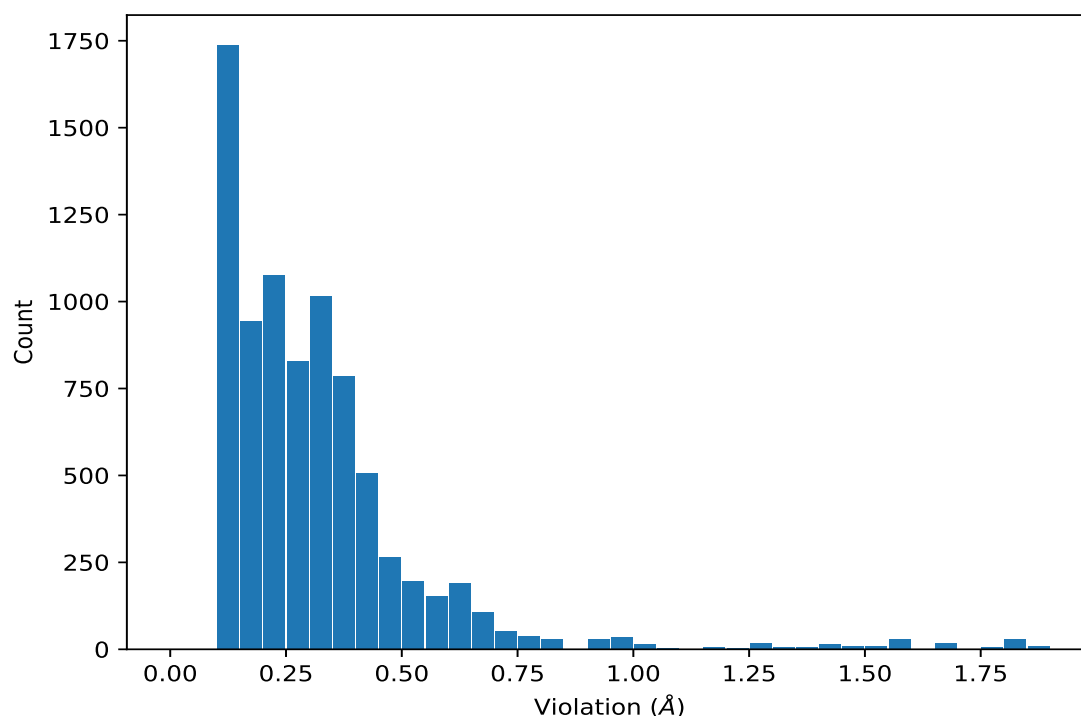
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1472)	1:601:A:LEU:HD23	1:601:A:LEU:HA	2	0.1	0.0	0.1
(2,226)	1:549:A:CYS:H	1:568:A:PHE:HA	2	0.1	0.0	0.1
(2,1487)	1:601:A:LEU:HD21	1:601:A:LEU:HA	2	0.1	0.0	0.1
(2,1487)	1:601:A:LEU:HD22	1:601:A:LEU:HA	2	0.1	0.0	0.1
(2,1487)	1:601:A:LEU:HD23	1:601:A:LEU:HA	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	12	1.87
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	12	1.87
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	12	1.87
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	15	1.87
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	15	1.87
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	15	1.87
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	18	1.87
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	18	1.87
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	18	1.87
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	16	1.84
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	16	1.84
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	16	1.84
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	1	1.83
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	1	1.83
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	1	1.83
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	5	1.83
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	5	1.83
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	5	1.83
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	9	1.82
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	9	1.82
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	9	1.82
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	14	1.82
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	14	1.82
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	14	1.82
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	3	1.81
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	3	1.81
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	3	1.81
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	7	1.81
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	7	1.81
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	7	1.81
(2,244)	1:550:A:SER:HA	1:553:A:GLN:HE21	2	1.8
(2,244)	1:550:A:SER:HA	1:553:A:GLN:HE21	10	1.8
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	6	1.8
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	6	1.8
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	6	1.8
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	8	1.8
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	8	1.8
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	8	1.8
(2,244)	1:550:A:SER:HA	1:553:A:GLN:HE21	11	1.79
(2,244)	1:550:A:SER:HA	1:553:A:GLN:HE21	17	1.79
(2,244)	1:550:A:SER:HA	1:553:A:GLN:HE21	19	1.79
(2,244)	1:550:A:SER:HA	1:553:A:GLN:HE21	20	1.79
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	13	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	13	1.78
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	13	1.78
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	2	1.69
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	2	1.69
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	2	1.69
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	19	1.67
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	19	1.67
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	19	1.67
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	10	1.66
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	10	1.66
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	10	1.66
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	17	1.66
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	17	1.66
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	17	1.66
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	20	1.66
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	20	1.66
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	20	1.66
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	11	1.65
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	11	1.65
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	11	1.65
(2,246)	1:550:A:SER:HB2	1:553:A:GLN:HE21	20	1.62
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	2	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	6	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	7	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	10	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	11	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	13	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	16	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	19	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	20	1.59
(2,246)	1:550:A:SER:HB2	1:553:A:GLN:HE21	10	1.59
(2,246)	1:550:A:SER:HB2	1:553:A:GLN:HE21	17	1.59
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	1	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	3	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	4	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	5	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	8	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	9	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	15	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	17	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	18	1.58
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	12	1.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,286)	1:551:A:GLY:HA2	1:572:A:HIS:HB2	14	1.57
(2,246)	1:550:A:SER:HB2	1:553:A:GLN:HE21	2	1.57
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	2	1.57
(2,246)	1:550:A:SER:HB2	1:553:A:GLN:HE21	19	1.56
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	20	1.56
(2,246)	1:550:A:SER:HB2	1:553:A:GLN:HE21	11	1.55
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	10	1.55
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	19	1.55
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	11	1.54
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	17	1.54
(2,245)	1:550:A:SER:HB3	1:553:A:GLN:HE21	20	1.53
(2,245)	1:550:A:SER:HB3	1:553:A:GLN:HE21	2	1.52
(2,245)	1:550:A:SER:HB3	1:553:A:GLN:HE21	10	1.52
(2,245)	1:550:A:SER:HB3	1:553:A:GLN:HE21	11	1.52
(2,245)	1:550:A:SER:HB3	1:553:A:GLN:HE21	17	1.52
(2,245)	1:550:A:SER:HB3	1:553:A:GLN:HE21	19	1.51
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	6	1.47
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	7	1.47
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	16	1.47
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	2	1.46
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	4	1.46
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	19	1.46
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	5	1.45
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	11	1.45
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	3	1.44
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	9	1.44
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	10	1.44
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	8	1.43
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	13	1.43
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	15	1.43
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	17	1.43
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	18	1.43
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	20	1.43
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	12	1.43
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	15	1.43
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	1	1.42
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	12	1.42
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	18	1.42
(2,285)	1:551:A:GLY:HA2	1:572:A:HIS:HB3	14	1.41
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	1	1.38
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	16	1.38
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	5	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	14	1.36
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	3	1.35
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	7	1.35
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	9	1.34
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	8	1.33
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	6	1.32
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	20	1.31
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	13	1.3
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	2	1.29
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	10	1.29
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	16	1.28
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	17	1.28
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	19	1.28
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	4	1.27
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	6	1.27
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	11	1.27
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	5	1.26
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	9	1.26
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	3	1.25
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	7	1.25
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	8	1.25
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	12	1.25
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	13	1.25
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	15	1.25
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	18	1.25
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	1	1.24
(2,288)	1:551:A:GLY:H	1:572:A:HIS:HB2	14	1.24
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	2	1.19
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	20	1.17
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	10	1.16
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	19	1.16
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	17	1.15
(2,166)	1:548:A:LEU:HB3	1:553:A:GLN:HE22	11	1.14
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	11	1.05
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	2	1.05
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	15	1.04
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	16	1.04
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	4	1.03
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	6	1.03
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	19	1.03
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	20	1.03
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	5	1.01
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	7	1.01
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	11	1.01
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	12	1.0
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	18	1.0
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	3	1.0
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	9	1.0
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	17	1.0
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	1	0.99
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	9	0.99
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	14	0.99
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	3	0.98
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	4	0.98
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	5	0.98
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	8	0.98
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	13	0.98
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	15	0.98
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	20	0.98
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	12	0.98
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	13	0.98
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	15	0.98
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	18	0.98
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	2	0.97
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	6	0.97
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	7	0.97
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	10	0.97
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	16	0.97
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	19	0.97
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	8	0.97
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	2	0.96
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	17	0.96
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	1	0.96
(2,287)	1:551:A:GLY:H	1:572:A:HIS:HB3	14	0.96
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	1	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	4	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	5	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	10	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	12	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	14	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	16	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	18	0.95
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	19	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	3	0.94
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	6	0.94
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	7	0.94
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	8	0.94
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	9	0.94
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	13	0.94
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	17	0.94
(2,619)	1:565:A:ALA:H	1:566:A:LYS:HB3	20	0.94
(2,303)	1:552:A:CYS:H	1:569:A:HIS:HB3	11	0.94
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	1	0.93
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	3	0.93
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	18	0.93
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	19	0.93
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	20	0.93
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	2	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	4	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	6	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	8	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	9	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	10	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	11	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	12	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	13	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	14	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	15	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	16	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	17	0.92
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	5	0.91
(2,849)	1:575:A:CYS:HB2	1:580:A:LYS:H	7	0.91
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	12	0.82
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	18	0.82
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	12	0.82
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	19	0.81
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	11	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	1	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	3	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	4	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	5	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	6	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	8	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	9	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	13	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	14	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	15	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	16	0.81
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	20	0.81
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	3	0.8
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	18	0.8
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	3	0.8
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	5	0.8
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	6	0.8
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	7	0.8
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	13	0.8
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	15	0.8
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	2	0.8
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	7	0.8
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	10	0.8
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	19	0.8
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	18	0.8
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	11	0.79
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	3	0.79
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	3	0.79
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	3	0.79
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	8	0.79
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	9	0.79
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	16	0.79
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	4	0.78
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	5	0.78
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	20	0.78
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	6	0.78
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	6	0.78
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	6	0.78
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	1	0.78
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	2	0.78
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	4	0.78
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	10	0.78
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	14	0.78
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	17	0.78
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	19	0.78
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	17	0.78
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	15	0.78
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	9	0.77
(2,304)	1:552:A:CYS:H	1:569:A:HIS:HB2	11	0.77
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	2	0.76
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	6	0.76
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	14	0.76
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	12	0.76
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	18	0.76
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	7	0.75
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	13	0.75
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	12	0.75
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	12	0.75
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	12	0.75
(2,431)	1:558:A:GLY:H	1:570:A:PRO:HG2	20	0.75
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	1	0.75
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	8	0.74
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	17	0.74
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	16	0.74
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	2	0.74
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	16	0.73
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	5	0.73
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	5	0.73
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	5	0.73
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	10	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	14	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	14	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	14	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	17	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	17	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	17	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	19	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	19	0.72
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	19	0.72
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	14	0.72
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	5	0.72
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	6	0.72
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	13	0.72
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	16	0.72
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	15	0.71
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	15	0.71
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	15	0.71
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	20	0.71
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	20	0.71
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	20	0.71
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	12	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	3	0.71
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	15	0.71
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	18	0.7
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	18	0.7
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	18	0.7
(2,1306)	1:592:A:ASP:HB2	1:593:A:LYS:HB3	15	0.7
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	3	0.7
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	3	0.7
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	3	0.7
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	2	0.7
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	2	0.7
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	2	0.7
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	7	0.7
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	7	0.7
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	7	0.7
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	3	0.7
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	9	0.7
(2,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	20	0.7
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	7	0.7
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	8	0.7
(1,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	20	0.7
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	7	0.7
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	8	0.7
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	1	0.69
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	1	0.69
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	1	0.69
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	8	0.69
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	8	0.69
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	8	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	4	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	4	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	4	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	18	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	18	0.69
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	18	0.69
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	5	0.69
(2,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	10	0.69
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	2	0.69
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	9	0.69
(1,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	10	0.69
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	2	0.69
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	9	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	2	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	2	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	2	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	3	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	3	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	3	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	4	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	4	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	4	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	5	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	5	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	5	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	7	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	7	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	7	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	9	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	9	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	9	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	10	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	10	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	10	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	11	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	11	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	11	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	13	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	13	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	13	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	14	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	14	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	14	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	17	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	17	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	17	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	19	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	19	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	19	0.68
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	6	0.68
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	6	0.68
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	6	0.68
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	16	0.68
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	16	0.68
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	16	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	7	0.68
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	8	0.68
(2,167)	1:548:A:LEU:HD11	1:553:A:GLN:HE22	4	0.68
(2,167)	1:548:A:LEU:HD12	1:553:A:GLN:HE22	4	0.68
(2,167)	1:548:A:LEU:HD13	1:553:A:GLN:HE22	4	0.68
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	6	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	6	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	6	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	12	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	12	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	12	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	16	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	16	0.67
(2,1459)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	16	0.67
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	3	0.67
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	9	0.67
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	9	0.67
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	9	0.67
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	4	0.67
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	18	0.66
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	19	0.66
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	14	0.66
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	14	0.66
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	14	0.66
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	3	0.66
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	3	0.66
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	3	0.66
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	10	0.66
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	4	0.65
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	6	0.65
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	14	0.65
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	19	0.65
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	19	0.65
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	19	0.65
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	6	0.65
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	6	0.65
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	6	0.65
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	14	0.65
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	14	0.65
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	14	0.65
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	13	0.65
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	13	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	13	0.65
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	1	0.65
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	12	0.65
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	5	0.64
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	12	0.64
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	12	0.64
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	12	0.64
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	17	0.64
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	17	0.64
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	17	0.64
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	12	0.64
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	12	0.64
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	12	0.64
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	19	0.64
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	19	0.64
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	19	0.64
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	14	0.64
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	20	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	1	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	4	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	5	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	6	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	7	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	8	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	9	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	11	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	13	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	16	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	19	0.64
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	20	0.64
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	20	0.64
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	13	0.64
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	14	0.64
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	17	0.64
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	14	0.64
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	17	0.64
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	9	0.63
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	11	0.63
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	20	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	1	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	2	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	5	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	7	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	8	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	9	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	11	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	12	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	13	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	14	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	15	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	17	0.63
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	19	0.63
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	4	0.63
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	4	0.63
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	4	0.63
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	18	0.63
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	18	0.63
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	18	0.63
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	17	0.63
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	17	0.63
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	17	0.63
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	18	0.63
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	18	0.63
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	18	0.63
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	1	0.63
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	12	0.63
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	13	0.63
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	17	0.63
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	18	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	2	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	3	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	10	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	12	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	14	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	15	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	17	0.63
(2,284)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	18	0.63
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	11	0.63
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	1	0.62
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	5	0.62
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	6	0.62
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	16	0.62
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	18	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	20	0.62
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	2	0.62
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	2	0.62
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	2	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	2	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	2	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	2	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	4	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	4	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	4	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	9	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	9	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	9	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	13	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	13	0.62
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	13	0.62
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	11	0.62
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	11	0.62
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	11	0.62
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	20	0.62
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	20	0.62
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	20	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	2	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	3	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	8	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	9	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	10	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	11	0.62
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	15	0.62
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	12	0.62
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	14	0.62
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	18	0.62
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	8	0.62
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	2	0.61
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	7	0.61
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	13	0.61
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	8	0.61
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	4	0.61
(2,1008)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	10	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	3	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	3	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	3	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	12	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	12	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	12	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	20	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	20	0.61
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	20	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	5	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	5	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	5	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	9	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	9	0.61
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	9	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	5	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	5	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	5	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	7	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	7	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	7	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	20	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	20	0.61
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	20	0.61
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	10	0.61
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	10	0.61
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	10	0.61
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	5	0.61
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	6	0.61
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	19	0.61
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	10	0.61
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	17	0.61
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	6	0.61
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	18	0.61
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	8	0.6
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	17	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	1	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	1	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	1	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	6	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	6	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	6	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	13	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	13	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	13	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	14	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	14	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	14	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	17	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	17	0.6
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	17	0.6
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	7	0.6
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	7	0.6
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	7	0.6
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	13	0.6
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	13	0.6
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	13	0.6
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	1	0.6
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	1	0.6
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	1	0.6
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	16	0.6
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	16	0.6
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	16	0.6
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	1	0.6
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	1	0.6
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	1	0.6
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	4	0.6
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	7	0.6
(2,464)	1:560:A:CYS:HA	1:570:A:PRO:HG2	16	0.6
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	1	0.6
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	14	0.6
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	16	0.59
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	10	0.59
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	15	0.59
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	15	0.59
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	15	0.59
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	19	0.59
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	19	0.59
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	19	0.59
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	8	0.59
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	8	0.59
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	8	0.59
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	11	0.59
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	13	0.59
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	10	0.58
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	1	0.58
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	11	0.58
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	20	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	5	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	5	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	5	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	9	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	9	0.58
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	9	0.58
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	16	0.58
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	16	0.58
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	16	0.58
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	18	0.58
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	18	0.58
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	18	0.58
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	18	0.58
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	19	0.58
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	8	0.58
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	9	0.58
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	1	0.58
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	12	0.58
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	14	0.58
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	7	0.58
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	13	0.58
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	12	0.57
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	6	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	4	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	4	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	4	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	8	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	8	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	8	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	10	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	10	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	10	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	11	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	11	0.57
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	11	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	8	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	8	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	8	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	10	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	10	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	15	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	15	0.57
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	15	0.57
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	1	0.57
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	7	0.57
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	8	0.57
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	13	0.57
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	1	0.57
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	6	0.57
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	7	0.57
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	13	0.57
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	17	0.57
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	2	0.57
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	3	0.57
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	5	0.57
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	8	0.57
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	9	0.57
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	13	0.57
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	15	0.57
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	18	0.57
(2,1304)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	15	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	2	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	3	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	4	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	12	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	15	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	16	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	17	0.56
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	15	0.56
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	15	0.56
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	15	0.56
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	2	0.56
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	2	0.56
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	2	0.56
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	16	0.56
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	16	0.56
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	16	0.56
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	20	0.56
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	20	0.56
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	20	0.56
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	5	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	11	0.56
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	14	0.56
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	15	0.56
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	19	0.56
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	20	0.56
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	20	0.56
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	20	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	2	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	3	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	8	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	10	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	12	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	14	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	15	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	16	0.56
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	20	0.56
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	11	0.56
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	3	0.56
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	15	0.56
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	4	0.56
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	6	0.56
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	7	0.56
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	16	0.56
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	9	0.56
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	19	0.56
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	9	0.55
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	13	0.55
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	14	0.55
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	18	0.55
(2,1149)	1:587:A:PHE:HB3	1:594:A:PRO:HA	19	0.55
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	11	0.55
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	16	0.55
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	1	0.55
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	1	0.55
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	1	0.55
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	2	0.55
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	3	0.55
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	4	0.55
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	6	0.55
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	9	0.55
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	10	0.55
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	17	0.55
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	4	0.55
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	2	0.55
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	10	0.55
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	17	0.55
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	19	0.55
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	19	0.55
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	10	0.55
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	19	0.55
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	20	0.55
(2,91)	1:545:A:ARG:HB3	1:546:A:GLY:HA3	13	0.55
(1,91)	1:545:A:ARG:HB3	1:546:A:GLY:HA3	13	0.55
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	18	0.54
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	15	0.54
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	7	0.54
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	7	0.54
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	7	0.54
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD21	15	0.54
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD22	15	0.54
(2,929)	1:577:A:PHE:HB3	1:603:A:LEU:HD23	15	0.54
(2,853)	1:575:A:CYS:HA	1:580:A:LYS:H	16	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	2	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	4	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	6	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	10	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	13	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	14	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	17	0.54
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	19	0.54
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	18	0.54
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	5	0.54
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	9	0.54
(2,296)	1:552:A:CYS:HB3	1:554:A:LYS:HD3	18	0.54
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	1	0.54
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	14	0.54
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	15	0.54
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	20	0.54
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	5	0.54
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	16	0.54
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	2	0.54
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	11	0.54
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	17	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,203)	1:549:A:CYS:HB3	1:553:A:GLN:H	20	0.54
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	20	0.53
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	10	0.53
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD21	11	0.53
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD22	11	0.53
(2,930)	1:577:A:PHE:HB2	1:603:A:LEU:HD23	11	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	1	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	3	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	5	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	8	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	9	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	11	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	12	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	15	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	16	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	18	0.53
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	20	0.53
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	20	0.53
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	7	0.53
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	7	0.53
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	7	0.53
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	14	0.53
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	14	0.53
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	14	0.53
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	3	0.53
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	12	0.53
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	13	0.53
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	6	0.53
(2,165)	1:548:A:LEU:HD21	1:553:A:GLN:HE21	2	0.53
(2,165)	1:548:A:LEU:HD22	1:553:A:GLN:HE21	2	0.53
(2,165)	1:548:A:LEU:HD23	1:553:A:GLN:HE21	2	0.53
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	1	0.52
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	2	0.52
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	4	0.52
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	17	0.52
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	18	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	2	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	4	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	9	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	13	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	14	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	15	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	16	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	18	0.52
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	19	0.52
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD11	18	0.52
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD12	18	0.52
(2,984)	1:580:A:LYS:HD3	1:582:A:LEU:HD13	18	0.52
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	8	0.52
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	8	0.52
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	8	0.52
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	10	0.52
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	10	0.52
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	10	0.52
(2,851)	1:575:A:CYS:H	1:580:A:LYS:HD3	7	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	1	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	2	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	4	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	7	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	8	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	9	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	12	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	13	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	14	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	15	0.52
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	19	0.52
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	1	0.52
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	12	0.52
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	13	0.52
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	20	0.52
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	4	0.52
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	5	0.52
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	6	0.52
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	8	0.52
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	9	0.52
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	18	0.52
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	7	0.52
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	11	0.52
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	1	0.51
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	6	0.51
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	8	0.51
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	9	0.51
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	12	0.51
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	13	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	19	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	1	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	6	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	7	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	8	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	10	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	11	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	12	0.51
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	20	0.51
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	3	0.51
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	5	0.51
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	8	0.51
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	10	0.51
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	3	0.51
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	5	0.51
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	6	0.51
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	10	0.51
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	11	0.51
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	17	0.51
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	8	0.51
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	8	0.51
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	8	0.51
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	12	0.51
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	14	0.51
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	17	0.51
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	8	0.51
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	14	0.51
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	7	0.51
(2,282)	1:551:A:GLY:H	1:568:A:PHE:HA	16	0.51
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	4	0.51
(2,253)	1:550:A:SER:H	1:556:A:ILE:HG13	4	0.51
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	12	0.5
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	3	0.5
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	5	0.5
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	8	0.5
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	11	0.5
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	15	0.5
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	7	0.5
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	14	0.5
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	20	0.5
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	3	0.5
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	17	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	11	0.5
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	11	0.5
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	11	0.5
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD21	15	0.5
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD22	15	0.5
(2,931)	1:577:A:PHE:H	1:603:A:LEU:HD23	15	0.5
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	1	0.5
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	6	0.5
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	7	0.5
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	11	0.5
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	12	0.5
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	18	0.5
(2,850)	1:575:A:CYS:H	1:580:A:LYS:HB3	16	0.5
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	7	0.5
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	9	0.5
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	11	0.5
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	12	0.5
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	15	0.5
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	17	0.5
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	18	0.5
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	5	0.5
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	5	0.5
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	5	0.5
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	13	0.5
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	13	0.5
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	13	0.5
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	1	0.5
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	8	0.5
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	10	0.5
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	13	0.5
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	18	0.5
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	20	0.5
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	3	0.5
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	15	0.5
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	17	0.5
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	18	0.5
(2,165)	1:548:A:LEU:HD21	1:553:A:GLN:HE21	19	0.5
(2,165)	1:548:A:LEU:HD22	1:553:A:GLN:HE21	19	0.5
(2,165)	1:548:A:LEU:HD23	1:553:A:GLN:HE21	19	0.5
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	6	0.49
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	17	0.49
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	9	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	10	0.49
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	12	0.49
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	13	0.49
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	17	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	1	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	3	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	7	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	8	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	11	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	15	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	18	0.49
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	20	0.49
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	3	0.49
(2,995)	1:580:A:LYS:HD3	1:596:A:CYS:H	5	0.49
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	11	0.49
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	11	0.49
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	11	0.49
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	4	0.49
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	16	0.49
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	2	0.49
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	4	0.49
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	6	0.49
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	13	0.49
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	16	0.49
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	19	0.49
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	1	0.49
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	1	0.49
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	1	0.49
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	3	0.49
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	3	0.49
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	3	0.49
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	6	0.49
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	6	0.49
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	6	0.49
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	3	0.49
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	16	0.49
(2,436)	1:559:A:ARG:HG3	1:559:A:ARG:HA	7	0.49
(2,436)	1:559:A:ARG:HG3	1:559:A:ARG:HA	11	0.49
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	3	0.49
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	9	0.49
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	15	0.49
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	6	0.49
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	10	0.49
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	11	0.49
(2,165)	1:548:A:LEU:HD21	1:553:A:GLN:HE21	10	0.49
(2,165)	1:548:A:LEU:HD22	1:553:A:GLN:HE21	10	0.49
(2,165)	1:548:A:LEU:HD23	1:553:A:GLN:HE21	10	0.49
(2,165)	1:548:A:LEU:HD21	1:553:A:GLN:HE21	17	0.49
(2,165)	1:548:A:LEU:HD22	1:553:A:GLN:HE21	17	0.49
(2,165)	1:548:A:LEU:HD23	1:553:A:GLN:HE21	17	0.49
(1,422)	1:559:A:ARG:HG3	1:559:A:ARG:HA	7	0.49
(1,422)	1:559:A:ARG:HG3	1:559:A:ARG:HA	11	0.49
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	17	0.48
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	3	0.48
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	5	0.48
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	2	0.48
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	4	0.48
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	6	0.48
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	7	0.48
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	14	0.48
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	19	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	2	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	5	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	9	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	12	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	13	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	17	0.48
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	19	0.48
(2,992)	1:580:A:LYS:HD3	1:596:A:CYS:HB3	5	0.48
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	13	0.48
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	13	0.48
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	13	0.48
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	2	0.48
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	17	0.48
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	19	0.48
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	20	0.48
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	3	0.48
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	14	0.48
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	4	0.48
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	4	0.48
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	4	0.48
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	19	0.48
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	19	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	19	0.48
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	6	0.48
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	13	0.48
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	15	0.48
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	5	0.48
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	12	0.48
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	18	0.48
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	5	0.48
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	11	0.48
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	16	0.48
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	19	0.48
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	2	0.48
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	9	0.48
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	16	0.48
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	19	0.48
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	15	0.47
(2,1420)	1:598:A:ASN:HB3	1:599:A:CYS:H	17	0.47
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	15	0.47
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	18	0.47
(2,1209)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	20	0.47
(2,1018)	1:581:A:GLN:HG2	1:582:A:LEU:HB2	16	0.47
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	6	0.47
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	14	0.47
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	14	0.47
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	14	0.47
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	14	0.47
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	9	0.47
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	1	0.47
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	10	0.47
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	20	0.47
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	2	0.47
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	2	0.47
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	2	0.47
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	15	0.47
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	15	0.47
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	15	0.47
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	20	0.47
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	20	0.47
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	20	0.47
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	1	0.47
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	4	0.47
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	5	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	8	0.47
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	10	0.47
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	11	0.47
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	14	0.47
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	17	0.47
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	11	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	6	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	9	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	10	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	12	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	15	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	16	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	17	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	18	0.47
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	19	0.47
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	9	0.47
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	13	0.47
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	14	0.47
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	16	0.47
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	2	0.47
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	7	0.47
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	4	0.47
(2,337)	1:554:A:LYS:HB3	1:555:A:PRO:HD3	7	0.47
(2,165)	1:548:A:LEU:HD21	1:553:A:GLN:HE21	11	0.47
(2,165)	1:548:A:LEU:HD22	1:553:A:GLN:HE21	11	0.47
(2,165)	1:548:A:LEU:HD23	1:553:A:GLN:HE21	11	0.47
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	2	0.47
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	6	0.47
(1,1405)	1:598:A:ASN:HB3	1:599:A:CYS:H	17	0.47
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	2	0.46
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	4	0.46
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	7	0.46
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	9	0.46
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	13	0.46
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	14	0.46
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	19	0.46
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	20	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	3	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	4	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	6	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	10	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	12	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	14	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	17	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	18	0.46
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	19	0.46
(2,1209)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	5	0.46
(2,1209)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	12	0.46
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	1	0.46
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	7	0.46
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	11	0.46
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	4	0.46
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	10	0.46
(2,1009)	1:581:A:GLN:HE22	1:581:A:GLN:HB3	16	0.46
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	13	0.46
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	14	0.46
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	8	0.46
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	17	0.46
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	17	0.46
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	17	0.46
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	7	0.46
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	9	0.46
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	19	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	1	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	2	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	3	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	4	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	5	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	7	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	8	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	13	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	14	0.46
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	20	0.46
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	18	0.46
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	18	0.46
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	18	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	1	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	2	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	3	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	4	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	6	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	10	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	15	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	17	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	19	0.46
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	20	0.46
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	4	0.46
(2,366)	1:555:A:PRO:HB3	1:556:A:ILE:HB	6	0.46
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	2	0.46
(2,165)	1:548:A:LEU:HD21	1:553:A:GLN:HE21	20	0.46
(2,165)	1:548:A:LEU:HD22	1:553:A:GLN:HE21	20	0.46
(2,165)	1:548:A:LEU:HD23	1:553:A:GLN:HE21	20	0.46
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	5	0.45
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	18	0.45
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	10	0.45
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	11	0.45
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	16	0.45
(2,1420)	1:598:A:ASN:HB3	1:599:A:CYS:H	15	0.45
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	1	0.45
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	8	0.45
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	10	0.45
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	11	0.45
(2,1402)	1:597:A:GLN:HA	1:600:A:PHE:HB2	16	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	1	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	2	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	5	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	7	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	8	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	9	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	11	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	13	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	15	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	16	0.45
(2,1343)	1:594:A:PRO:HB3	1:595:A:TYR:HA	20	0.45
(2,1209)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	3	0.45
(2,1209)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	6	0.45
(2,1209)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	17	0.45
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	17	0.45
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	17	0.45
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	17	0.45
(2,905)	1:576:A:ALA:H	1:594:A:PRO:HG3	15	0.45
(2,843)	1:575:A:CYS:HB3	1:580:A:LYS:HB3	5	0.45
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	9	0.45
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	9	0.45
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	9	0.45
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	12	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	12	0.45
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	12	0.45
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	2	0.45
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	12	0.45
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	8	0.45
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	11	0.45
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	10	0.45
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	20	0.45
(1,1405)	1:598:A:ASN:HB3	1:599:A:CYS:H	15	0.45
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	1	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	2	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	3	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	4	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	6	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	7	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	9	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	12	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	13	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	14	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	19	0.44
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	20	0.44
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	5	0.44
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	20	0.44
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	8	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	9	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	9	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	9	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	12	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	12	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	12	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	16	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	16	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	16	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	19	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	19	0.44
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	19	0.44
(2,751)	1:572:A:HIS:H	1:573:A:PHE:HB3	18	0.44
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	8	0.44
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	8	0.44
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	8	0.44
(2,484)	1:561:A:ILE:HB	1:563:A:ALA:HA	7	0.44
(2,438)	1:559:A:ARG:HG2	1:559:A:ARG:H	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,438)	1:559:A:ARG:HG2	1:559:A:ARG:H	16	0.44
(2,438)	1:559:A:ARG:HG2	1:559:A:ARG:H	19	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	4	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	4	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	4	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	6	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	6	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	6	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	7	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	7	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	7	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	9	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	9	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	9	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	12	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	12	0.44
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	12	0.44
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	11	0.44
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	17	0.44
(2,247)	1:550:A:SER:HA	1:553:A:GLN:HE22	19	0.44
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	17	0.44
(1,424)	1:559:A:ARG:HG2	1:559:A:ARG:H	4	0.44
(1,424)	1:559:A:ARG:HG2	1:559:A:ARG:H	16	0.44
(1,424)	1:559:A:ARG:HG2	1:559:A:ARG:H	19	0.44
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	1	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	1	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	1	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	2	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	2	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	2	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	4	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	4	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	4	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	7	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	7	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	7	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	8	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	8	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	8	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	10	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	10	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	8	0.43
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	10	0.43
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	11	0.43
(2,1456)	1:599:A:CYS:H	1:603:A:LEU:HG	16	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	1	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	2	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	3	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	4	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	6	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	8	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	9	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	12	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	14	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	15	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	19	0.43
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	20	0.43
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	5	0.43
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	6	0.43
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	12	0.43
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	17	0.43
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	5	0.43
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	7	0.43
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	5	0.43
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	15	0.43
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	11	0.43
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	11	0.43
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	11	0.43
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	3	0.43
(2,600)	1:564:A:MET:HB2	1:565:A:ALA:H	11	0.43
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	5	0.43
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	5	0.43
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	5	0.43
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	7	0.43
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	7	0.43
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	7	0.43
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	10	0.43
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	10	0.43
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	10	0.43
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	11	0.43
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	11	0.43
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	11	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	1	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	1	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	1	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	3	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	3	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	3	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	5	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	5	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	5	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	8	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	8	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	8	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	13	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	13	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	13	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	14	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	14	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	14	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	15	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	15	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	15	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	16	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	16	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	16	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	18	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	18	0.43
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	18	0.43
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	20	0.43
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	5	0.43
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	5	0.43
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	5	0.43
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	4	0.43
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	5	0.43
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	10	0.43
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	16	0.43
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	3	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	3	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	3	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	5	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	5	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	5	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	6	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	6	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	9	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	9	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	9	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	11	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	11	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	11	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	12	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	12	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	12	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	13	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	13	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	13	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	14	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	14	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	14	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	15	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	15	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	15	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	16	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	16	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	16	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	17	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	17	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	17	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	18	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	18	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	18	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	19	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	19	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	19	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD11	20	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD12	20	0.42
(2,1542)	1:602:A:LYS:H	1:603:A:LEU:HD13	20	0.42
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	10	0.42
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	11	0.42
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	16	0.42
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	7	0.42
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	13	0.42
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	17	0.42
(2,1448)	1:599:A:CYS:HA	1:602:A:LYS:HG2	18	0.42
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	17	0.42
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	12	0.42
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	2	0.42
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	8	0.42
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	9	0.42
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	10	0.42
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	12	0.42
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	17	0.42
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	18	0.42
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	2	0.42
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	7	0.42
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	9	0.42
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	12	0.42
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	16	0.42
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	17	0.42
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	6	0.42
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	13	0.42
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	19	0.42
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	2	0.42
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	2	0.42
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	2	0.42
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	15	0.42
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	10	0.42
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	10	0.42
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	10	0.42
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	5	0.42
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	13	0.42
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	20	0.42
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	6	0.42
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	6	0.42
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	6	0.42
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	7	0.42
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	11	0.42
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	16	0.42
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	11	0.42
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	11	0.42
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	11	0.42
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	20	0.42
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	20	0.42
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	20	0.42
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	6	0.42
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	6	0.42
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	12	0.42
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	12	0.42
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	12	0.42
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	15	0.42
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	15	0.42
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	15	0.42
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	15	0.42
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	12	0.42
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	2	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	3	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	4	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	6	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	7	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	8	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	14	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	18	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	19	0.41
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	20	0.41
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	5	0.41
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	5	0.41
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	5	0.41
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	17	0.41
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	17	0.41
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	17	0.41
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	20	0.41
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	3	0.41
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	6	0.41
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	5	0.41
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	3	0.41
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	9	0.41
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	12	0.41
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	14	0.41
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	17	0.41
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	15	0.41
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	15	0.41
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	15	0.41
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	7	0.41
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	7	0.41
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	7	0.41
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	13	0.41
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	14	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	19	0.41
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	6	0.41
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	1	0.41
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	2	0.41
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	4	0.41
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	7	0.41
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	8	0.41
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	14	0.41
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	2	0.41
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	2	0.41
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	2	0.41
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	3	0.41
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	3	0.41
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	3	0.41
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	4	0.41
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	4	0.41
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	4	0.41
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	16	0.41
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	16	0.41
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	16	0.41
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	4	0.41
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	5	0.41
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	6	0.41
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	10	0.41
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	15	0.41
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	19	0.41
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	12	0.41
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	14	0.41
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	18	0.41
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	17	0.41
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	17	0.41
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	17	0.41
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	19	0.41
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	19	0.41
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	19	0.41
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	20	0.41
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	20	0.41
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	20	0.41
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	11	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	1	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	1	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	1	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	2	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	2	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	2	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	3	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	3	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	3	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	4	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	4	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	4	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	8	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	8	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	8	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	10	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	10	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	10	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	11	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	11	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	11	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	13	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	13	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	13	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	14	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	14	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	14	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	16	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	16	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	16	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	17	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	17	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	17	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	18	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	18	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	18	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	19	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	19	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	19	0.41
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	20	0.41
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	20	0.41
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	20	0.41
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	2	0.41
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	4	0.41
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	6	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	7	0.41
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	11	0.41
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	19	0.41
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	8	0.41
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	20	0.41
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	1	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	2	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	3	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	4	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	5	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	6	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	7	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	8	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	9	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	13	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	14	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	15	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	18	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	19	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	20	0.4
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	1	0.4
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	5	0.4
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	9	0.4
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	12	0.4
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	13	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	1	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	1	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	1	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	3	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	3	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	3	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	6	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	6	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	6	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	7	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	7	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	7	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	8	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	8	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	8	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	9	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	9	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	9	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	10	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	10	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	10	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	11	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	11	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	11	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	12	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	12	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	12	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	13	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	13	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	13	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	14	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	14	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	14	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	16	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	16	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	16	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	19	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	19	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	19	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	20	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	20	0.4
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	20	0.4
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	16	0.4
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	5	0.4
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	2	0.4
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	4	0.4
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	18	0.4
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	19	0.4
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	20	0.4
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	8	0.4
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	19	0.4
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	11	0.4
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	2	0.4
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	4	0.4
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	16	0.4
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	20	0.4
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	18	0.4
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	13	0.4
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	13	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	13	0.4
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	14	0.4
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	14	0.4
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	14	0.4
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	2	0.4
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	2	0.4
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	4	0.4
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	7	0.4
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	16	0.4
(2,798)	1:574:A:VAL:HG11	1:580:A:LYS:HA	16	0.4
(2,798)	1:574:A:VAL:HG12	1:580:A:LYS:HA	16	0.4
(2,798)	1:574:A:VAL:HG13	1:580:A:LYS:HA	16	0.4
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	6	0.4
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	9	0.4
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	9	0.4
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	9	0.4
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	17	0.4
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	17	0.4
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	17	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	1	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	2	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	3	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	8	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	9	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	12	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	13	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	14	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	17	0.4
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	18	0.4
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	4	0.4
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	16	0.4
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	19	0.4
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	2	0.4
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	2	0.4
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	2	0.4
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD11	10	0.4
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD12	10	0.4
(2,324)	1:553:A:GLN:H	1:556:A:ILE:HD13	10	0.4
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	17	0.4
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	17	0.4
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	17	0.4
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	19	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	12	0.4
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	14	0.4
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	17	0.4
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	20	0.4
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	20	0.4
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	7	0.4
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	7	0.4
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	7	0.4
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	16	0.4
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	20	0.4
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	6	0.4
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	19	0.4
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	12	0.39
(2,1531)	1:602:A:LYS:HB2	1:603:A:LEU:HG	17	0.39
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	10	0.39
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	11	0.39
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	16	0.39
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	17	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	2	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	2	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	2	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	4	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	4	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	4	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	15	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	15	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	15	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD21	18	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD22	18	0.39
(2,1431)	1:598:A:ASN:H	1:601:A:LEU:HD23	18	0.39
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	10	0.39
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	11	0.39
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	3	0.39
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	6	0.39
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	20	0.39
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	3	0.39
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	18	0.39
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	3	0.39
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	5	0.39
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	3	0.39
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	6	0.39
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	11	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	14	0.39
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	7	0.39
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	5	0.39
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	18	0.39
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	11	0.39
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	15	0.39
(2,1117)	1:584:A:LYS:HD3	1:587:A:PHE:H	18	0.39
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	10	0.39
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	18	0.39
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	18	0.39
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	7	0.39
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	9	0.39
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	11	0.39
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	12	0.39
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	16	0.39
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	17	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	3	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	5	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	10	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	12	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	14	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	17	0.39
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	19	0.39
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	18	0.39
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	8	0.39
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	12	0.39
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	12	0.39
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	12	0.39
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	6	0.39
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	4	0.39
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	17	0.39
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	20	0.39
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	2	0.39
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	2	0.39
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	2	0.39
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	10	0.39
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	17	0.39
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	20	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	1	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	3	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	5	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	8	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	9	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	10	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	11	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	13	0.39
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	18	0.39
(2,177)	1:548:A:LEU:HD11	1:554:A:LYS:H	9	0.39
(2,177)	1:548:A:LEU:HD12	1:554:A:LYS:H	9	0.39
(2,177)	1:548:A:LEU:HD13	1:554:A:LYS:H	9	0.39
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	3	0.39
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	5	0.39
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	10	0.39
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	13	0.39
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	15	0.39
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	20	0.39
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	9	0.39
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	14	0.39
(1,1102)	1:584:A:LYS:HD3	1:587:A:PHE:H	18	0.39
(2,1470)	1:600:A:PHE:HA	1:603:A:LEU:HB3	15	0.38
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	18	0.38
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	19	0.38
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	12	0.38
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	17	0.38
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	14	0.38
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	18	0.38
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	15	0.38
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	18	0.38
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	19	0.38
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	1	0.38
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	9	0.38
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	13	0.38
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	16	0.38
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	18	0.38
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	19	0.38
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	8	0.38
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	14	0.38
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	7	0.38
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	20	0.38
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	7	0.38
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	15	0.38
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	13	0.38
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	16	0.38
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	18	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	20	0.38
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	1	0.38
(2,1028)	1:581:A:GLN:HG2	1:582:A:LEU:HA	10	0.38
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	10	0.38
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	20	0.38
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	19	0.38
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	19	0.38
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	19	0.38
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	1	0.38
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	3	0.38
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	4	0.38
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	6	0.38
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	8	0.38
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	9	0.38
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	11	0.38
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	2	0.38
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	2	0.38
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	2	0.38
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	3	0.38
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	3	0.38
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	3	0.38
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	9	0.38
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	10	0.38
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	12	0.38
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	16	0.38
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	17	0.38
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	19	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	1	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	2	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	5	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	7	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	9	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	10	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	12	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	14	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	17	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	18	0.38
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	19	0.38
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	19	0.38
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	19	0.38
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	19	0.38
(2,509)	1:561:A:ILE:H	1:570:A:PRO:HG2	20	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	1	0.38
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	7	0.38
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	16	0.38
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	12	0.38
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	12	0.38
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	12	0.38
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	14	0.38
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	14	0.38
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	14	0.38
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	17	0.38
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	17	0.38
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	17	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	6	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	6	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	6	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	9	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	9	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	9	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	10	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	10	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	10	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	14	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	14	0.38
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	14	0.38
(2,276)	1:551:A:GLY:H	1:553:A:GLN:HG3	2	0.38
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	2	0.38
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	4	0.38
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	6	0.38
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	15	0.38
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	19	0.38
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	17	0.38
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	12	0.38
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	1	0.38
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	8	0.38
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	9	0.38
(2,126)	1:547:A:SER:HA	1:567:A:LYS:HE3	17	0.38
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	10	0.38
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	16	0.38
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	18	0.38
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	4	0.38
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	3	0.37
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	3	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	5	0.37
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	5	0.37
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	5	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	6	0.37
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	6	0.37
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	6	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	12	0.37
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	12	0.37
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	12	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	15	0.37
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	15	0.37
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	15	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	17	0.37
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	17	0.37
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	17	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	20	0.37
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	20	0.37
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	20	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	1	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	2	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	4	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	7	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	9	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	10	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	11	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	13	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	14	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	15	0.37
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	16	0.37
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	1	0.37
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	4	0.37
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	7	0.37
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	8	0.37
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	10	0.37
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	11	0.37
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	4	0.37
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	19	0.37
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	19	0.37
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	4	0.37
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	6	0.37
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	12	0.37
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	7	0.37
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	8	0.37
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	10	0.37
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	12	0.37
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	15	0.37
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	17	0.37
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	3	0.37
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	4	0.37
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	6	0.37
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	12	0.37
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	14	0.37
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	16	0.37
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	2	0.37
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	4	0.37
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	5	0.37
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	6	0.37
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	11	0.37
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	2	0.37
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	9	0.37
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	13	0.37
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	14	0.37
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	15	0.37
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	16	0.37
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	19	0.37
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	2	0.37
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	9	0.37
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	12	0.37
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	13	0.37
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	14	0.37
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	17	0.37
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	19	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	1	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	2	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	3	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	4	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	9	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	10	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	12	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	14	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	17	0.37
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1087)	1:583:A:ASN:HB2	1:583:A:ASN:H	20	0.37
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	18	0.37
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	1	0.37
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	11	0.37
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	15	0.37
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	16	0.37
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	15	0.37
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	17	0.37
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	17	0.37
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	17	0.37
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	18	0.37
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	18	0.37
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	18	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	1	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	1	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	1	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	2	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	2	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	2	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	3	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	3	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	3	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	4	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	4	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	4	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	5	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	5	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	5	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	6	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	6	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	6	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	7	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	7	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	7	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	8	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	8	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	8	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	9	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	9	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	9	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	10	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	10	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	10	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	11	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	11	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	11	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	12	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	12	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	12	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	13	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	13	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	13	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	16	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	16	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	16	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	17	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	17	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	17	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	18	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	18	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	18	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	19	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	19	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	19	0.37
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	20	0.37
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	20	0.37
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	20	0.37
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	5	0.37
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	8	0.37
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	10	0.37
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	20	0.37
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	1	0.37
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	13	0.37
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	15	0.37
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	9	0.37
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	9	0.37
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	9	0.37
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	17	0.37
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	17	0.37
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	17	0.37
(2,610)	1:564:A:MET:HB3	1:566:A:LYS:H	15	0.37
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	9	0.37
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	10	0.37
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	12	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	17	0.37
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	18	0.37
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	19	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	3	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	4	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	6	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	13	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	15	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	16	0.37
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	20	0.37
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	1	0.37
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	1	0.37
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	1	0.37
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	18	0.37
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	18	0.37
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	18	0.37
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	15	0.37
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	15	0.37
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	15	0.37
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	2	0.37
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	3	0.37
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	5	0.37
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	13	0.37
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	15	0.37
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	19	0.37
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	7	0.37
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	8	0.37
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	8	0.37
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	8	0.37
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	20	0.37
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	20	0.37
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	20	0.37
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	11	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	3	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	3	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	3	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	5	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	5	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	5	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	7	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	7	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	7	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	8	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	8	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	8	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	11	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	11	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	11	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	12	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	12	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	12	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	13	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	13	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	13	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	18	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	18	0.37
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	18	0.37
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	7	0.37
(2,237)	1:550:A:SER:H	1:551:A:GLY:HA2	16	0.37
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	1	0.37
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	2	0.37
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	5	0.37
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	10	0.37
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	13	0.37
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	15	0.37
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	18	0.37
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	14	0.37
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	17	0.37
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	1	0.37
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	7	0.37
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	13	0.37
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	18	0.37
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	1	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	1	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	1	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	2	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	2	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	2	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	4	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	4	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	4	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	7	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	7	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	7	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	8	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	8	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	8	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	9	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	9	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	9	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	13	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	13	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	13	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	14	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	14	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	14	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	18	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	18	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	18	0.36
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	19	0.36
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	19	0.36
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	19	0.36
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	10	0.36
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	11	0.36
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	16	0.36
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	8	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	2	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	9	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	13	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	14	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	15	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	16	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	18	0.36
(2,1367)	1:596:A:CYS:HA	1:597:A:GLN:HB3	19	0.36
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	6	0.36
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	3	0.36
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	5	0.36
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	9	0.36
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	14	0.36
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	1	0.36
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	2	0.36
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	7	0.36
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	8	0.36
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	13	0.36
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	14	0.36
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	17	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	5	0.36
(2,1262)	1:590:A:GLN:H	1:591:A:ASN:HB3	20	0.36
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	2	0.36
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	13	0.36
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	15	0.36
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	17	0.36
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	13	0.36
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	4	0.36
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	11	0.36
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	18	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	1	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	3	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	4	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	6	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	8	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	11	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	16	0.36
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	20	0.36
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	6	0.36
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	15	0.36
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	8	0.36
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	11	0.36
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	18	0.36
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	9	0.36
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	9	0.36
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	9	0.36
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	12	0.36
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	12	0.36
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	12	0.36
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	14	0.36
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	14	0.36
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	14	0.36
(2,964)	1:579:A:LEU:HD11	1:580:A:LYS:H	15	0.36
(2,964)	1:579:A:LEU:HD12	1:580:A:LYS:H	15	0.36
(2,964)	1:579:A:LEU:HD13	1:580:A:LYS:H	15	0.36
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	18	0.36
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	12	0.36
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	12	0.36
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	12	0.36
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	18	0.36
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	18	0.36
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	1	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	4	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	6	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	7	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	8	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	14	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	15	0.36
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	16	0.36
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	11	0.36
(2,578)	1:563:A:ALA:HA	1:565:A:ALA:H	11	0.36
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	13	0.36
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	13	0.36
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	13	0.36
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	8	0.36
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	8	0.36
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	8	0.36
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	8	0.36
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	9	0.36
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	10	0.36
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	11	0.36
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	14	0.36
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	18	0.36
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	20	0.36
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	1	0.36
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	1	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	1	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	1	0.36
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	2	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	2	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	2	0.36
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	3	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	3	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	3	0.36
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	9	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	9	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	9	0.36
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	13	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	13	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	13	0.36
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	15	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	15	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	15	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	18	0.36
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	18	0.36
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	18	0.36
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	16	0.36
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	16	0.36
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	16	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	3	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	7	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	8	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	10	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	11	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	13	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	16	0.36
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	17	0.36
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	2	0.36
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	4	0.36
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	10	0.36
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	16	0.36
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	17	0.36
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	19	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	1	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	1	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	1	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	15	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	15	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	15	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	16	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	16	0.36
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	16	0.36
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	3	0.36
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	8	0.36
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	12	0.36
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	14	0.36
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	10	0.36
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	14	0.36
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	12	0.36
(2,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	18	0.36
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	3	0.36
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	9	0.36
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	11	0.36
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	19	0.36
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	10	0.35
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	10	0.35
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	10	0.35
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	11	0.35
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	11	0.35
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	11	0.35
(2,1496)	1:601:A:LEU:HD21	1:602:A:LYS:H	16	0.35
(2,1496)	1:601:A:LEU:HD22	1:602:A:LYS:H	16	0.35
(2,1496)	1:601:A:LEU:HD23	1:602:A:LYS:H	16	0.35
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	3	0.35
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	6	0.35
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	12	0.35
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	17	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	1	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	2	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	4	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	7	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	8	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	13	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	18	0.35
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	19	0.35
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	3	0.35
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	4	0.35
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	11	0.35
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	18	0.35
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	19	0.35
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	2	0.35
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	12	0.35
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	13	0.35
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	16	0.35
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	4	0.35
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	7	0.35
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	17	0.35
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	10	0.35
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	11	0.35
(2,1264)	1:590:A:GLN:HB3	1:591:A:ASN:HA	16	0.35
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	1	0.35
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	7	0.35
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	8	0.35
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	9	0.35
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	10	0.35
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	1	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	9	0.35
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	10	0.35
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	12	0.35
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	16	0.35
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	17	0.35
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	18	0.35
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	20	0.35
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	1	0.35
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	10	0.35
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	5	0.35
(2,1145)	1:587:A:PHE:HB3	1:588:A:LYS:H	10	0.35
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	5	0.35
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	8	0.35
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	3	0.35
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	6	0.35
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	18	0.35
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	11	0.35
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	16	0.35
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	4	0.35
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	7	0.35
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	9	0.35
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	1	0.35
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	7	0.35
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	8	0.35
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	11	0.35
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	11	0.35
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	11	0.35
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	18	0.35
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	18	0.35
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	18	0.35
(2,891)	1:576:A:ALA:H	1:582:A:LEU:HB3	18	0.35
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	1	0.35
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	3	0.35
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	14	0.35
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	18	0.35
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	20	0.35
(2,820)	1:574:A:VAL:HA	1:582:A:LEU:HG	20	0.35
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	20	0.35
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	2	0.35
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	15	0.35
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	15	0.35
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	2	0.35
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	2	0.35
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	2	0.35
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	7	0.35
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	7	0.35
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	7	0.35
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	9	0.35
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	9	0.35
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	9	0.35
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	10	0.35
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	10	0.35
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	10	0.35
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	17	0.35
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	17	0.35
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	17	0.35
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	19	0.35
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	19	0.35
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	19	0.35
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	11	0.35
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	11	0.35
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	11	0.35
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	18	0.35
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	18	0.35
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	18	0.35
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	18	0.35
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	6	0.35
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	8	0.35
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	10	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	1	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	4	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	12	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	14	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	15	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	17	0.35
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	19	0.35
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	9	0.35
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	5	0.35
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	5	0.35
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	5	0.35
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	6	0.35
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	6	0.35
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	10	0.35
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	10	0.35
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	10	0.35
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	7	0.35
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	7	0.35
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	7	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	1	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	2	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	9	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	14	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	15	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	18	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	19	0.35
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	20	0.35
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	11	0.35
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	16	0.35
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	19	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	3	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	6	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	7	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	8	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	9	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	13	0.35
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	15	0.35
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	4	0.35
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	4	0.35
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	4	0.35
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD11	19	0.35
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD12	19	0.35
(2,301)	1:552:A:CYS:H	1:556:A:ILE:HD13	19	0.35
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	6	0.35
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	7	0.35
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	11	0.35
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	15	0.35
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	11	0.35
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	12	0.35
(2,82)	1:545:A:ARG:HA	1:545:A:ARG:HG3	3	0.35
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	1	0.35
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	15	0.35
(1,82)	1:545:A:ARG:HA	1:545:A:ARG:HG3	3	0.35
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	10	0.34
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	1	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	2	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	4	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	7	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	8	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	9	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	13	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	14	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	18	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	19	0.34
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	5	0.34
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	3	0.34
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	6	0.34
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	20	0.34
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	15	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	1	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	2	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	5	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	7	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	8	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	9	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	10	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	13	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	14	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	15	0.34
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	16	0.34
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	17	0.34
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	2	0.34
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	6	0.34
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	11	0.34
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	15	0.34
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	1	0.34
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	2	0.34
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	11	0.34
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	20	0.34
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	3	0.34
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	19	0.34
(2,1203)	1:588:A:LYS:H	1:597:A:GLN:HB3	8	0.34
(2,1138)	1:586:A:THR:HB	1:597:A:GLN:HG3	7	0.34
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	4	0.34
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	8	0.34
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	20	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	2	0.34
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	5	0.34
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	14	0.34
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	19	0.34
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	10	0.34
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	13	0.34
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	16	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	1	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	1	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	1	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	2	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	2	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	2	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	3	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	3	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	3	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	16	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	16	0.34
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	16	0.34
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	4	0.34
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	4	0.34
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	4	0.34
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	6	0.34
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	6	0.34
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	6	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	4	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	6	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	9	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	11	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	13	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	17	0.34
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	19	0.34
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	4	0.34
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	4	0.34
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	4	0.34
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	13	0.34
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	13	0.34
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	13	0.34
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	14	0.34
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	14	0.34
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	14	0.34
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	15	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	15	0.34
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	15	0.34
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	19	0.34
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	19	0.34
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	19	0.34
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	20	0.34
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	20	0.34
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	20	0.34
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	20	0.34
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	3	0.34
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	5	0.34
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	13	0.34
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	20	0.34
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	4	0.34
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	4	0.34
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	4	0.34
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	10	0.34
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	10	0.34
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	10	0.34
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	18	0.34
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	18	0.34
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	18	0.34
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	20	0.34
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	20	0.34
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	20	0.34
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	5	0.34
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	5	0.34
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	5	0.34
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	12	0.34
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	12	0.34
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	12	0.34
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	13	0.34
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	13	0.34
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	13	0.34
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	14	0.34
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	14	0.34
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	14	0.34
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	16	0.34
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	16	0.34
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	16	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	7	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	7	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	9	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	9	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	9	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	10	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	10	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	10	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	12	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	12	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	12	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	17	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	17	0.34
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	17	0.34
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	12	0.34
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	17	0.34
(2,458)	1:560:A:CYS:HB2	1:568:A:PHE:H	20	0.34
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	2	0.34
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	3	0.34
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	5	0.34
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	15	0.34
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	17	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	2	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	3	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	5	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	6	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	8	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	9	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	10	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	11	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	13	0.34
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	16	0.34
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	8	0.34
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	10	0.34
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	7	0.34
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	7	0.34
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	7	0.34
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	11	0.34
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	11	0.34
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	11	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	4	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	4	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	4	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	11	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	11	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	11	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	19	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	19	0.34
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	19	0.34
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	4	0.34
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	5	0.34
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	6	0.34
(2,368)	1:555:A:PRO:HG2	1:556:A:ILE:H	12	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	2	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	3	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	4	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	6	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	7	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	8	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	10	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	13	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	15	0.34
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	17	0.34
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	1	0.34
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	5	0.34
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	12	0.34
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	18	0.34
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	20	0.34
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	10	0.34
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	17	0.34
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	4	0.34
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	9	0.34
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	16	0.34
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	17	0.34
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	18	0.34
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	1	0.34
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	2	0.34
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	9	0.34
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	18	0.34
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	19	0.34
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	8	0.34
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	12	0.34
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	14	0.34
(2,90)	1:545:A:ARG:H	1:546:A:GLY:HA3	20	0.34
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	7	0.34
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	14	0.34
(1,90)	1:545:A:ARG:H	1:546:A:GLY:HA3	20	0.34
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	14	0.34
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	3	0.33
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	5	0.33
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	6	0.33
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	12	0.33
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	15	0.33
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	17	0.33
(2,1469)	1:600:A:PHE:H	1:602:A:LYS:H	20	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	1	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	2	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	4	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	7	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	8	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	10	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	11	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	13	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	15	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	16	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	18	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	19	0.33
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	12	0.33
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	6	0.33
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	12	0.33
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	17	0.33
(2,1345)	1:594:A:PRO:HG3	1:595:A:TYR:H	20	0.33
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	7	0.33
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	9	0.33
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	10	0.33
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	3	0.33
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	14	0.33
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	8	0.33
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	10	0.33
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	12	0.33
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	13	0.33
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	16	0.33
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	13	0.33
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	15	0.33
(2,1233)	1:589:A:GLU:HB2	1:592:A:ASP:H	15	0.33
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	14	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	15	0.33
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	18	0.33
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	6	0.33
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	11	0.33
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	20	0.33
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	11	0.33
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	3	0.33
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	4	0.33
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	5	0.33
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	10	0.33
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	2	0.33
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	13	0.33
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	14	0.33
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	6	0.33
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	6	0.33
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	6	0.33
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	20	0.33
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	20	0.33
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	20	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	2	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	5	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	7	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	8	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	10	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	12	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	15	0.33
(2,864)	1:575:A:CYS:H	1:582:A:LEU:HG	16	0.33
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	6	0.33
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	6	0.33
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	6	0.33
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	16	0.33
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	16	0.33
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	16	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	1	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	1	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	1	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	2	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	2	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	2	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	3	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	3	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	5	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	5	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	5	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	6	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	6	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	6	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	9	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	9	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	9	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	11	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	11	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	11	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	12	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	12	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	12	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	14	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	14	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	14	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	15	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	15	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	15	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	16	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	16	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	16	0.33
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	17	0.33
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	17	0.33
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	17	0.33
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	14	0.33
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	14	0.33
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	14	0.33
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	1	0.33
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	1	0.33
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	1	0.33
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	4	0.33
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	4	0.33
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	4	0.33
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	6	0.33
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	6	0.33
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	6	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	2	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	2	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	2	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	4	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	4	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	4	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	14	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	14	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	14	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	16	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	16	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	16	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	19	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	19	0.33
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	19	0.33
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	7	0.33
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	7	0.33
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	7	0.33
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	1	0.33
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	12	0.33
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	14	0.33
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	18	0.33
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	9	0.33
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	11	0.33
(2,440)	1:559:A:ARG:HA	1:560:A:CYS:HB3	7	0.33
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	13	0.33
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	16	0.33
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	16	0.33
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	16	0.33
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	19	0.33
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	19	0.33
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	19	0.33
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	1	0.33
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	5	0.33
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	9	0.33
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	12	0.33
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	14	0.33
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	18	0.33
(2,361)	1:555:A:PRO:HA	1:556:A:ILE:HG12	20	0.33
(2,360)	1:555:A:PRO:HA	1:556:A:ILE:HG13	14	0.33
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	12	0.33
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	18	0.33
(2,221)	1:549:A:CYS:H	1:556:A:ILE:HG12	19	0.33
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	3	0.33
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	5	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	8	0.33
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	13	0.33
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	15	0.33
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	7	0.33
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	16	0.33
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	4	0.33
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	4	0.33
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	4	0.33
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	6	0.33
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	6	0.33
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	6	0.33
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	11	0.33
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	11	0.33
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	11	0.33
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	19	0.33
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	19	0.33
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	19	0.33
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	1	0.33
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	14	0.33
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	11	0.33
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	9	0.32
(2,1406)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	14	0.32
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	2	0.32
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	4	0.32
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	7	0.32
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	8	0.32
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	13	0.32
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	18	0.32
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	1	0.32
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	8	0.32
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	20	0.32
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	4	0.32
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	6	0.32
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	18	0.32
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	19	0.32
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	1	0.32
(2,1312)	1:593:A:LYS:HB3	1:593:A:LYS:H	20	0.32
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	4	0.32
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	6	0.32
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	10	0.32
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	11	0.32
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	20	0.32
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	3	0.32
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	4	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	1	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	2	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	6	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	7	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	9	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	11	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	12	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	13	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	15	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	16	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	17	0.32
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	19	0.32
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	7	0.32
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	9	0.32
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	10	0.32
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	13	0.32
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	14	0.32
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	17	0.32
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	19	0.32
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	2	0.32
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	4	0.32
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	9	0.32
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	19	0.32
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	20	0.32
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	4	0.32
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	4	0.32
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	4	0.32
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	3	0.32
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	3	0.32
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	3	0.32
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	7	0.32
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	7	0.32
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	7	0.32
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	5	0.32
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	6	0.32
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	10	0.32
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	16	0.32
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	12	0.32
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	20	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	15	0.32
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	11	0.32
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	7	0.32
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	7	0.32
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	7	0.32
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	8	0.32
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	8	0.32
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	8	0.32
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	13	0.32
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	13	0.32
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	13	0.32
(2,553)	1:562:A:THR:HG21	1:563:A:ALA:HA	19	0.32
(2,553)	1:562:A:THR:HG22	1:563:A:ALA:HA	19	0.32
(2,553)	1:562:A:THR:HG23	1:563:A:ALA:HA	19	0.32
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	20	0.32
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	20	0.32
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	20	0.32
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	3	0.32
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	3	0.32
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	3	0.32
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	11	0.32
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	11	0.32
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	11	0.32
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	15	0.32
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	15	0.32
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	15	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	1	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	1	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	1	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	5	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	5	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	5	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	6	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	6	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	6	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	8	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	8	0.32
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	8	0.32
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	4	0.32
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	4	0.32
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	4	0.32
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	18	0.32
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	18	0.32
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	8	0.32
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	9	0.32
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	10	0.32
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	13	0.32
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	15	0.32
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	17	0.32
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	20	0.32
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	6	0.32
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	6	0.32
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	6	0.32
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	2	0.32
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	4	0.32
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	5	0.32
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	9	0.32
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	19	0.32
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	4	0.32
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	11	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	3	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	5	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	8	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	11	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	13	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	18	0.32
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	19	0.32
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	7	0.32
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	7	0.32
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	7	0.32
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	16	0.32
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	16	0.32
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	16	0.32
(2,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	17	0.32
(2,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	5	0.32
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	2	0.31
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	5	0.31
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	11	0.31
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	14	0.31
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	17	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	3	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	5	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	8	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	9	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	12	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	13	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	17	0.31
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	20	0.31
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	3	0.31
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	9	0.31
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	12	0.31
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	17	0.31
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	18	0.31
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	19	0.31
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	20	0.31
(2,1465)	1:600:A:PHE:HB2	1:601:A:LEU:H	20	0.31
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	15	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	1	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	5	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	9	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	10	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	11	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	14	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	16	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	17	0.31
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	19	0.31
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	15	0.31
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	2	0.31
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	13	0.31
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	16	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	3	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	5	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	8	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	9	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	12	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	16	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	18	0.31
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	19	0.31
(2,1237)	1:589:A:GLU:HG2	1:593:A:LYS:H	5	0.31
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	13	0.31
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	18	0.31
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	19	0.31
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	3	0.31
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	6	0.31
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	12	0.31
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	17	0.31
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	13	0.31
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	1	0.31
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	16	0.31
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	16	0.31
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	5	0.31
(2,1017)	1:581:A:GLN:HG3	1:582:A:LEU:H	14	0.31
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	1	0.31
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	4	0.31
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	12	0.31
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	20	0.31
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	3	0.31
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	6	0.31
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	12	0.31
(2,994)	1:580:A:LYS:HD3	1:596:A:CYS:HB2	17	0.31
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	5	0.31
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	12	0.31
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	17	0.31
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	2	0.31
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	4	0.31
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	7	0.31
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	8	0.31
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	10	0.31
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	18	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	1	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	2	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	3	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	4	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	7	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	8	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	9	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	11	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	12	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	13	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	17	0.31
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	18	0.31
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	9	0.31
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	10	0.31
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	17	0.31
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	18	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	1	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	2	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	3	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	4	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	5	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	6	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	7	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	8	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	9	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	10	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	11	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	12	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	13	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	14	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	15	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	16	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	17	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	18	0.31
(2,663)	1:568:A:PHE:HA	1:569:A:HIS:HB3	19	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	7	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	8	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	9	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	10	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	12	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	16	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	17	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	18	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	19	0.31
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	20	0.31
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	18	0.31
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	18	0.31
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	18	0.31
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	20	0.31
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	20	0.31
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	20	0.31
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	18	0.31
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	18	0.31
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	18	0.31
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	13	0.31
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	13	0.31
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	13	0.31
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	20	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	20	0.31
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	20	0.31
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	5	0.31
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	5	0.31
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	5	0.31
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	6	0.31
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	6	0.31
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	6	0.31
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	8	0.31
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	8	0.31
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	8	0.31
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	11	0.31
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	11	0.31
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	11	0.31
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	16	0.31
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	16	0.31
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	16	0.31
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	19	0.31
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	19	0.31
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	19	0.31
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	2	0.31
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	3	0.31
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	5	0.31
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	6	0.31
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	19	0.31
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	13	0.31
(2,383)	1:556:A:ILE:HG21	1:557:A:THR:HA	4	0.31
(2,383)	1:556:A:ILE:HG22	1:557:A:THR:HA	4	0.31
(2,383)	1:556:A:ILE:HG23	1:557:A:THR:HA	4	0.31
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	2	0.31
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	2	0.31
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	2	0.31
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	1	0.31
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	8	0.31
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	11	0.31
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	12	0.31
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	13	0.31
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	20	0.31
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	1	0.31
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	3	0.31
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	7	0.31
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	14	0.31
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	16	0.31
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	6	0.31
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	7	0.31
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	15	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	2	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	4	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	6	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	9	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	10	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	12	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	15	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	17	0.31
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	20	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	2	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	2	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	2	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	3	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	3	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	3	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	5	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	5	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	5	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	10	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	10	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	10	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	13	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	13	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	13	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	15	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	15	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	15	0.31
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	17	0.31
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	17	0.31
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	17	0.31
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	1	0.31
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	2	0.31
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	3	0.31
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	8	0.31
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	13	0.31
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	15	0.31
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	16	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	5	0.31
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	16	0.31
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	2	0.31
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	20	0.31
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	19	0.31
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	19	0.31
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	1	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	3	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	4	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	6	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	7	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	8	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	9	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	10	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	12	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	13	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	15	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	16	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	18	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	19	0.3
(2,1578)	1:604:A:PHE:H	1:605:A:CYS:HB3	20	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	1	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	2	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	4	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	7	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	14	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	15	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	18	0.3
(2,1516)	1:602:A:LYS:HD3	1:602:A:LYS:H	19	0.3
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	15	0.3
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	15	0.3
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	15	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	2	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	4	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	5	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	6	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	7	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	10	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	11	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	13	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	14	0.3
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	16	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	1	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	2	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	4	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	7	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	8	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	13	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	18	0.3
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	19	0.3
(2,1399)	1:597:A:GLN:HB3	1:598:A:ASN:HB3	17	0.3
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	3	0.3
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	6	0.3
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	12	0.3
(2,1377)	1:596:A:CYS:H	1:598:A:ASN:H	20	0.3
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	11	0.3
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	16	0.3
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	20	0.3
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	7	0.3
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	2	0.3
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	9	0.3
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	20	0.3
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	3	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	2	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	7	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	9	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	12	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	14	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	15	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	17	0.3
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	19	0.3
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	13	0.3
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	3	0.3
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	6	0.3
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	8	0.3
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	6	0.3
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	7	0.3
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	7	0.3
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	7	0.3
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	10	0.3
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	10	0.3
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	10	0.3
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	1	0.3
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	1	0.3
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	10	0.3
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	10	0.3
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	10	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	1	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	3	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	6	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	9	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	11	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	12	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	13	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	14	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	15	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	16	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	19	0.3
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	20	0.3
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	14	0.3
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	15	0.3
(2,765)	1:573:A:PHE:HB2	1:574:A:VAL:H	19	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	1	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	2	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	3	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	4	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	5	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	6	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	8	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	14	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	16	0.3
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	19	0.3
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	9	0.3
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	12	0.3
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	14	0.3
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	17	0.3
(2,623)	1:566:A:LYS:HA	1:566:A:LYS:HG3	11	0.3
(2,623)	1:566:A:LYS:HA	1:566:A:LYS:HG3	15	0.3
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	3	0.3
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	11	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	1	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	2	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	3	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	4	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	5	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	6	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	13	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	14	0.3
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	15	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	1	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	1	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	1	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	2	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	2	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	2	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	4	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	4	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	4	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	5	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	5	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	5	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	6	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	6	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	6	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	7	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	7	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	7	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	9	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	9	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	9	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	10	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	10	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	10	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	12	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	12	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	12	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	14	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	14	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	14	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	15	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	15	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	15	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	16	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	16	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	16	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	17	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	17	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	19	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	19	0.3
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	19	0.3
(2,525)	1:561:A:ILE:HD11	1:572:A:HIS:H	20	0.3
(2,525)	1:561:A:ILE:HD12	1:572:A:HIS:H	20	0.3
(2,525)	1:561:A:ILE:HD13	1:572:A:HIS:H	20	0.3
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB1	3	0.3
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB2	3	0.3
(2,486)	1:561:A:ILE:HB	1:563:A:ALA:HB3	3	0.3
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	1	0.3
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	1	0.3
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	1	0.3
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	2	0.3
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	2	0.3
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	2	0.3
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	9	0.3
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	9	0.3
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	9	0.3
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	13	0.3
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	13	0.3
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	13	0.3
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	14	0.3
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	14	0.3
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	14	0.3
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	4	0.3
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	16	0.3
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	15	0.3
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	5	0.3
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	5	0.3
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	5	0.3
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	9	0.3
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	9	0.3
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	9	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	3	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	5	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	6	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	10	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	14	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	15	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	18	0.3
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	19	0.3
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	6	0.3
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	13	0.3
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	20	0.3
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	20	0.3
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	20	0.3
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	5	0.3
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	6	0.3
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	16	0.3
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	19	0.3
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	1	0.3
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	1	0.3
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	1	0.3
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	1	0.3
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	8	0.3
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	8	0.3
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	8	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	5	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	6	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	9	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	10	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	11	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	12	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	19	0.3
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	20	0.3
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	2	0.3
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	2	0.3
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	2	0.3
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	10	0.3
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	10	0.3
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	10	0.3
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	11	0.3
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	11	0.3
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	11	0.3
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	17	0.3
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	17	0.3
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	17	0.3
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	19	0.3
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	19	0.3
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	19	0.3
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	20	0.3
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	20	0.3
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	3	0.3
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	7	0.3
(1,609)	1:566:A:LYS:HA	1:566:A:LYS:HG3	11	0.3
(1,609)	1:566:A:LYS:HA	1:566:A:LYS:HG3	15	0.3
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	3	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	4	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	6	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	7	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	9	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	11	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	13	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	14	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	17	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	18	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	19	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	20	0.29
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	5	0.29
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	5	0.29
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	5	0.29
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	10	0.29
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	10	0.29
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	10	0.29
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	11	0.29
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	11	0.29
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	11	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	1	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	2	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	4	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	7	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	9	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	10	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	11	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	13	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	14	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	15	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	16	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	18	0.29
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	19	0.29
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	1	0.29
(2,1477)	1:600:A:PHE:HA	1:604:A:PHE:HA	8	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	12	0.29
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	1	0.29
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	8	0.29
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	10	0.29
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	12	0.29
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	17	0.29
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	20	0.29
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	4	0.29
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	16	0.29
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	2	0.29
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	14	0.29
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	19	0.29
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	12	0.29
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	17	0.29
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	16	0.29
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	7	0.29
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	3	0.29
(2,991)	1:580:A:LYS:H	1:596:A:CYS:H	3	0.29
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	5	0.29
(2,872)	1:575:A:CYS:HA	1:596:A:CYS:H	17	0.29
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	10	0.29
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	10	0.29
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	10	0.29
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	11	0.29
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	11	0.29
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	11	0.29
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	7	0.29
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	13	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	1	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	7	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	8	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	10	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	11	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	13	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	15	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	16	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	18	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	19	0.29
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	20	0.29
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	11	0.29
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	13	0.29
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	20	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	11	0.29
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	15	0.29
(2,571)	1:563:A:ALA:HA	1:564:A:MET:H	11	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	3	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	3	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	3	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	8	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	8	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	8	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	11	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	11	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	11	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB1	13	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB2	13	0.29
(2,546)	1:562:A:THR:HA	1:563:A:ALA:HB3	13	0.29
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	3	0.29
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	3	0.29
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	3	0.29
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	10	0.29
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	10	0.29
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	10	0.29
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	12	0.29
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	12	0.29
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	12	0.29
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	15	0.29
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	15	0.29
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	15	0.29
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	17	0.29
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	17	0.29
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	17	0.29
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	2	0.29
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	3	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	3	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	3	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	3	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	10	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	10	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	10	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	13	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	13	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	13	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	15	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	15	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	15	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	17	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	17	0.29
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	17	0.29
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	2	0.29
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	4	0.29
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	7	0.29
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	9	0.29
(2,339)	1:554:A:LYS:HB2	1:555:A:PRO:HD3	16	0.29
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	11	0.29
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	7	0.29
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	1	0.29
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	2	0.29
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	4	0.29
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	8	0.29
(2,190)	1:548:A:LEU:HA	1:556:A:ILE:H	14	0.29
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	18	0.29
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	18	0.29
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	18	0.29
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	20	0.29
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	20	0.29
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	20	0.29
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	4	0.29
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	14	0.29
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	17	0.29
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	18	0.29
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	5	0.29
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	5	0.29
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	5	0.29
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	6	0.29
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	6	0.29
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	6	0.29
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	15	0.29
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	15	0.29
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	15	0.29
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	16	0.29
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	16	0.29
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	16	0.29
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	9	0.29
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	10	0.29
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	3	0.29
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	3	0.29
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	1	0.28
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	2	0.28
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	5	0.28
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	8	0.28
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	10	0.28
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	12	0.28
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	15	0.28
(2,1573)	1:603:A:LEU:HG	1:605:A:CYS:H	16	0.28
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	1	0.28
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	1	0.28
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	1	0.28
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	2	0.28
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	2	0.28
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	2	0.28
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	8	0.28
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	8	0.28
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	8	0.28
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	16	0.28
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	16	0.28
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	16	0.28
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	20	0.28
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	20	0.28
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	20	0.28
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	3	0.28
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	5	0.28
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	6	0.28
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	8	0.28
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	12	0.28
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	17	0.28
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	11	0.28
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	16	0.28
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	3	0.28
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	6	0.28
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	20	0.28
(2,1328)	1:593:A:LYS:HA	1:594:A:PRO:HG2	5	0.28
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	11	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	1	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	2	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	3	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	5	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	6	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	7	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	8	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	9	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	10	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	11	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	12	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	13	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	14	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	15	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	16	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	17	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	18	0.28
(2,1254)	1:590:A:GLN:HE21	1:590:A:GLN:HG3	19	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	4	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	7	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	8	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	9	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	10	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	11	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	13	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	15	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	16	0.28
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	18	0.28
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	6	0.28
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	6	0.28
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	11	0.28
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	2	0.28
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	9	0.28
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	6	0.28
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	8	0.28
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	8	0.28
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	8	0.28
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	20	0.28
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	20	0.28
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	20	0.28
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	11	0.28
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	11	0.28
(2,707)	1:569:A:HIS:H	1:572:A:HIS:H	15	0.28
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	2	0.28
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	20	0.28
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	14	0.28
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	2	0.28
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	5	0.28
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	20	0.28
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	3	0.28
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	3	0.28
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	3	0.28
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	6	0.28
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	6	0.28
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	6	0.28
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	7	0.28
(2,453)	1:560:A:CYS:HB3	1:561:A:ILE:H	11	0.28
(2,444)	1:559:A:ARG:HD3	1:560:A:CYS:H	7	0.28
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	5	0.28
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	8	0.28
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	8	0.28
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	8	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	1	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	3	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	4	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	5	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	6	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	8	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	9	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	13	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	14	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	15	0.28
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	16	0.28
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	20	0.28
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	20	0.28
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	20	0.28
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	15	0.28
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	17	0.28
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	17	0.28
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	17	0.28
(2,200)	1:549:A:CYS:HB2	1:551:A:GLY:H	16	0.28
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	3	0.28
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	13	0.28
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	12	0.28
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	12	0.28
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	12	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	14	0.28
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	14	0.28
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	14	0.28
(2,176)	1:548:A:LEU:HB2	1:554:A:LYS:H	7	0.28
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	4	0.28
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	4	0.28
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	4	0.28
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	7	0.28
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	7	0.28
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	7	0.28
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	6	0.28
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	8	0.28
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	4	0.28
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	17	0.28
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	19	0.28
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	17	0.28
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	18	0.28
(1,430)	1:559:A:ARG:HD3	1:560:A:CYS:H	7	0.28
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	13	0.28
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	10	0.27
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	11	0.27
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	16	0.27
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	9	0.27
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	9	0.27
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	9	0.27
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	13	0.27
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	13	0.27
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	13	0.27
(2,1491)	1:601:A:LEU:HG	1:601:A:LEU:H	20	0.27
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	11	0.27
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	11	0.27
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	11	0.27
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	16	0.27
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	16	0.27
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	16	0.27
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	10	0.27
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	18	0.27
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	3	0.27
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	20	0.27
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	7	0.27
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	9	0.27
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	7	0.27
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	3	0.27
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	9	0.27
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	18	0.27
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	19	0.27
(2,1155)	1:588:A:LYS:HB3	1:588:A:LYS:H	1	0.27
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	1	0.27
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	5	0.27
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	7	0.27
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	1	0.27
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	3	0.27
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	4	0.27
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	12	0.27
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	17	0.27
(2,996)	1:580:A:LYS:HG2	1:596:A:CYS:H	5	0.27
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	5	0.27
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	5	0.27
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	5	0.27
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	20	0.27
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	3	0.27
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	20	0.27
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	4	0.27
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	5	0.27
(2,666)	1:568:A:PHE:HB2	1:569:A:HIS:H	6	0.27
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	1	0.27
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	2	0.27
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	5	0.27
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	10	0.27
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	12	0.27
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	18	0.27
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	19	0.27
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	14	0.27
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	3	0.27
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	5	0.27
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	13	0.27
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	20	0.27
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	16	0.27
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	11	0.27
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	11	0.27
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	11	0.27
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	19	0.27
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	20	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	20	0.27
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	20	0.27
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	7	0.27
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	12	0.27
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	18	0.27
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	10	0.27
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	10	0.27
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	10	0.27
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	9	0.27
(2,182)	1:548:A:LEU:HD11	1:555:A:PRO:HG2	9	0.27
(2,182)	1:548:A:LEU:HD12	1:555:A:PRO:HG2	9	0.27
(2,182)	1:548:A:LEU:HD13	1:555:A:PRO:HG2	9	0.27
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	3	0.27
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	3	0.27
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	3	0.27
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	8	0.27
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	8	0.27
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	8	0.27
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	9	0.27
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	9	0.27
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	9	0.27
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	12	0.27
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	12	0.27
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	12	0.27
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	13	0.27
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	13	0.27
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	13	0.27
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	14	0.27
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	14	0.27
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	14	0.27
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	18	0.27
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	18	0.27
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	18	0.27
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	5	0.27
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	6	0.27
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	15	0.27
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	8	0.27
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	9	0.27
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	12	0.27
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	13	0.27
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	14	0.27
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	16	0.27
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	8	0.26
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	15	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	3	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	3	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	3	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	6	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	6	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	6	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	10	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	10	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	10	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	11	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	11	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	11	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	12	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	12	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	12	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	14	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	14	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	14	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	16	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	16	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	16	0.26
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	17	0.26
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	17	0.26
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	17	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	3	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	5	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	6	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	7	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	8	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	12	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	15	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	17	0.26
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	20	0.26
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	4	0.26
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	4	0.26
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	4	0.26
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	6	0.26
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	6	0.26
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	6	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	14	0.26
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	14	0.26
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	14	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	2	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	2	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	2	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	4	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	4	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	4	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	6	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	6	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	6	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	7	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	7	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	7	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	9	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	9	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	9	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	10	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	10	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	10	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	13	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	13	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	13	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	19	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	19	0.26
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	19	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	1	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	3	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	4	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	6	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	7	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	9	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	13	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	14	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	15	0.26
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	19	0.26
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	12	0.26
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	11	0.26
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	5	0.26
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	4	0.26
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	14	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	16	0.26
(2,1255)	1:590:A:GLN:HE22	1:590:A:GLN:HA	17	0.26
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	8	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	4	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	8	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	9	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	10	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	13	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	14	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	15	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	16	0.26
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	20	0.26
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	20	0.26
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	8	0.26
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	12	0.26
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	17	0.26
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	20	0.26
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD11	5	0.26
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD12	5	0.26
(2,989)	1:580:A:LYS:HG3	1:582:A:LEU:HD13	5	0.26
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	8	0.26
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	8	0.26
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	8	0.26
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	18	0.26
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	4	0.26
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	6	0.26
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	7	0.26
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	13	0.26
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	1	0.26
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	5	0.26
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	8	0.26
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	18	0.26
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	20	0.26
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	11	0.26
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	6	0.26
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	7	0.26
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	8	0.26
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	16	0.26
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	17	0.26
(2,605)	1:564:A:MET:HB2	1:565:A:ALA:HA	11	0.26
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	1	0.26
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	6	0.26
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	7	0.26
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	8	0.26
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	16	0.26
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	5	0.26
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	11	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	1	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	2	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	4	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	6	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	8	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	14	0.26
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	16	0.26
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	19	0.26
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	11	0.26
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	11	0.26
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	11	0.26
(2,541)	1:561:A:ILE:HG21	1:584:A:LYS:HG3	20	0.26
(2,541)	1:561:A:ILE:HG22	1:584:A:LYS:HG3	20	0.26
(2,541)	1:561:A:ILE:HG23	1:584:A:LYS:HG3	20	0.26
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	16	0.26
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	1	0.26
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	1	0.26
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	1	0.26
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	18	0.26
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	18	0.26
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	18	0.26
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	2	0.26
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	10	0.26
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	11	0.26
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	19	0.26
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	17	0.26
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	17	0.26
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	17	0.26
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	14	0.26
(2,171)	1:548:A:LEU:HD11	1:553:A:GLN:H	1	0.26
(2,171)	1:548:A:LEU:HD12	1:553:A:GLN:H	1	0.26
(2,171)	1:548:A:LEU:HD13	1:553:A:GLN:H	1	0.26
(2,164)	1:548:A:LEU:HB3	1:553:A:GLN:HE21	13	0.26
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	2	0.26
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	2	0.26
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	10	0.26
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	10	0.26
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	10	0.26
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	11	0.26
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	11	0.26
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	11	0.26
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	17	0.26
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	17	0.26
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	17	0.26
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	20	0.26
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	20	0.26
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	20	0.26
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	9	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	1	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	2	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	3	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	5	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	6	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	7	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	10	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	11	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	19	0.26
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	20	0.26
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	17	0.26
(1,549)	1:562:A:THR:HB	1:567:A:LYS:HE3	20	0.26
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	17	0.26
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	1	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	2	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	4	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	5	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	7	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	10	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	11	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	13	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	18	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	19	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	20	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	1	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	1	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	1	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	2	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	2	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	4	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	4	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	4	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	5	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	5	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	5	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	7	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	7	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	7	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	8	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	8	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	8	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	9	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	9	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	9	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	13	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	13	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	13	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	15	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	15	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	15	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	18	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	18	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	18	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	19	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	19	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	19	0.25
(2,1567)	1:603:A:LEU:HD21	1:604:A:PHE:H	20	0.25
(2,1567)	1:603:A:LEU:HD22	1:604:A:PHE:H	20	0.25
(2,1567)	1:603:A:LEU:HD23	1:604:A:PHE:H	20	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	1	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	2	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	3	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	4	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	6	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	7	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	8	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	9	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	13	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	14	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	15	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	18	0.25
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	19	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	1	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	2	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	4	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	9	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	13	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	14	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	18	0.25
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	19	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	4	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	9	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	10	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	11	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	14	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	15	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	16	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	18	0.25
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	19	0.25
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	12	0.25
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	12	0.25
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	12	0.25
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	18	0.25
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	18	0.25
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	18	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	1	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	1	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	1	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	3	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	3	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	3	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	5	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	5	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	5	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	8	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	8	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	8	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	12	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	12	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	12	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	14	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	14	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	18	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	18	0.25
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	18	0.25
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	2	0.25
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	5	0.25
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	8	0.25
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	12	0.25
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	17	0.25
(2,1454)	1:599:A:CYS:HA	1:603:A:LEU:HG	20	0.25
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	10	0.25
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	11	0.25
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	16	0.25
(2,1411)	1:598:A:ASN:HA	1:598:A:ASN:HD21	15	0.25
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	1	0.25
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	5	0.25
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	10	0.25
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	19	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	1	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	2	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	6	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	7	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	10	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	11	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	12	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	13	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	15	0.25
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	17	0.25
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	20	0.25
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	7	0.25
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	2	0.25
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	19	0.25
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	8	0.25
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	10	0.25
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	1	0.25
(2,808)	1:574:A:VAL:HG11	1:581:A:GLN:HG3	1	0.25
(2,808)	1:574:A:VAL:HG12	1:581:A:GLN:HG3	1	0.25
(2,808)	1:574:A:VAL:HG13	1:581:A:GLN:HG3	1	0.25
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	7	0.25
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	2	0.25
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	5	0.25
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	19	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	2	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	4	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	6	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	7	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	9	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	10	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	11	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	12	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	13	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	14	0.25
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	17	0.25
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	15	0.25
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	3	0.25
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	4	0.25
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	9	0.25
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	13	0.25
(2,636)	1:566:A:LYS:HA	1:567:A:LYS:HE3	20	0.25
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	9	0.25
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	15	0.25
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	17	0.25
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	19	0.25
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	2	0.25
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	3	0.25
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	6	0.25
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	13	0.25
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	14	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	7	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	9	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	10	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	12	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	15	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	17	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	18	0.25
(2,599)	1:564:A:MET:HB3	1:565:A:ALA:H	19	0.25
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	4	0.25
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	6	0.25
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	7	0.25
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	14	0.25
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	14	0.25
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	14	0.25
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	17	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,305)	1:552:A:CYS:H	1:569:A:HIS:H	20	0.25
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	2	0.25
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	2	0.25
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	2	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	2	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	2	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	2	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	12	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	12	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	12	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	18	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	18	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	18	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	19	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	19	0.25
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	19	0.25
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	12	0.25
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	18	0.25
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	10	0.25
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	18	0.25
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	19	0.25
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	19	0.25
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	19	0.25
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	1	0.25
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	3	0.25
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	7	0.25
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	13	0.25
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	14	0.25
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	16	0.25
(2,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	20	0.25
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	12	0.25
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	16	0.25
(1,1396)	1:598:A:ASN:HA	1:598:A:ASN:HD21	15	0.25
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	18	0.25
(1,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	20	0.25
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	12	0.25
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	16	0.25
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	3	0.24
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	6	0.24
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	9	0.24
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	12	0.24
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	16	0.24
(2,1577)	1:604:A:PHE:H	1:605:A:CYS:HA	17	0.24
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	5	0.24
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	12	0.24
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	20	0.24
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	11	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	1	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	2	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	3	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	5	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	6	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	7	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	8	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	12	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	13	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	17	0.24
(2,1510)	1:602:A:LYS:HA	1:602:A:LYS:HG2	20	0.24
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	7	0.24
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	7	0.24
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	7	0.24
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	17	0.24
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	17	0.24
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	17	0.24
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	19	0.24
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	19	0.24
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	19	0.24
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	17	0.24
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	17	0.24
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	17	0.24
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	20	0.24
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	20	0.24
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	20	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	1	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	2	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	4	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	9	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	11	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	13	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	14	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	15	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	16	0.24
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	19	0.24
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	6	0.24
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	7	0.24
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	8	0.24
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	9	0.24
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	18	0.24
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	9	0.24
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	1	0.24
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	6	0.24
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	12	0.24
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	17	0.24
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	11	0.24
(2,1131)	1:586:A:THR:HB	1:587:A:PHE:H	5	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	1	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	3	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	5	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	7	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	8	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	9	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	11	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	12	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	15	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	17	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	18	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	19	0.24
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	20	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	2	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	3	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	4	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	5	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	6	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	8	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	9	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	10	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	12	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	13	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	14	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	15	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	16	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	17	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	18	0.24
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	20	0.24
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	8	0.24
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	8	0.24
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	8	0.24
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	1	0.24
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	8	0.24
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	11	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	1	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	8	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	9	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	10	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	12	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	14	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	15	0.24
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	17	0.24
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	3	0.24
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	15	0.24
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	16	0.24
(2,678)	1:568:A:PHE:HB2	1:573:A:PHE:H	19	0.24
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	10	0.24
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	12	0.24
(2,604)	1:564:A:MET:HB3	1:565:A:ALA:HA	18	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	1	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	4	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	7	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	8	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	9	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	12	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	16	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	17	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	18	0.24
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	19	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	3	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	3	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	3	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	4	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	4	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	4	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	7	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	7	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	7	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	8	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	8	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	13	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	13	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	13	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	14	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	14	0.24
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	14	0.24
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	1	0.24
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	1	0.24
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	1	0.24
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	1	0.24
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	1	0.24
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	1	0.24
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG21	12	0.24
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG22	12	0.24
(2,369)	1:555:A:PRO:HB3	1:557:A:THR:HG23	12	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	1	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	3	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	6	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	8	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	12	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	13	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	14	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	15	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	16	0.24
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	18	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	1	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	1	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	1	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	10	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	10	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	10	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	17	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	17	0.24
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	17	0.24
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	11	0.24
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	11	0.24
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	11	0.24
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	14	0.24
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	14	0.24
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	14	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	8	0.24
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	9	0.24
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	12	0.24
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	14	0.24
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	15	0.24
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	17	0.24
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	12	0.24
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	8	0.24
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	12	0.24
(2,153)	1:548:A:LEU:HB3	1:551:A:GLY:H	18	0.24
(2,146)	1:548:A:LEU:HB2	1:549:A:CYS:H	4	0.24
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	1	0.24
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	17	0.24
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	20	0.24
(2,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	18	0.24
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	5	0.24
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	8	0.24
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	9	0.24
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	12	0.24
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	14	0.24
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	15	0.24
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	17	0.24
(1,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	18	0.24
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	5	0.24
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	2	0.23
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	8	0.23
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	10	0.23
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	11	0.23
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	15	0.23
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	16	0.23
(2,1540)	1:602:A:LYS:H	1:603:A:LEU:HB3	17	0.23
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	10	0.23
(2,1524)	1:602:A:LYS:HG2	1:602:A:LYS:H	16	0.23
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	11	0.23
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	14	0.23
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	15	0.23
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD21	15	0.23
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD22	15	0.23
(2,1455)	1:599:A:CYS:H	1:603:A:LEU:HD23	15	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	1	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	2	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	4	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	6	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	7	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	8	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	9	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	13	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	14	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	18	0.23
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	19	0.23
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	10	0.23
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	11	0.23
(2,1418)	1:598:A:ASN:H	1:598:A:ASN:HD22	16	0.23
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	7	0.23
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	8	0.23
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	10	0.23
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	4	0.23
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	14	0.23
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	16	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	1	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	2	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	3	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	4	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	5	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	6	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	8	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	9	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	10	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	11	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	12	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	14	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	15	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	17	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	18	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	19	0.23
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	20	0.23
(2,1323)	1:593:A:LYS:H	1:594:A:PRO:HD3	5	0.23
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	17	0.23
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	5	0.23
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	8	0.23
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	5	0.23
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	1	0.23
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	10	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1142)	1:587:A:PHE:HA	1:588:A:LYS:HG3	18	0.23
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	10	0.23
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	5	0.23
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	7	0.23
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	2	0.23
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	6	0.23
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	10	0.23
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	13	0.23
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	14	0.23
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	1	0.23
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	7	0.23
(2,1005)	1:581:A:GLN:HG2	1:581:A:GLN:HE22	11	0.23
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	4	0.23
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	10	0.23
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	16	0.23
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	3	0.23
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	5	0.23
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	15	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	1	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	2	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	3	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	4	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	6	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	10	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	12	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	13	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	14	0.23
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	16	0.23
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	10	0.23
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	15	0.23
(2,602)	1:564:A:MET:H	1:565:A:ALA:HA	20	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	1	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	1	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	1	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	6	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	6	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	6	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	16	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	16	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	16	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	19	0.23
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	19	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	19	0.23
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	14	0.23
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	14	0.23
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	14	0.23
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	20	0.23
(2,406)	1:556:A:ILE:HG13	1:568:A:PHE:HA	11	0.23
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	4	0.23
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	5	0.23
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	7	0.23
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	9	0.23
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	10	0.23
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	10	0.23
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	10	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	8	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	8	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	8	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	13	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	13	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	13	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	14	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	14	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	14	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	15	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	15	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	15	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	18	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	18	0.23
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	18	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	1	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	1	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	1	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	8	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	8	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	8	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	9	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	9	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	9	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	13	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	13	0.23
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	13	0.23
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	18	0.23
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	1	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	3	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	4	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	5	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	6	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	7	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	13	0.23
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	16	0.23
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	17	0.23
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	2	0.23
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	4	0.23
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	4	0.23
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	4	0.23
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	5	0.23
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	5	0.23
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	5	0.23
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	6	0.23
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	6	0.23
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	6	0.23
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	15	0.23
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	15	0.23
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	15	0.23
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	16	0.23
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	16	0.23
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	16	0.23
(2,90)	1:545:A:ARG:H	1:546:A:GLY:HA3	18	0.23
(2,68)	1:542:A:HIS:HB3	1:543:A:GLU:H	15	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	1	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	3	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	4	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	5	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	6	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	7	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	13	0.23
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	16	0.23
(1,90)	1:545:A:ARG:H	1:546:A:GLY:HA3	18	0.23
(1,68)	1:542:A:HIS:HB3	1:543:A:GLU:H	15	0.23
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	1	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	3	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	4	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	5	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	7	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	12	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	13	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	14	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	17	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	19	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	20	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	1	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	2	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	3	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	4	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	6	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	7	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	8	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	9	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	10	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	12	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	13	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	16	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	17	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	18	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	19	0.22
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	20	0.22
(2,1504)	1:601:A:LEU:HD21	1:605:A:CYS:HB2	3	0.22
(2,1504)	1:601:A:LEU:HD22	1:605:A:CYS:HB2	3	0.22
(2,1504)	1:601:A:LEU:HD23	1:605:A:CYS:HB2	3	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	1	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	7	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	8	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	9	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	10	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	14	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	16	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	17	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	18	0.22
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	19	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	1	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	2	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	4	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	7	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	8	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	13	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	14	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	18	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	19	0.22
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	20	0.22
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	5	0.22
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	12	0.22
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	20	0.22
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	20	0.22
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	2	0.22
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	11	0.22
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	13	0.22
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	17	0.22
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	7	0.22
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	13	0.22
(2,1341)	1:594:A:PRO:HB2	1:595:A:TYR:HA	16	0.22
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	2	0.22
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	4	0.22
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	10	0.22
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	7	0.22
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	18	0.22
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	13	0.22
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	14	0.22
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	15	0.22
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	4	0.22
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	11	0.22
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	13	0.22
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	19	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	2	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	4	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	6	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	8	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	10	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	11	0.22
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	16	0.22
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	4	0.22
(2,1010)	1:581:A:GLN:HE22	1:581:A:GLN:HB2	16	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	1	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	2	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	3	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	5	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	7	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	8	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	9	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	11	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	12	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	13	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	14	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	15	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	17	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	18	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	19	0.22
(2,1000)	1:581:A:GLN:HG3	1:581:A:GLN:HE21	20	0.22
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD11	5	0.22
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD12	5	0.22
(2,985)	1:580:A:LYS:HE3	1:582:A:LEU:HD13	5	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	2	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	3	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	4	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	6	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	7	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	9	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	11	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	12	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	13	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	14	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	15	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	16	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	17	0.22
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	19	0.22
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	2	0.22
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	9	0.22
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	17	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	3	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	4	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	9	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	12	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	13	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	14	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	17	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	18	0.22
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	19	0.22
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,726)	1:571:A:GLU:HB2	1:571:A:GLU:H	18	0.22
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	5	0.22
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	7	0.22
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	8	0.22
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	17	0.22
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	19	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	2	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	2	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	2	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	5	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	5	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	5	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	9	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	9	0.22
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	9	0.22
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	1	0.22
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	7	0.22
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	8	0.22
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	14	0.22
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	15	0.22
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	18	0.22
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	19	0.22
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	2	0.22
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	2	0.22
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	2	0.22
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	9	0.22
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	9	0.22
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	9	0.22
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	13	0.22
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	13	0.22
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	13	0.22
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	17	0.22
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	17	0.22
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	17	0.22
(2,433)	1:559:A:ARG:HA	1:559:A:ARG:HG2	11	0.22
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	9	0.22
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	9	0.22
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	9	0.22
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	17	0.22
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	17	0.22
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	17	0.22
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	18	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	18	0.22
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	18	0.22
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	19	0.22
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	19	0.22
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	19	0.22
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	20	0.22
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	20	0.22
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	20	0.22
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	2	0.22
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	10	0.22
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	11	0.22
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	17	0.22
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	19	0.22
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	12	0.22
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	12	0.22
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	12	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	3	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	3	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	3	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	9	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	9	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	9	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	12	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	12	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	12	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	16	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	16	0.22
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	16	0.22
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	3	0.22
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	3	0.22
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	3	0.22
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	16	0.22
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	16	0.22
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	16	0.22
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	20	0.22
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	2	0.22
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	10	0.22
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	11	0.22
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	19	0.22
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	10	0.22
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	11	0.22
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	19	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	20	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	3	0.22
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	3	0.22
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	3	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	7	0.22
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	7	0.22
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	7	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	8	0.22
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	8	0.22
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	8	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	12	0.22
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	12	0.22
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	12	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	13	0.22
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	13	0.22
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	13	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	14	0.22
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	14	0.22
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	14	0.22
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	18	0.22
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	18	0.22
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	18	0.22
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	16	0.22
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	16	0.22
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	16	0.22
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	8	0.22
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	9	0.22
(2,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	1	0.22
(2,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	10	0.22
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	5	0.22
(1,419)	1:559:A:ARG:HA	1:559:A:ARG:HG2	11	0.22
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	2	0.22
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	10	0.22
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	11	0.22
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	19	0.22
(1,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	1	0.22
(1,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	10	0.22
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	9	0.21
(2,1564)	1:603:A:LEU:H	1:604:A:PHE:HA	18	0.21
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	5	0.21
(2,1507)	1:601:A:LEU:HB2	1:605:A:CYS:H	15	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	3	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	4	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	5	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	6	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	11	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	12	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	13	0.21
(2,1466)	1:600:A:PHE:H	1:601:A:LEU:HB3	20	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	3	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	5	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	6	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	10	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	11	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	12	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	15	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	16	0.21
(2,1462)	1:600:A:PHE:HA	1:601:A:LEU:HB3	17	0.21
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	15	0.21
(2,1411)	1:598:A:ASN:HA	1:598:A:ASN:HD21	17	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	1	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	2	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	3	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	4	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	5	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	6	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	7	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	8	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	9	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	10	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	11	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	12	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	13	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	14	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	15	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	16	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	17	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	18	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	19	0.21
(2,1289)	1:591:A:ASN:HB2	1:591:A:ASN:HD22	20	0.21
(2,1265)	1:590:A:GLN:HB2	1:591:A:ASN:HA	20	0.21
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	3	0.21
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	11	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	15	0.21
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	18	0.21
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	19	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	2	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	6	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	12	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	13	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	14	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	15	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	17	0.21
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	19	0.21
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	19	0.21
(2,1109)	1:584:A:LYS:HD3	1:585:A:GLY:HA3	18	0.21
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	2	0.21
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	14	0.21
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	16	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	1	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	3	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	9	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	12	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	13	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	14	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	15	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	17	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	19	0.21
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	20	0.21
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	18	0.21
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	1	0.21
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	5	0.21
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	8	0.21
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	10	0.21
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	18	0.21
(2,979)	1:580:A:LYS:HB3	1:581:A:GLN:H	20	0.21
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	18	0.21
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	18	0.21
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	4	0.21
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	12	0.21
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	2	0.21
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	6	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	2	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	3	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	5	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	6	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	7	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	8	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	11	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	12	0.21
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	19	0.21
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	2	0.21
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	9	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	10	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	10	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	10	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	12	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	12	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	12	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	15	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	15	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	15	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	17	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	17	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	17	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	18	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	18	0.21
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	18	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	2	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	3	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	5	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	9	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	11	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	12	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	13	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	17	0.21
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	20	0.21
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	12	0.21
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	12	0.21
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	12	0.21
(2,479)	1:561:A:ILE:HG21	1:562:A:THR:HA	20	0.21
(2,479)	1:561:A:ILE:HG22	1:562:A:THR:HA	20	0.21
(2,479)	1:561:A:ILE:HG23	1:562:A:THR:HA	20	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	2	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	2	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	3	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	3	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	3	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	5	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	5	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	5	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	6	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	6	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	6	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	7	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	7	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	7	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	10	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	10	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	10	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	11	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	11	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	11	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	12	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	12	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	12	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	13	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	13	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	13	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	15	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	15	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	15	0.21
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	16	0.21
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	16	0.21
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	16	0.21
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	11	0.21
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	16	0.21
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	19	0.21
(2,294)	1:552:A:CYS:H	1:553:A:GLN:HA	20	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	2	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	2	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	2	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	14	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	14	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	14	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	18	0.21
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	18	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	5	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	5	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	5	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	6	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	6	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	6	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	7	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	7	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	7	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	11	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	11	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	11	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	19	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	19	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	19	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	20	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	20	0.21
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	20	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	4	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	4	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	4	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	5	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	5	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	5	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	15	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	15	0.21
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	15	0.21
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	10	0.21
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	11	0.21
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	14	0.21
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	17	0.21
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	17	0.21
(2,198)	1:549:A:CYS:H	1:550:A:SER:HA	20	0.21
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	16	0.21
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	17	0.21
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	1	0.21
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	1	0.21
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	1	0.21
(2,154)	1:548:A:LEU:HD11	1:552:A:CYS:H	9	0.21
(2,154)	1:548:A:LEU:HD12	1:552:A:CYS:H	9	0.21
(2,154)	1:548:A:LEU:HD13	1:552:A:CYS:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	3	0.21
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	3	0.21
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	3	0.21
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	10	0.21
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	10	0.21
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	10	0.21
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	12	0.21
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	12	0.21
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	12	0.21
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	13	0.21
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	13	0.21
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	13	0.21
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	6	0.21
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	17	0.21
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	10	0.21
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	12	0.21
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	14	0.21
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	11	0.21
(2,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	18	0.21
(2,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	14	0.21
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	8	0.21
(1,1396)	1:598:A:ASN:HA	1:598:A:ASN:HD21	17	0.21
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	8	0.21
(1,1094)	1:584:A:LYS:HD3	1:585:A:GLY:HA3	18	0.21
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	3	0.21
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	5	0.21
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	8	0.21
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	10	0.21
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	11	0.21
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	12	0.21
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	14	0.21
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	17	0.21
(1,192)	1:549:A:CYS:H	1:550:A:SER:HA	20	0.21
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	11	0.21
(1,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	18	0.21
(1,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	14	0.21
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	8	0.21
(2,1451)	1:599:A:CYS:H	1:602:A:LYS:HB3	17	0.2
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	15	0.2
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	3	0.2
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	6	0.2
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	17	0.2
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	14	0.2
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	18	0.2
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	19	0.2
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	15	0.2
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	3	0.2
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	11	0.2
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	2	0.2
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	9	0.2
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	12	0.2
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	14	0.2
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	16	0.2
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	17	0.2
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	9	0.2
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	11	0.2
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	16	0.2
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	7	0.2
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	9	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	1	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	10	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	13	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	14	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	15	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	19	0.2
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	20	0.2
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	1	0.2
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	1	0.2
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	1	0.2
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	13	0.2
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	13	0.2
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	13	0.2
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	11	0.2
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	15	0.2
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	8	0.2
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	2	0.2
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	7	0.2
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	14	0.2
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	15	0.2
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	5	0.2
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	8	0.2
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	10	0.2
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	10	0.2
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	16	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	1	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	9	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	10	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	13	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	14	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	15	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	16	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	17	0.2
(2,746)	1:572:A:HIS:HB3	1:572:A:HIS:H	18	0.2
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	6	0.2
(2,653)	1:567:A:LYS:HB2	1:568:A:PHE:H	18	0.2
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	2	0.2
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	10	0.2
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	17	0.2
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	19	0.2
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB1	20	0.2
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB2	20	0.2
(2,551)	1:562:A:THR:H	1:563:A:ALA:HB3	20	0.2
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	4	0.2
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	6	0.2
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	10	0.2
(2,549)	1:562:A:THR:HB	1:563:A:ALA:H	16	0.2
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	19	0.2
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	19	0.2
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	19	0.2
(2,433)	1:559:A:ARG:HA	1:559:A:ARG:HG2	7	0.2
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	8	0.2
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	8	0.2
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	8	0.2
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	14	0.2
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	14	0.2
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	14	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	1	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	2	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	3	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	4	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	5	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	6	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	7	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	9	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	10	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	12	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	13	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	14	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	15	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	17	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	18	0.2
(2,358)	1:555:A:PRO:HB3	1:555:A:PRO:HD2	20	0.2
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	4	0.2
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	19	0.2
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	9	0.2
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	9	0.2
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	9	0.2
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	11	0.2
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	11	0.2
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	11	0.2
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	6	0.2
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	6	0.2
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	6	0.2
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD11	7	0.2
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD12	7	0.2
(2,250)	1:550:A:SER:HA	1:556:A:ILE:HD13	7	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	1	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	2	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	3	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	4	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	5	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	8	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	9	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	12	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	13	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	15	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	18	0.2
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	19	0.2
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	12	0.2
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	14	0.2
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	18	0.2
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	20	0.2
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	6	0.2
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	7	0.2
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	15	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	1	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	1	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	1	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	2	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	2	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	2	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	5	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	5	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	5	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	7	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	7	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	7	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	8	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	8	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	8	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	11	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	11	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	11	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	14	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	14	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	14	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	15	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	15	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	15	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	18	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	18	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	18	0.2
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	20	0.2
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	20	0.2
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	20	0.2
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	19	0.2
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	4	0.2
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	7	0.2
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	11	0.2
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	18	0.2
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	19	0.2
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	4	0.2
(2,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	14	0.2
(2,68)	1:542:A:HIS:HB3	1:543:A:GLU:H	12	0.2
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	15	0.2
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	15	0.2
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	6	0.2
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	7	0.2
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	11	0.2
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	12	0.2
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	18	0.2
(1,419)	1:559:A:ARG:HA	1:559:A:ARG:HG2	7	0.2
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	3	0.2
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	5	0.2
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	6	0.2
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	7	0.2
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	13	0.2
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	15	0.2
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	1	0.2
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	8	0.2
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	10	0.2
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	13	0.2
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	18	0.2
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	20	0.2
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	4	0.2
(1,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	14	0.2
(1,68)	1:542:A:HIS:HB3	1:543:A:GLU:H	12	0.2
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	3	0.19
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	3	0.19
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	3	0.19
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	5	0.19
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	5	0.19
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	5	0.19
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	6	0.19
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	6	0.19
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	6	0.19
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	12	0.19
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	12	0.19
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	12	0.19
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	17	0.19
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	17	0.19
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	17	0.19
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	18	0.19
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	18	0.19
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	18	0.19
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	19	0.19
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	19	0.19
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	17	0.19
(2,1386)	1:597:A:GLN:HA	1:597:A:GLN:HG3	5	0.19
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	16	0.19
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	12	0.19
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	3	0.19
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	4	0.19
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	13	0.19
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	3	0.19
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	4	0.19
(2,1100)	1:584:A:LYS:HB3	1:584:A:LYS:HE3	1	0.19
(2,1041)	1:582:A:LEU:HG	1:582:A:LEU:H	18	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	2	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	3	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	4	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	5	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	6	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	7	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	8	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	9	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	11	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	12	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	16	0.19
(2,1013)	1:581:A:GLN:HA	1:582:A:LEU:HG	17	0.19
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	14	0.19
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	14	0.19
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	14	0.19
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	16	0.19
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	8	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	1	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	4	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	6	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	8	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	11	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	13	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	19	0.19
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	20	0.19
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	6	0.19
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	13	0.19
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	15	0.19
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	19	0.19
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	4	0.19
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	10	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	15	0.19
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	16	0.19
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	20	0.19
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	11	0.19
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	1	0.19
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	8	0.19
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	9	0.19
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	12	0.19
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	14	0.19
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	16	0.19
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	1	0.19
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	4	0.19
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	4	0.19
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	4	0.19
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	4	0.19
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	15	0.19
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	15	0.19
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	15	0.19
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	16	0.19
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	16	0.19
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	16	0.19
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	17	0.19
(2,433)	1:559:A:ARG:HA	1:559:A:ARG:HG2	4	0.19
(2,424)	1:557:A:THR:HG21	1:558:A:GLY:HA2	4	0.19
(2,424)	1:557:A:THR:HG22	1:558:A:GLY:HA2	4	0.19
(2,424)	1:557:A:THR:HG23	1:558:A:GLY:HA2	4	0.19
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	18	0.19
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	18	0.19
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	18	0.19
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	2	0.19
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	6	0.19
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	7	0.19
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	11	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	1	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	1	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	1	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	3	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	3	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	3	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	8	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	8	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	13	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	13	0.19
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	13	0.19
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	6	0.19
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	7	0.19
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	10	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	3	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	4	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	5	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	6	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	13	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	14	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	15	0.19
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	16	0.19
(2,193)	1:549:A:CYS:HA	1:550:A:SER:HB2	20	0.19
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	4	0.19
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	13	0.19
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	4	0.19
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	4	0.19
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	4	0.19
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	6	0.19
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	6	0.19
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	6	0.19
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	17	0.19
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	17	0.19
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	17	0.19
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	19	0.19
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	19	0.19
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	19	0.19
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	7	0.19
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	11	0.19
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	3	0.19
(2,104)	1:547:A:SER:HB3	1:547:A:SER:H	1	0.19
(2,104)	1:547:A:SER:HB3	1:547:A:SER:H	4	0.19
(2,104)	1:547:A:SER:HB3	1:547:A:SER:H	10	0.19
(2,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	10	0.19
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	17	0.19
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	12	0.19
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	10	0.19
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	4	0.19
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	16	0.19
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,419)	1:559:A:ARG:HA	1:559:A:ARG:HG2	4	0.19
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	8	0.19
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	9	0.19
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	16	0.19
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	3	0.19
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	9	0.19
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	15	0.19
(1,104)	1:547:A:SER:HB3	1:547:A:SER:H	1	0.19
(1,104)	1:547:A:SER:HB3	1:547:A:SER:H	4	0.19
(1,104)	1:547:A:SER:HB3	1:547:A:SER:H	10	0.19
(1,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	10	0.19
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	1	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	1	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	1	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	2	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	2	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	2	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	4	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	4	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	4	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	7	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	7	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	7	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	8	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	8	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	8	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	9	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	9	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	9	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	10	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	10	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	10	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	11	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	11	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	11	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	13	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	13	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	13	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	14	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	14	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	14	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	15	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	15	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	16	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	16	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	16	0.18
(2,1490)	1:601:A:LEU:HD21	1:601:A:LEU:H	20	0.18
(2,1490)	1:601:A:LEU:HD22	1:601:A:LEU:H	20	0.18
(2,1490)	1:601:A:LEU:HD23	1:601:A:LEU:H	20	0.18
(2,1347)	1:594:A:PRO:HB2	1:596:A:CYS:H	15	0.18
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	7	0.18
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	12	0.18
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	13	0.18
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	17	0.18
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	6	0.18
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	6	0.18
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	7	0.18
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	10	0.18
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	3	0.18
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	5	0.18
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	1	0.18
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	5	0.18
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	10	0.18
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	15	0.18
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	8	0.18
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	8	0.18
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	8	0.18
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	15	0.18
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	15	0.18
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	15	0.18
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	13	0.18
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	14	0.18
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	18	0.18
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	1	0.18
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	10	0.18
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	3	0.18
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	5	0.18
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	10	0.18
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	9	0.18
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	10	0.18
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	12	0.18
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	16	0.18
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	1	0.18
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	7	0.18
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	11	0.18
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	2	0.18
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	4	0.18
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	7	0.18
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	11	0.18
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	12	0.18
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	19	0.18
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	3	0.18
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	12	0.18
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	14	0.18
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	19	0.18
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	3	0.18
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	4	0.18
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	7	0.18
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	11	0.18
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	4	0.18
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	6	0.18
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	16	0.18
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	3	0.18
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	4	0.18
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	5	0.18
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	7	0.18
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	13	0.18
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	18	0.18
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	10	0.18
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	10	0.18
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	10	0.18
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	7	0.18
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	8	0.18
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	10	0.18
(2,433)	1:559:A:ARG:HA	1:559:A:ARG:HG2	16	0.18
(2,433)	1:559:A:ARG:HA	1:559:A:ARG:HG2	19	0.18
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	12	0.18
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	12	0.18
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	12	0.18
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	14	0.18
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	14	0.18
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	14	0.18
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	3	0.18
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	9	0.18
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	10	0.18
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	15	0.18
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	16	0.18
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	17	0.18
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	3	0.18
(2,311)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	2	0.18
(2,311)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	10	0.18
(2,311)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	11	0.18
(2,311)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	17	0.18
(2,311)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	19	0.18
(2,311)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	20	0.18
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	5	0.18
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	5	0.18
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	5	0.18
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	19	0.18
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	19	0.18
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	19	0.18
(2,238)	1:550:A:SER:H	1:551:A:GLY:H	16	0.18
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	1	0.18
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	10	0.18
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	11	0.18
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	17	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	1	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	2	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	7	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	8	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	9	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	11	0.18
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	12	0.18
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	1	0.18
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	3	0.18
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	5	0.18
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	8	0.18
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	2	0.18
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	4	0.18
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	9	0.18
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	18	0.18
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	13	0.18
(2,104)	1:547:A:SER:HB3	1:547:A:SER:H	20	0.18
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	14	0.18
(2,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	9	0.18
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	16	0.18
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	17	0.18
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	3	0.18
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	5	0.18
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	1	0.18
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	7	0.18
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	11	0.18
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	20	0.18
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	2	0.18
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	17	0.18
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	19	0.18
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	20	0.18
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	2	0.18
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	4	0.18
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	7	0.18
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	11	0.18
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	12	0.18
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	19	0.18
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	3	0.18
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	4	0.18
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	7	0.18
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	11	0.18
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	4	0.18
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	6	0.18
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	16	0.18
(1,419)	1:559:A:ARG:HA	1:559:A:ARG:HG2	16	0.18
(1,419)	1:559:A:ARG:HA	1:559:A:ARG:HG2	19	0.18
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	1	0.18
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	2	0.18
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	4	0.18
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	10	0.18
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	14	0.18
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	17	0.18
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	19	0.18
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	5	0.18
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	11	0.18
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	16	0.18
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	19	0.18
(1,297)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	2	0.18
(1,297)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	10	0.18
(1,297)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,297)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	17	0.18
(1,297)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	19	0.18
(1,297)	1:553:A:GLN:HG3	1:553:A:GLN:HE21	20	0.18
(1,104)	1:547:A:SER:HB3	1:547:A:SER:H	20	0.18
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	14	0.18
(1,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	4	0.18
(1,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	9	0.18
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	16	0.18
(2,1411)	1:598:A:ASN:HA	1:598:A:ASN:HD21	5	0.17
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	20	0.17
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	7	0.17
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	18	0.17
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	12	0.17
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	15	0.17
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	17	0.17
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	10	0.17
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	16	0.17
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	8	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	1	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	2	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	6	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	10	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	12	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	13	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	14	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	17	0.17
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	19	0.17
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	8	0.17
(2,1141)	1:587:A:PHE:HB2	1:587:A:PHE:H	20	0.17
(2,1081)	1:582:A:LEU:HG	1:596:A:CYS:HB2	18	0.17
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	14	0.17
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	7	0.17
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	7	0.17
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	7	0.17
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	19	0.17
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	19	0.17
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	19	0.17
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	2	0.17
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	7	0.17
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	9	0.17
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	10	0.17
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	19	0.17
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	5	0.17
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	18	0.17
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	1	0.17
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	6	0.17
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	7	0.17
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	3	0.17
(2,807)	1:574:A:VAL:HA	1:581:A:GLN:HG3	14	0.17
(2,749)	1:572:A:HIS:HB3	1:573:A:PHE:H	20	0.17
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	1	0.17
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	5	0.17
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	9	0.17
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	11	0.17
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	13	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	2	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	5	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	6	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	8	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	10	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	13	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	16	0.17
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	17	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	1	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	2	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	3	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	4	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	5	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	6	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	7	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	8	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	9	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	10	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	11	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	12	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	13	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	14	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	15	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	16	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	18	0.17
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	19	0.17
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	1	0.17
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	19	0.17
(2,584)	1:563:A:ALA:H	1:566:A:LYS:HB3	6	0.17
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	6	0.17
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	7	0.17
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	7	0.17
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	7	0.17
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	9	0.17
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	12	0.17
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	3	0.17
(2,444)	1:559:A:ARG:HD3	1:560:A:CYS:H	11	0.17
(2,444)	1:559:A:ARG:HD3	1:560:A:CYS:H	16	0.17
(2,444)	1:559:A:ARG:HD3	1:560:A:CYS:H	19	0.17
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	17	0.17
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	17	0.17
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	17	0.17
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	1	0.17
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	8	0.17
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	13	0.17
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	18	0.17
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	9	0.17
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	6	0.17
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	6	0.17
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	6	0.17
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	15	0.17
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	15	0.17
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	15	0.17
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	1	0.17
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	15	0.17
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	16	0.17
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	1	0.17
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	12	0.17
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	14	0.17
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	18	0.17
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	19	0.17
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	10	0.17
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	18	0.17
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	19	0.17
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	9	0.17
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	12	0.17
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	18	0.17
(2,147)	1:548:A:LEU:HD11	1:549:A:CYS:H	9	0.17
(2,147)	1:548:A:LEU:HD12	1:549:A:CYS:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,147)	1:548:A:LEU:HD13	1:549:A:CYS:H	9	0.17
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	16	0.17
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	16	0.17
(2,69)	1:542:A:HIS:HB2	1:543:A:GLU:H	7	0.17
(2,67)	1:542:A:HIS:HA	1:543:A:GLU:H	6	0.17
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	13	0.17
(1,1396)	1:598:A:ASN:HA	1:598:A:ASN:HD21	5	0.17
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	3	0.17
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	10	0.17
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	16	0.17
(1,1194)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	20	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	1	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	2	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	6	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	10	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	12	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	13	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	14	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	17	0.17
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	19	0.17
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	6	0.17
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	14	0.17
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	9	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	2	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	5	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	6	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	8	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	10	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	13	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	16	0.17
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	17	0.17
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	11	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	6	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	9	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	10	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	12	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	15	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	16	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	17	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	18	0.17
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	19	0.17
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	3	0.17
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	19	0.17
(1,430)	1:559:A:ARG:HD3	1:560:A:CYS:H	11	0.17
(1,430)	1:559:A:ARG:HD3	1:560:A:CYS:H	16	0.17
(1,430)	1:559:A:ARG:HD3	1:560:A:CYS:H	19	0.17
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	2	0.17
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	7	0.17
(1,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	2	0.17
(1,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	6	0.17
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	16	0.17
(1,69)	1:542:A:HIS:HB2	1:543:A:GLU:H	7	0.17
(1,67)	1:542:A:HIS:HA	1:543:A:GLU:H	6	0.17
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	13	0.17
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	10	0.16
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	11	0.16
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	16	0.16
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	9	0.16
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	14	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	3	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	5	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	6	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	12	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	13	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	14	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	15	0.16
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	17	0.16
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	9	0.16
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	11	0.16
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	20	0.16
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	9	0.16
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	9	0.16
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	1	0.16
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	5	0.16
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	11	0.16
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	4	0.16
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	8	0.16
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	9	0.16
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	16	0.16
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	18	0.16
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	1	0.16
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	13	0.16
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	5	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	5	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	5	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	11	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	11	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	11	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	12	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	12	0.16
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	12	0.16
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	1	0.16
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	4	0.16
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	12	0.16
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	4	0.16
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	7	0.16
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	9	0.16
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	20	0.16
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	4	0.16
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	11	0.16
(2,875)	1:575:A:CYS:H	1:596:A:CYS:H	5	0.16
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	3	0.16
(2,724)	1:571:A:GLU:HA	1:571:A:GLU:HG3	6	0.16
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	7	0.16
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	18	0.16
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	1	0.16
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	9	0.16
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	14	0.16
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	19	0.16
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	17	0.16
(2,660)	1:567:A:LYS:H	1:568:A:PHE:H	20	0.16
(2,595)	1:564:A:MET:HG2	1:564:A:MET:H	11	0.16
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	2	0.16
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	7	0.16
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	10	0.16
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	13	0.16
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	15	0.16
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	2	0.16
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	3	0.16
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	10	0.16
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	15	0.16
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	8	0.16
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	8	0.16
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	8	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	2	0.16
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	5	0.16
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	11	0.16
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	13	0.16
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	20	0.16
(2,444)	1:559:A:ARG:HD3	1:560:A:CYS:H	4	0.16
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	12	0.16
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	14	0.16
(2,347)	1:554:A:LYS:H	1:555:A:PRO:HD3	20	0.16
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	13	0.16
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	14	0.16
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	20	0.16
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	4	0.16
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	4	0.16
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	4	0.16
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	7	0.16
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	7	0.16
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	7	0.16
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	14	0.16
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	7	0.16
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	16	0.16
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	8	0.16
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	9	0.16
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	2	0.16
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	3	0.16
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	5	0.16
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	8	0.16
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	9	0.16
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	13	0.16
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	17	0.16
(2,170)	1:548:A:LEU:HB2	1:553:A:GLN:H	14	0.16
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	5	0.16
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	15	0.16
(2,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	4	0.16
(2,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	9	0.16
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	1	0.16
(2,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	9	0.16
(2,67)	1:542:A:HIS:HA	1:543:A:GLU:H	12	0.16
(2,67)	1:542:A:HIS:HA	1:543:A:GLU:H	16	0.16
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	5	0.16
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	9	0.16
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	18	0.16
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	19	0.16
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	9	0.16
(1,1194)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	5	0.16
(1,1194)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	12	0.16
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	4	0.16
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	8	0.16
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	9	0.16
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	16	0.16
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	18	0.16
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	2	0.16
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	3	0.16
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	4	0.16
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	12	0.16
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	15	0.16
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	16	0.16
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	17	0.16
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	1	0.16
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	7	0.16
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	11	0.16
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	1	0.16
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	13	0.16
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	15	0.16
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	13	0.16
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	14	0.16
(1,737)	1:572:A:HIS:H	1:573:A:PHE:HB3	20	0.16
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	3	0.16
(1,710)	1:571:A:GLU:HA	1:571:A:GLU:HG3	6	0.16
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	1	0.16
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	9	0.16
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	14	0.16
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	19	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	1	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	2	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	3	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	4	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	5	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	7	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	8	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	13	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	14	0.16
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:564:A:MET:HG2	1:564:A:MET:H	11	0.16
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	2	0.16
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	7	0.16
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	10	0.16
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	13	0.16
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	15	0.16
(1,430)	1:559:A:ARG:HD3	1:560:A:CYS:H	4	0.16
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	12	0.16
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	18	0.16
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	16	0.16
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	16	0.16
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	16	0.16
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	4	0.16
(1,352)	1:555:A:PRO:HB3	1:556:A:ILE:HB	6	0.16
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	7	0.16
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	16	0.16
(1,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	4	0.16
(1,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	9	0.16
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	1	0.16
(1,70)	1:543:A:GLU:HA	1:543:A:GLU:HG3	9	0.16
(1,67)	1:542:A:HIS:HA	1:543:A:GLU:H	12	0.16
(1,67)	1:542:A:HIS:HA	1:543:A:GLU:H	16	0.16
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	5	0.16
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	1	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	2	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	3	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	4	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	5	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	6	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	7	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	8	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	12	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	13	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	14	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	15	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	17	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	18	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	19	0.15
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	20	0.15
(2,1411)	1:598:A:ASN:HA	1:598:A:ASN:HD21	9	0.15
(2,1411)	1:598:A:ASN:HA	1:598:A:ASN:HD21	14	0.15
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	4	0.15
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	7	0.15
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	8	0.15
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	18	0.15
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	19	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	1	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	2	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	4	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	7	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	8	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	9	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	10	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	11	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	16	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	18	0.15
(2,1390)	1:597:A:GLN:HE21	1:597:A:GLN:HG3	19	0.15
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	4	0.15
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	8	0.15
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	10	0.15
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	14	0.15
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	16	0.15
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	19	0.15
(2,1235)	1:589:A:GLU:HA	1:593:A:LYS:H	15	0.15
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	5	0.15
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	8	0.15
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	7	0.15
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	11	0.15
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	15	0.15
(2,1150)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	20	0.15
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	1	0.15
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	1	0.15
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	1	0.15
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	18	0.15
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	18	0.15
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	18	0.15
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	18	0.15
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	19	0.15
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	20	0.15
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	9	0.15
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	9	0.15
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	9	0.15
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	17	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	17	0.15
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	17	0.15
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	6	0.15
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	8	0.15
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	20	0.15
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	15	0.15
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	16	0.15
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	11	0.15
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	16	0.15
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	19	0.15
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	12	0.15
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	16	0.15
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	20	0.15
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	1	0.15
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	7	0.15
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	8	0.15
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	11	0.15
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	15	0.15
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	8	0.15
(2,699)	1:569:A:HIS:HB3	1:572:A:HIS:HB3	17	0.15
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	12	0.15
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	15	0.15
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	18	0.15
(2,668)	1:568:A:PHE:HB3	1:570:A:PRO:HA	20	0.15
(2,645)	1:567:A:LYS:HE3	1:567:A:LYS:HG3	20	0.15
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	5	0.15
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	8	0.15
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	9	0.15
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	14	0.15
(2,580)	1:563:A:ALA:HA	1:566:A:LYS:HB3	11	0.15
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	15	0.15
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	16	0.15
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	18	0.15
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	19	0.15
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	4	0.15
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	14	0.15
(2,434)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	4	0.15
(2,434)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	16	0.15
(2,434)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	19	0.15
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	1	0.15
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	1	0.15
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	8	0.15
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	8	0.15
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	8	0.15
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	9	0.15
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	9	0.15
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	9	0.15
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	10	0.15
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	10	0.15
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	10	0.15
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	5	0.15
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	8	0.15
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	16	0.15
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	17	0.15
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	18	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	3	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	4	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	5	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	6	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	8	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	9	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	12	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	13	0.15
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	18	0.15
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD11	16	0.15
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD12	16	0.15
(2,281)	1:551:A:GLY:H	1:556:A:ILE:HD13	16	0.15
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD11	4	0.15
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD12	4	0.15
(2,251)	1:550:A:SER:HB2	1:556:A:ILE:HD13	4	0.15
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	20	0.15
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	6	0.15
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	13	0.15
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	4	0.15
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	15	0.15
(2,197)	1:549:A:CYS:H	1:550:A:SER:H	20	0.15
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	3	0.15
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	8	0.15
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	10	0.15
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	13	0.15
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	16	0.15
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	15	0.15
(2,91)	1:545:A:ARG:HB3	1:546:A:GLY:HA3	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	18	0.15
(2,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	17	0.15
(2,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	3	0.15
(2,67)	1:542:A:HIS:HA	1:543:A:GLU:H	15	0.15
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	6	0.15
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	20	0.15
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	10	0.15
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	11	0.15
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	16	0.15
(1,1396)	1:598:A:ASN:HA	1:598:A:ASN:HD21	9	0.15
(1,1396)	1:598:A:ASN:HA	1:598:A:ASN:HD21	14	0.15
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	2	0.15
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	4	0.15
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	7	0.15
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	8	0.15
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	18	0.15
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	19	0.15
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	3	0.15
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	4	0.15
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	11	0.15
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	18	0.15
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	19	0.15
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	4	0.15
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	6	0.15
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	14	0.15
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	5	0.15
(1,1194)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	3	0.15
(1,1194)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	6	0.15
(1,1194)	1:588:A:LYS:HD2	1:597:A:GLN:HE21	17	0.15
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	7	0.15
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	11	0.15
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	15	0.15
(1,1135)	1:587:A:PHE:HB3	1:594:A:PRO:HB2	20	0.15
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	9	0.15
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	13	0.15
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	14	0.15
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	18	0.15
(1,1134)	1:587:A:PHE:HB3	1:594:A:PRO:HA	19	0.15
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	18	0.15
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	19	0.15
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	20	0.15
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	16	0.15
(1,891)	1:576:A:ALA:H	1:594:A:PRO:HG3	15	0.15
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	1	0.15
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	7	0.15
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	8	0.15
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	11	0.15
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	15	0.15
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	12	0.15
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	15	0.15
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	18	0.15
(1,654)	1:568:A:PHE:HB3	1:570:A:PRO:HA	20	0.15
(1,631)	1:567:A:LYS:HE3	1:567:A:LYS:HG3	20	0.15
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	5	0.15
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	8	0.15
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	9	0.15
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	14	0.15
(1,566)	1:563:A:ALA:HA	1:566:A:LYS:HB3	11	0.15
(1,420)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	4	0.15
(1,420)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	16	0.15
(1,420)	1:559:A:ARG:HB3	1:559:A:ARG:HD3	19	0.15
(1,417)	1:558:A:GLY:H	1:570:A:PRO:HG2	20	0.15
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	7	0.15
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	7	0.15
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	7	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	3	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	4	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	5	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	6	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	8	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	9	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	12	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	13	0.15
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	18	0.15
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	20	0.15
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	6	0.15
(1,91)	1:545:A:ARG:HB3	1:546:A:GLY:HA3	18	0.15
(1,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	18	0.15
(1,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	17	0.15
(1,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	3	0.15
(1,67)	1:542:A:HIS:HA	1:543:A:GLU:H	15	0.15
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	6	0.15
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	1	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	2	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	3	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	4	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	5	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	6	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	7	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	8	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	9	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	10	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	11	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	12	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	13	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	14	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	15	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	16	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	17	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	18	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	19	0.14
(2,1551)	1:603:A:LEU:HB3	1:603:A:LEU:H	20	0.14
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	9	0.14
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	10	0.14
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	11	0.14
(2,1550)	1:603:A:LEU:HA	1:603:A:LEU:HG	16	0.14
(2,1421)	1:598:A:ASN:HB2	1:599:A:CYS:H	9	0.14
(2,1421)	1:598:A:ASN:HB2	1:599:A:CYS:H	14	0.14
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	1	0.14
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	5	0.14
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	10	0.14
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	11	0.14
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	13	0.14
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	16	0.14
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	1	0.14
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	2	0.14
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	13	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	1	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	3	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	4	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	5	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	6	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	7	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	9	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	10	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	11	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	12	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	13	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	14	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	15	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	16	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	18	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	19	0.14
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	20	0.14
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	1	0.14
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	8	0.14
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	10	0.14
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	11	0.14
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	19	0.14
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	1	0.14
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	8	0.14
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	11	0.14
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	14	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	6	0.14
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	6	0.14
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	6	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	9	0.14
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	9	0.14
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	9	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	11	0.14
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	11	0.14
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	11	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	13	0.14
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	13	0.14
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	13	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	14	0.14
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	14	0.14
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	14	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	16	0.14
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	16	0.14
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	16	0.14
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	17	0.14
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	17	0.14
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	17	0.14
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	9	0.14
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	10	0.14
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	11	0.14
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	12	0.14
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	17	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	3	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	3	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	3	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	6	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	6	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	6	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	20	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	20	0.14
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	20	0.14
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	5	0.14
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	10	0.14
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	3	0.14
(2,967)	1:580:A:LYS:HA	1:580:A:LYS:HD3	5	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	2	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	4	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	7	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	8	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	9	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	10	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	11	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	12	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	17	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	18	0.14
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	20	0.14
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	2	0.14
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	3	0.14
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	12	0.14
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	13	0.14
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	15	0.14
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	19	0.14
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	7	0.14
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	7	0.14
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	7	0.14
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	5	0.14
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	12	0.14
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	13	0.14
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	18	0.14
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	19	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	1	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	9	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	11	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	12	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	14	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	15	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	17	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	18	0.14
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	19	0.14
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	11	0.14
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	20	0.14
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	12	0.14
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	17	0.14
(2,580)	1:563:A:ALA:HA	1:566:A:LYS:HB3	15	0.14
(2,538)	1:561:A:ILE:HG21	1:584:A:LYS:HD3	5	0.14
(2,538)	1:561:A:ILE:HG22	1:584:A:LYS:HD3	5	0.14
(2,538)	1:561:A:ILE:HG23	1:584:A:LYS:HD3	5	0.14
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	1	0.14
(2,460)	1:560:A:CYS:HA	1:570:A:PRO:HD2	11	0.14
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	11	0.14
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	11	0.14
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	11	0.14
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	14	0.14
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	14	0.14
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	14	0.14
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	2	0.14
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	2	0.14
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	2	0.14
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	13	0.14
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	13	0.14
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	13	0.14
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	20	0.14
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	20	0.14
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	20	0.14
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	2	0.14
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	10	0.14
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	12	0.14
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	1	0.14
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	7	0.14
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	15	0.14
(2,316)	1:553:A:GLN:HG2	1:553:A:GLN:H	16	0.14
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	9	0.14
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	12	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	3	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	4	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	5	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	8	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	13	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	15	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	18	0.14
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	19	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	1	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	2	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	3	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	4	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	5	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	6	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	7	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	8	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	9	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	10	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	12	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	13	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	14	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	15	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	16	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	17	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	18	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	19	0.14
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	20	0.14
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	2	0.14
(2,123)	1:547:A:SER:H	1:556:A:ILE:HB	4	0.14
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	12	0.14
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	14	0.14
(2,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	6	0.14
(2,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	18	0.14
(2,83)	1:545:A:ARG:HB3	1:545:A:ARG:HD3	4	0.14
(2,82)	1:545:A:ARG:HA	1:545:A:ARG:HG3	14	0.14
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	5	0.14
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	19	0.14
(2,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	8	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	1	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	2	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	3	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	4	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	5	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	6	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	7	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	8	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	9	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	10	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	11	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	12	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	13	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	14	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	15	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	16	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	17	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	18	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	19	0.14
(1,1536)	1:603:A:LEU:HB3	1:603:A:LEU:H	20	0.14
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	5	0.14
(1,1406)	1:598:A:ASN:HB2	1:599:A:CYS:H	9	0.14
(1,1406)	1:598:A:ASN:HB2	1:599:A:CYS:H	14	0.14
(1,1391)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	20	0.14
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	1	0.14
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	5	0.14
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	10	0.14
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	11	0.14
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	13	0.14
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	16	0.14
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	15	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	1	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	2	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	5	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	7	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	8	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	9	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	10	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	13	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	14	0.14
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	16	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	1	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	3	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	4	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	5	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	6	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	7	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	8	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	9	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	10	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	11	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	12	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	13	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	14	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	15	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	16	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	18	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	19	0.14
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	20	0.14
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	5	0.14
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	11	0.14
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	19	0.14
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	1	0.14
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	8	0.14
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	11	0.14
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	8	0.14
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	3	0.14
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	9	0.14
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	10	0.14
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	11	0.14
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	12	0.14
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	17	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	2	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	4	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	7	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	8	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	9	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	10	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	11	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	12	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	17	0.14
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	20	0.14
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	5	0.14
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	12	0.14
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	13	0.14
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	14	0.14
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	18	0.14
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	19	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	1	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	9	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	11	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	12	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	14	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	15	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	17	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	18	0.14
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	19	0.14
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	11	0.14
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	20	0.14
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	12	0.14
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	17	0.14
(1,566)	1:563:A:ALA:HA	1:566:A:LYS:HB3	15	0.14
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	11	0.14
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	11	0.14
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	11	0.14
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	14	0.14
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	14	0.14
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	14	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	4	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	4	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	4	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	11	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	11	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	11	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	19	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	19	0.14
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	19	0.14
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	1	0.14
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	7	0.14
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	14	0.14
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	15	0.14
(1,302)	1:553:A:GLN:HG2	1:553:A:GLN:H	16	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	4	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	5	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	6	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	7	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	8	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	9	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	11	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	13	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	16	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	19	0.14
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	20	0.14
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	12	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	3	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	4	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	5	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	8	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	13	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	15	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	18	0.14
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	19	0.14
(1,123)	1:547:A:SER:H	1:556:A:ILE:HB	4	0.14
(1,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	6	0.14
(1,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	18	0.14
(1,83)	1:545:A:ARG:HB3	1:545:A:ARG:HD3	4	0.14
(1,82)	1:545:A:ARG:HA	1:545:A:ARG:HG3	14	0.14
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	17	0.14
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	5	0.14
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	19	0.14
(1,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	7	0.14
(1,62)	1:541:A:TYR:HB2	1:541:A:TYR:H	8	0.14
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	14	0.13
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	5	0.13
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	9	0.13
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	14	0.13
(2,1421)	1:598:A:ASN:HB2	1:599:A:CYS:H	5	0.13
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	2	0.13
(2,1337)	1:594:A:PRO:HA	1:595:A:TYR:HB3	17	0.13
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	5	0.13
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	7	0.13
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	8	0.13
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	10	0.13
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	2	0.13
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	4	0.13
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	7	0.13
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	10	0.13
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	13	0.13
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	15	0.13
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	18	0.13
(2,1171)	1:588:A:LYS:HA	1:589:A:GLU:HB3	20	0.13
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG21	18	0.13
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG22	18	0.13
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG23	18	0.13
(2,1114)	1:584:A:LYS:HB3	1:586:A:THR:H	15	0.13
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	2	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	2	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	2	0.13
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	3	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	3	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	3	0.13
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	4	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	4	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	4	0.13
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	8	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	8	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	8	0.13
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	12	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	12	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	12	0.13
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	15	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	15	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	15	0.13
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	20	0.13
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	20	0.13
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	20	0.13
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	4	0.13
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	5	0.13
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	6	0.13
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	8	0.13
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	16	0.13
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	2	0.13
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	2	0.13
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	2	0.13
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	10	0.13
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	10	0.13
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	1	0.13
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	3	0.13
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	4	0.13
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	6	0.13
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	8	0.13
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	1	0.13
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	3	0.13
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	5	0.13
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	6	0.13
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	13	0.13
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	14	0.13
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	6	0.13
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	14	0.13
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	2	0.13
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	9	0.13
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	14	0.13
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	17	0.13
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	14	0.13
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	14	0.13
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	14	0.13
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	18	0.13
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	18	0.13
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	18	0.13
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	3	0.13
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	9	0.13
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	17	0.13
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	20	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	2	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	3	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	4	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	5	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	6	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	7	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	8	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	10	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	13	0.13
(2,764)	1:573:A:PHE:HB3	1:574:A:VAL:H	16	0.13
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	13	0.13
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	3	0.13
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	6	0.13
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	12	0.13
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	18	0.13
(2,432)	1:559:A:ARG:HA	1:559:A:ARG:HD3	7	0.13
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	15	0.13
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	15	0.13
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	15	0.13
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	5	0.13
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	5	0.13
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	5	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	1	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	2	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	8	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	12	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	14	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	15	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	18	0.13
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	20	0.13
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	4	0.13
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	6	0.13
(2,265)	1:550:A:SER:H	1:567:A:LYS:HB3	20	0.13
(2,264)	1:550:A:SER:HB2	1:567:A:LYS:H	20	0.13
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	3	0.13
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	4	0.13
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	9	0.13
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	10	0.13
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	14	0.13
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	17	0.13
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	18	0.13
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	1	0.13
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	2	0.13
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	9	0.13
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	11	0.13
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	12	0.13
(2,232)	1:550:A:SER:HB3	1:550:A:SER:H	11	0.13
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	3	0.13
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	15	0.13
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	6	0.13
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	7	0.13
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	17	0.13
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	20	0.13
(2,123)	1:547:A:SER:H	1:556:A:ILE:HB	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,123)	1:547:A:SER:H	1:556:A:ILE:HB	20	0.13
(2,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	16	0.13
(2,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	19	0.13
(2,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	3	0.13
(2,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	8	0.13
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	10	0.13
(2,69)	1:542:A:HIS:HB2	1:543:A:GLU:H	2	0.13
(2,67)	1:542:A:HIS:HA	1:543:A:GLU:H	5	0.13
(2,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	1	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	1	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	2	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	3	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	4	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	6	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	8	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	9	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	12	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	14	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	15	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	19	0.13
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	20	0.13
(1,1406)	1:598:A:ASN:HB2	1:599:A:CYS:H	5	0.13
(1,1391)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	5	0.13
(1,1391)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	6	0.13
(1,1391)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	12	0.13
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	6	0.13
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	12	0.13
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	17	0.13
(1,1330)	1:594:A:PRO:HG3	1:595:A:TYR:H	20	0.13
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	2	0.13
(1,1322)	1:594:A:PRO:HA	1:595:A:TYR:HB3	17	0.13
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	9	0.13
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	11	0.13
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	20	0.13
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	5	0.13
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	7	0.13
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	8	0.13
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	10	0.13
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	18	0.13
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	2	0.13
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	4	0.13
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	10	0.13
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	13	0.13
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	15	0.13
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	18	0.13
(1,1188)	1:588:A:LYS:H	1:597:A:GLN:HB3	17	0.13
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG21	18	0.13
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG22	18	0.13
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG23	18	0.13
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	5	0.13
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	15	0.13
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	4	0.13
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	5	0.13
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	6	0.13
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	8	0.13
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	16	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	1	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	2	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	3	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	5	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	7	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	8	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	9	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	11	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	12	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	13	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	14	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	15	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	17	0.13
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	19	0.13
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	1	0.13
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	3	0.13
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	5	0.13
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	6	0.13
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	13	0.13
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	14	0.13
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	3	0.13
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	9	0.13
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	17	0.13
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	20	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	2	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	3	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	5	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	6	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	7	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	8	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	10	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	13	0.13
(1,750)	1:573:A:PHE:HB3	1:574:A:VAL:H	16	0.13
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	3	0.13
(1,586)	1:564:A:MET:HB2	1:565:A:ALA:H	11	0.13
(1,418)	1:559:A:ARG:HA	1:559:A:ARG:HD3	7	0.13
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	15	0.13
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	15	0.13
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	15	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	2	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	3	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	10	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	12	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	14	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	15	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	17	0.13
(1,274)	1:551:A:GLY:HA3	1:572:A:HIS:HB2	18	0.13
(1,254)	1:550:A:SER:HB2	1:567:A:LYS:H	20	0.13
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	4	0.13
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	9	0.13
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	10	0.13
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	14	0.13
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	17	0.13
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	18	0.13
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	1	0.13
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	2	0.13
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	9	0.13
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	11	0.13
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	12	0.13
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	17	0.13
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	20	0.13
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	5	0.13
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	5	0.13
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	5	0.13
(1,123)	1:547:A:SER:H	1:556:A:ILE:HB	1	0.13
(1,123)	1:547:A:SER:H	1:556:A:ILE:HB	20	0.13
(1,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	4	0.13
(1,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	16	0.13
(1,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	19	0.13
(1,85)	1:545:A:ARG:HB2	1:545:A:ARG:HD3	3	0.13
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	10	0.13
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	16	0.13
(1,77)	1:544:A:ARG:HB3	1:544:A:ARG:HD3	8	0.13
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	10	0.13
(1,69)	1:542:A:HIS:HB2	1:543:A:GLU:H	2	0.13
(1,67)	1:542:A:HIS:HA	1:543:A:GLU:H	5	0.13
(1,61)	1:541:A:TYR:HB3	1:541:A:TYR:H	1	0.13
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	3	0.12
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	3	0.12
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	3	0.12
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	6	0.12
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	6	0.12
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	6	0.12
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	14	0.12
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	14	0.12
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	14	0.12
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	17	0.12
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	17	0.12
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	17	0.12
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	18	0.12
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	18	0.12
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	18	0.12
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	3	0.12
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	6	0.12
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	9	0.12
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	16	0.12
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	18	0.12
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	20	0.12
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	20	0.12
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	20	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	1	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	2	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	3	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	4	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	6	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	7	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	8	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	12	0.12
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	19	0.12
(2,1403)	1:597:A:GLN:HA	1:600:A:PHE:H	20	0.12
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	3	0.12
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	6	0.12
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	12	0.12
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	5	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	2	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	3	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	4	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	6	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	7	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	8	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	9	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	14	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	16	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	17	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	18	0.12
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	19	0.12
(2,1314)	1:593:A:LYS:HD3	1:593:A:LYS:HA	13	0.12
(2,1252)	1:590:A:GLN:HE21	1:590:A:GLN:HB3	20	0.12
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	9	0.12
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	12	0.12
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	15	0.12
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	16	0.12
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	17	0.12
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	9	0.12
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	14	0.12
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	15	0.12
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	17	0.12
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	18	0.12
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	19	0.12
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	9	0.12
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	14	0.12
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	16	0.12
(2,1206)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	19	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG21	14	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG22	14	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG23	14	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG21	15	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG22	15	0.12
(2,1121)	1:585:A:GLY:HA2	1:586:A:THR:HG23	15	0.12
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	5	0.12
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	5	0.12
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	7	0.12
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	7	0.12
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	7	0.12
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	10	0.12
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	10	0.12
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	10	0.12
(2,1039)	1:582:A:LEU:HD11	1:582:A:LEU:H	19	0.12
(2,1039)	1:582:A:LEU:HD12	1:582:A:LEU:H	19	0.12
(2,1039)	1:582:A:LEU:HD13	1:582:A:LEU:H	19	0.12
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	2	0.12
(2,1025)	1:581:A:GLN:H	1:582:A:LEU:HG	7	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	4	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	4	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	4	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	16	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	16	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	16	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD21	18	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD22	18	0.12
(2,988)	1:580:A:LYS:H	1:582:A:LEU:HD23	18	0.12
(2,948)	1:578:A:CYS:H	1:595:A:TYR:HA	19	0.12
(2,911)	1:576:A:ALA:H	1:596:A:CYS:H	17	0.12
(2,899)	1:576:A:ALA:HA	1:594:A:PRO:HB3	13	0.12
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	5	0.12
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	5	0.12
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	5	0.12
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	8	0.12
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	8	0.12
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	8	0.12
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	2	0.12
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	4	0.12
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	6	0.12
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	4	0.12
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	7	0.12
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	10	0.12
(2,632)	1:566:A:LYS:H	1:566:A:LYS:HE3	15	0.12
(2,587)	1:563:A:ALA:H	1:567:A:LYS:HD2	18	0.12
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	1	0.12
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	13	0.12
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	11	0.12
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	14	0.12
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	1	0.12
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	13	0.12
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	14	0.12
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	1	0.12
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	1	0.12
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	1	0.12
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	3	0.12
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	3	0.12
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	3	0.12
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	8	0.12
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	8	0.12
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	8	0.12
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	13	0.12
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	13	0.12
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	13	0.12
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	3	0.12
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	3	0.12
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	3	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	3	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	4	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	5	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	6	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	7	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	9	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	10	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	11	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	13	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	16	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	17	0.12
(2,359)	1:555:A:PRO:HB2	1:555:A:PRO:HD3	19	0.12
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	1	0.12
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	15	0.12
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	19	0.12
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	5	0.12
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	1	0.12
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	3	0.12
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	6	0.12
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	7	0.12
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	8	0.12
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	16	0.12
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	10	0.12
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	14	0.12
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	19	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	2	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	5	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	7	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	8	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	9	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	10	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	12	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	16	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	18	0.12
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	19	0.12
(2,123)	1:547:A:SER:H	1:556:A:ILE:HB	10	0.12
(2,113)	1:547:A:SER:HB3	1:555:A:PRO:HB3	20	0.12
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	5	0.12
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	12	0.12
(2,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	11	0.12
(2,83)	1:545:A:ARG:HB3	1:545:A:ARG:HD3	11	0.12
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	6	0.12
(2,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	11	0.12
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	9	0.12
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	19	0.12
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	10	0.12
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	11	0.12
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	16	0.12
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	20	0.12
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	20	0.12
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	20	0.12
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	7	0.12
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	13	0.12
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	17	0.12
(1,1433)	1:599:A:CYS:HA	1:602:A:LYS:HG2	18	0.12
(1,1391)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	3	0.12
(1,1391)	1:597:A:GLN:HE21	1:601:A:LEU:HB3	17	0.12
(1,1388)	1:597:A:GLN:HA	1:600:A:PHE:H	20	0.12
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	3	0.12
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	6	0.12
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	12	0.12
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	2	0.12
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	7	0.12
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	8	0.12
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	13	0.12
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	18	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	2	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	3	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	4	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	6	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	7	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	8	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	9	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	14	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	16	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	17	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	18	0.12
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	19	0.12
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	1	0.12
(1,1237)	1:590:A:GLN:HE21	1:590:A:GLN:HB3	20	0.12
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	9	0.12
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	12	0.12
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	15	0.12
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	16	0.12
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	17	0.12
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	9	0.12
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	14	0.12
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	15	0.12
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	17	0.12
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	18	0.12
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	19	0.12
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	9	0.12
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	14	0.12
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	16	0.12
(1,1191)	1:588:A:LYS:HG2	1:597:A:GLN:HB3	19	0.12
(1,1188)	1:588:A:LYS:H	1:597:A:GLN:HB3	12	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG21	14	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG22	14	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG23	14	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG21	15	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG22	15	0.12
(1,1106)	1:585:A:GLY:HA2	1:586:A:THR:HG23	15	0.12
(1,1072)	1:583:A:ASN:HB2	1:583:A:ASN:H	2	0.12
(1,1072)	1:583:A:ASN:HB2	1:583:A:ASN:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:583:A:ASN:HB2	1:583:A:ASN:H	9	0.12
(1,1072)	1:583:A:ASN:HB2	1:583:A:ASN:H	12	0.12
(1,1072)	1:583:A:ASN:HB2	1:583:A:ASN:H	16	0.12
(1,1072)	1:583:A:ASN:HB2	1:583:A:ASN:H	17	0.12
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	6	0.12
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	13	0.12
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	19	0.12
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	2	0.12
(1,1010)	1:581:A:GLN:H	1:582:A:LEU:HG	7	0.12
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	6	0.12
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	16	0.12
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	18	0.12
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	20	0.12
(1,934)	1:578:A:CYS:H	1:595:A:TYR:HA	19	0.12
(1,877)	1:576:A:ALA:H	1:582:A:LEU:HB3	15	0.12
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	2	0.12
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	4	0.12
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	6	0.12
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	4	0.12
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	7	0.12
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	10	0.12
(1,622)	1:566:A:LYS:HA	1:567:A:LYS:HE3	15	0.12
(1,618)	1:566:A:LYS:H	1:566:A:LYS:HE3	15	0.12
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	5	0.12
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	13	0.12
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	20	0.12
(1,573)	1:563:A:ALA:H	1:567:A:LYS:HD2	18	0.12
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	7	0.12
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	11	0.12
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	16	0.12
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	1	0.12
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	13	0.12
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	14	0.12
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	1	0.12
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	1	0.12
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	1	0.12
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	3	0.12
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	3	0.12
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	3	0.12
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	8	0.12
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	8	0.12
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	13	0.12
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	13	0.12
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	13	0.12
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	6	0.12
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	6	0.12
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	6	0.12
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	1	0.12
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	3	0.12
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	6	0.12
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	7	0.12
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	8	0.12
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	13	0.12
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	16	0.12
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	10	0.12
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	14	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	2	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	5	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	7	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	8	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	9	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	10	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	12	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	16	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	18	0.12
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	19	0.12
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	6	0.12
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	6	0.12
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	6	0.12
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	12	0.12
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	12	0.12
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	12	0.12
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	15	0.12
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	15	0.12
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	15	0.12
(1,123)	1:547:A:SER:H	1:556:A:ILE:HB	10	0.12
(1,114)	1:547:A:SER:HB2	1:555:A:PRO:HB3	15	0.12
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	12	0.12
(1,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	11	0.12
(1,83)	1:545:A:ARG:HB3	1:545:A:ARG:HD3	11	0.12
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	12	0.12
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	6	0.12
(1,76)	1:544:A:ARG:HA	1:544:A:ARG:HG3	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	9	0.12
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	19	0.12
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	4	0.11
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	4	0.11
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	4	0.11
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	7	0.11
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	7	0.11
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	7	0.11
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	9	0.11
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	9	0.11
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	9	0.11
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	13	0.11
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	13	0.11
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	13	0.11
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	19	0.11
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	19	0.11
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	19	0.11
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	20	0.11
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	20	0.11
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	20	0.11
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	4	0.11
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	10	0.11
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	11	0.11
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	17	0.11
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	19	0.11
(2,1522)	1:602:A:LYS:HG3	1:602:A:LYS:H	10	0.11
(2,1522)	1:602:A:LYS:HG3	1:602:A:LYS:H	11	0.11
(2,1522)	1:602:A:LYS:HG3	1:602:A:LYS:H	16	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	1	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	1	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	1	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	2	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	2	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	2	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	3	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	3	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	3	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	4	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	4	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	4	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	5	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	5	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	6	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	6	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	6	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	8	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	8	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	8	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	12	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	12	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	12	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	13	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	13	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	13	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	17	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	17	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	17	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	18	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	18	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	18	0.11
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	19	0.11
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	19	0.11
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	19	0.11
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	15	0.11
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	18	0.11
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	20	0.11
(2,1378)	1:596:A:CYS:HB3	1:599:A:CYS:H	15	0.11
(2,1372)	1:596:A:CYS:HB2	1:597:A:GLN:H	17	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	1	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	5	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	10	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	11	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	12	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	13	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	15	0.11
(2,1335)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	20	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	1	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	2	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	3	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	4	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	6	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	13	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	18	0.11
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	19	0.11
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	1	0.11
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	7	0.11
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	8	0.11
(2,1234)	1:589:A:GLU:HG3	1:592:A:ASP:H	11	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	2	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	3	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	4	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	7	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	12	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	13	0.11
(2,1230)	1:589:A:GLU:H	1:590:A:GLN:H	16	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	1	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	2	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	3	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	4	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	5	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	6	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	7	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	8	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	9	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	10	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	11	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	12	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	13	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	16	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	17	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	18	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	19	0.11
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	20	0.11
(2,1147)	1:587:A:PHE:H	1:588:A:LYS:H	8	0.11
(2,997)	1:581:A:GLN:HB3	1:581:A:GLN:H	1	0.11
(2,997)	1:581:A:GLN:HB3	1:581:A:GLN:H	7	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	2	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	9	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	12	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	13	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	14	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	16	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	17	0.11
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,970)	1:580:A:LYS:HB3	1:580:A:LYS:HE3	20	0.11
(2,926)	1:577:A:PHE:H	1:595:A:TYR:HA	9	0.11
(2,926)	1:577:A:PHE:H	1:595:A:TYR:HA	18	0.11
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	10	0.11
(2,766)	1:573:A:PHE:H	1:574:A:VAL:HA	16	0.11
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	3	0.11
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	5	0.11
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	6	0.11
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	13	0.11
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	16	0.11
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	19	0.11
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	2	0.11
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	4	0.11
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	7	0.11
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	11	0.11
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	19	0.11
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	18	0.11
(2,649)	1:567:A:LYS:H	1:567:A:LYS:HD2	20	0.11
(2,646)	1:567:A:LYS:HE3	1:567:A:LYS:H	20	0.11
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	2	0.11
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	3	0.11
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	5	0.11
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	11	0.11
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	13	0.11
(2,563)	1:562:A:THR:HB	1:567:A:LYS:HE3	7	0.11
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	4	0.11
(2,489)	1:561:A:ILE:HA	1:568:A:PHE:HB2	14	0.11
(2,488)	1:561:A:ILE:HG21	1:563:A:ALA:H	7	0.11
(2,488)	1:561:A:ILE:HG22	1:563:A:ALA:H	7	0.11
(2,488)	1:561:A:ILE:HG23	1:563:A:ALA:H	7	0.11
(2,488)	1:561:A:ILE:HG21	1:563:A:ALA:H	11	0.11
(2,488)	1:561:A:ILE:HG22	1:563:A:ALA:H	11	0.11
(2,488)	1:561:A:ILE:HG23	1:563:A:ALA:H	11	0.11
(2,488)	1:561:A:ILE:HG21	1:563:A:ALA:H	16	0.11
(2,488)	1:561:A:ILE:HG22	1:563:A:ALA:H	16	0.11
(2,488)	1:561:A:ILE:HG23	1:563:A:ALA:H	16	0.11
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	5	0.11
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	7	0.11
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	16	0.11
(2,476)	1:561:A:ILE:HB	1:562:A:THR:H	19	0.11
(2,460)	1:560:A:CYS:HA	1:570:A:PRO:HD2	7	0.11
(2,460)	1:560:A:CYS:HA	1:570:A:PRO:HD2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	4	0.11
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	10	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	2	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	3	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	4	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	5	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	6	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	8	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	9	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	10	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	12	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	15	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	17	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	18	0.11
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	20	0.11
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	2	0.11
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	2	0.11
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	2	0.11
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	12	0.11
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	12	0.11
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	12	0.11
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	17	0.11
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	17	0.11
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	17	0.11
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	15	0.11
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	15	0.11
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	15	0.11
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	19	0.11
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	19	0.11
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	19	0.11
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	7	0.11
(2,342)	1:554:A:LYS:HG3	1:555:A:PRO:HD3	11	0.11
(2,264)	1:550:A:SER:HB2	1:567:A:LYS:H	17	0.11
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	7	0.11
(2,249)	1:550:A:SER:HB2	1:553:A:GLN:HE22	8	0.11
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	2	0.11
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	5	0.11
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	19	0.11
(2,235)	1:550:A:SER:HB3	1:551:A:GLY:H	17	0.11
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	5	0.11
(2,210)	1:549:A:CYS:HA	1:556:A:ILE:HG13	16	0.11
(2,201)	1:549:A:CYS:HB3	1:552:A:CYS:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	1	0.11
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	3	0.11
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	4	0.11
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	6	0.11
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	11	0.11
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	13	0.11
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	14	0.11
(2,196)	1:549:A:CYS:HB2	1:550:A:SER:H	15	0.11
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	2	0.11
(2,111)	1:547:A:SER:HB3	1:548:A:LEU:H	6	0.11
(2,98)	1:546:A:GLY:H	1:547:A:SER:HB2	5	0.11
(2,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	14	0.11
(2,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	19	0.11
(2,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	20	0.11
(2,67)	1:542:A:HIS:HA	1:543:A:GLU:H	11	0.11
(2,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	3	0.11
(1,1507)	1:602:A:LYS:HG3	1:602:A:LYS:H	10	0.11
(1,1507)	1:602:A:LYS:HG3	1:602:A:LYS:H	11	0.11
(1,1507)	1:602:A:LYS:HG3	1:602:A:LYS:H	16	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	1	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	1	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	1	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	2	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	2	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	2	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	3	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	3	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	3	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	4	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	4	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	4	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	5	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	5	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	5	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	6	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	6	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	6	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	8	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	8	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	8	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	12	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	12	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	13	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	13	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	13	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	17	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	17	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	17	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	18	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	18	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	18	0.11
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	19	0.11
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	19	0.11
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	19	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	3	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	9	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	12	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	17	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	18	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	19	0.11
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	20	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	2	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	3	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	4	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	6	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	7	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	8	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	14	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	18	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	19	0.11
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	20	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	15	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	15	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	15	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD21	20	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD22	20	0.11
(1,1444)	1:599:A:CYS:HB2	1:603:A:LEU:HD23	20	0.11
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	5	0.11
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	5	0.11
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	5	0.11
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	17	0.11
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	17	0.11
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	1	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	5	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	9	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	10	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	11	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	14	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	16	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	17	0.11
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	19	0.11
(1,1357)	1:596:A:CYS:HB2	1:597:A:GLN:H	17	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	1	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	5	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	10	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	11	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	12	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	13	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	15	0.11
(1,1320)	1:594:A:PRO:HD3	1:594:A:PRO:HB2	20	0.11
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	2	0.11
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	7	0.11
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	13	0.11
(1,1249)	1:590:A:GLN:HB3	1:591:A:ASN:HA	20	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	1	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	2	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	3	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	4	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	6	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	13	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	14	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	18	0.11
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	19	0.11
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	1	0.11
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	7	0.11
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	8	0.11
(1,1219)	1:589:A:GLU:HG3	1:592:A:ASP:H	11	0.11
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	2	0.11
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	3	0.11
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	4	0.11
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	7	0.11
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	12	0.11
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	13	0.11
(1,1215)	1:589:A:GLU:H	1:590:A:GLN:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1188)	1:588:A:LYS:H	1:597:A:GLN:HB3	3	0.11
(1,1188)	1:588:A:LYS:H	1:597:A:GLN:HB3	6	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	1	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	2	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	3	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	4	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	5	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	6	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	7	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	8	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	9	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	10	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	11	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	12	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	13	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	16	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	17	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	18	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	19	0.11
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	20	0.11
(1,1132)	1:587:A:PHE:H	1:588:A:LYS:H	8	0.11
(1,1099)	1:584:A:LYS:HB3	1:586:A:THR:H	5	0.11
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	3	0.11
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	9	0.11
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	12	0.11
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	14	0.11
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	17	0.11
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	4	0.11
(1,993)	1:581:A:GLN:HE21	1:581:A:GLN:HB2	10	0.11
(1,982)	1:581:A:GLN:HB3	1:581:A:GLN:H	1	0.11
(1,982)	1:581:A:GLN:HB3	1:581:A:GLN:H	7	0.11
(1,877)	1:576:A:ALA:H	1:582:A:LEU:HB3	13	0.11
(1,877)	1:576:A:ALA:H	1:582:A:LEU:HB3	14	0.11
(1,877)	1:576:A:ALA:H	1:582:A:LEU:HB3	19	0.11
(1,806)	1:574:A:VAL:HA	1:582:A:LEU:HG	6	0.11
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	10	0.11
(1,752)	1:573:A:PHE:H	1:574:A:VAL:HA	16	0.11
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	3	0.11
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	5	0.11
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	6	0.11
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	13	0.11
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	19	0.11
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	2	0.11
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	4	0.11
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	7	0.11
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	11	0.11
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	19	0.11
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	18	0.11
(1,635)	1:567:A:LYS:H	1:567:A:LYS:HD2	20	0.11
(1,632)	1:567:A:LYS:HE3	1:567:A:LYS:H	20	0.11
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	1	0.11
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	2	0.11
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	4	0.11
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	7	0.11
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	8	0.11
(1,596)	1:564:A:MET:HB3	1:566:A:LYS:H	14	0.11
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	2	0.11
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	3	0.11
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	5	0.11
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	11	0.11
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	13	0.11
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	4	0.11
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	5	0.11
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	6	0.11
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	10	0.11
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	15	0.11
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	19	0.11
(1,474)	1:561:A:ILE:HG21	1:563:A:ALA:H	7	0.11
(1,474)	1:561:A:ILE:HG22	1:563:A:ALA:H	7	0.11
(1,474)	1:561:A:ILE:HG23	1:563:A:ALA:H	7	0.11
(1,474)	1:561:A:ILE:HG21	1:563:A:ALA:H	11	0.11
(1,474)	1:561:A:ILE:HG22	1:563:A:ALA:H	11	0.11
(1,474)	1:561:A:ILE:HG23	1:563:A:ALA:H	11	0.11
(1,474)	1:561:A:ILE:HG21	1:563:A:ALA:H	16	0.11
(1,474)	1:561:A:ILE:HG22	1:563:A:ALA:H	16	0.11
(1,474)	1:561:A:ILE:HG23	1:563:A:ALA:H	16	0.11
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	4	0.11
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	10	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	2	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	3	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	4	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	5	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	8	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	9	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	10	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	12	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	15	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	17	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	18	0.11
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	20	0.11
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	2	0.11
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	2	0.11
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	2	0.11
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	12	0.11
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	12	0.11
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	12	0.11
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	17	0.11
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	17	0.11
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	17	0.11
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG21	2	0.11
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG22	2	0.11
(1,355)	1:555:A:PRO:HB3	1:557:A:THR:HG23	2	0.11
(1,288)	1:552:A:CYS:H	1:556:A:ILE:HD11	20	0.11
(1,288)	1:552:A:CYS:H	1:556:A:ILE:HD12	20	0.11
(1,288)	1:552:A:CYS:H	1:556:A:ILE:HD13	20	0.11
(1,254)	1:550:A:SER:HB2	1:567:A:LYS:H	17	0.11
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	2	0.11
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	5	0.11
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	19	0.11
(1,229)	1:550:A:SER:HB3	1:551:A:GLY:H	17	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	1	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	3	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	4	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	6	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	11	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	13	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	14	0.11
(1,190)	1:549:A:CYS:HB2	1:550:A:SER:H	15	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	1	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	1	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	1	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	2	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	2	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	3	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	3	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	3	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	4	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	4	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	4	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	8	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	8	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	8	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	10	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	10	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	10	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	11	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	11	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	11	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	13	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	13	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	13	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	14	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	14	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	14	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	16	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	16	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	16	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	17	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	17	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	17	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	18	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	18	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	18	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	19	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	19	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	19	0.11
(1,171)	1:548:A:LEU:HD11	1:554:A:LYS:H	20	0.11
(1,171)	1:548:A:LEU:HD12	1:554:A:LYS:H	20	0.11
(1,171)	1:548:A:LEU:HD13	1:554:A:LYS:H	20	0.11
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	2	0.11
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	4	0.11
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	6	0.11
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	7	0.11
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	11	0.11
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:546:A:GLY:H	1:547:A:SER:HB2	5	0.11
(1,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	14	0.11
(1,92)	1:545:A:ARG:HB2	1:546:A:GLY:HA3	19	0.11
(1,87)	1:545:A:ARG:H	1:545:A:ARG:HD3	20	0.11
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	8	0.11
(1,81)	1:545:A:ARG:HA	1:545:A:ARG:HD3	20	0.11
(1,67)	1:542:A:HIS:HA	1:543:A:GLU:H	11	0.11
(1,66)	1:542:A:HIS:H	1:542:A:HIS:HB3	3	0.11
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	1	0.1
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	1	0.1
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	1	0.1
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	2	0.1
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	2	0.1
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	2	0.1
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	11	0.1
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	11	0.1
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	11	0.1
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	12	0.1
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	12	0.1
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	12	0.1
(2,1566)	1:603:A:LEU:HD11	1:604:A:PHE:H	16	0.1
(2,1566)	1:603:A:LEU:HD12	1:604:A:PHE:H	16	0.1
(2,1566)	1:603:A:LEU:HD13	1:604:A:PHE:H	16	0.1
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	12	0.1
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	13	0.1
(2,1561)	1:603:A:LEU:HB3	1:604:A:PHE:H	20	0.1
(2,1544)	1:602:A:LYS:H	1:603:A:LEU:HG	2	0.1
(2,1544)	1:602:A:LYS:H	1:603:A:LEU:HG	10	0.1
(2,1544)	1:602:A:LYS:H	1:603:A:LEU:HG	11	0.1
(2,1487)	1:601:A:LEU:HD21	1:601:A:LEU:HA	17	0.1
(2,1487)	1:601:A:LEU:HD22	1:601:A:LEU:HA	17	0.1
(2,1487)	1:601:A:LEU:HD23	1:601:A:LEU:HA	17	0.1
(2,1487)	1:601:A:LEU:HD21	1:601:A:LEU:HA	20	0.1
(2,1487)	1:601:A:LEU:HD22	1:601:A:LEU:HA	20	0.1
(2,1487)	1:601:A:LEU:HD23	1:601:A:LEU:HA	20	0.1
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	7	0.1
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	7	0.1
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	7	0.1
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	9	0.1
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	9	0.1
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	9	0.1
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	10	0.1
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	10	0.1
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	11	0.1
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	11	0.1
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	11	0.1
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	14	0.1
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	14	0.1
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	14	0.1
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	15	0.1
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	15	0.1
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	15	0.1
(2,1486)	1:601:A:LEU:HD11	1:601:A:LEU:H	16	0.1
(2,1486)	1:601:A:LEU:HD12	1:601:A:LEU:H	16	0.1
(2,1486)	1:601:A:LEU:HD13	1:601:A:LEU:H	16	0.1
(2,1434)	1:598:A:ASN:HA	1:601:A:LEU:H	17	0.1
(2,1430)	1:598:A:ASN:H	1:601:A:LEU:HB2	20	0.1
(2,1411)	1:598:A:ASN:HA	1:598:A:ASN:HD21	10	0.1
(2,1400)	1:597:A:GLN:HB3	1:599:A:CYS:H	20	0.1
(2,1250)	1:590:A:GLN:HG2	1:590:A:GLN:H	20	0.1
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	14	0.1
(2,1181)	1:588:A:LYS:H	1:589:A:GLU:H	15	0.1
(2,1174)	1:588:A:LYS:HB2	1:589:A:GLU:H	5	0.1
(2,1147)	1:587:A:PHE:H	1:588:A:LYS:H	5	0.1
(2,1147)	1:587:A:PHE:H	1:588:A:LYS:H	20	0.1
(2,997)	1:581:A:GLN:HB3	1:581:A:GLN:H	5	0.1
(2,997)	1:581:A:GLN:HB3	1:581:A:GLN:H	8	0.1
(2,997)	1:581:A:GLN:HB3	1:581:A:GLN:H	11	0.1
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	1	0.1
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	1	0.1
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	1	0.1
(2,799)	1:574:A:VAL:HG11	1:580:A:LYS:H	13	0.1
(2,799)	1:574:A:VAL:HG12	1:580:A:LYS:H	13	0.1
(2,799)	1:574:A:VAL:HG13	1:580:A:LYS:H	13	0.1
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	2	0.1
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	14	0.1
(2,716)	1:570:A:PRO:HB3	1:571:A:GLU:H	15	0.1
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	6	0.1
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	10	0.1
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	12	0.1
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	16	0.1
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	18	0.1
(2,711)	1:570:A:PRO:HA	1:570:A:PRO:HG2	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	2	0.1
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	4	0.1
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	9	0.1
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	16	0.1
(2,670)	1:568:A:PHE:HA	1:572:A:HIS:H	17	0.1
(2,632)	1:566:A:LYS:H	1:566:A:LYS:HE3	11	0.1
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	6	0.1
(2,603)	1:564:A:MET:H	1:565:A:ALA:H	14	0.1
(2,488)	1:561:A:ILE:HG21	1:563:A:ALA:H	5	0.1
(2,488)	1:561:A:ILE:HG22	1:563:A:ALA:H	5	0.1
(2,488)	1:561:A:ILE:HG23	1:563:A:ALA:H	5	0.1
(2,488)	1:561:A:ILE:HG21	1:563:A:ALA:H	9	0.1
(2,488)	1:561:A:ILE:HG22	1:563:A:ALA:H	9	0.1
(2,488)	1:561:A:ILE:HG23	1:563:A:ALA:H	9	0.1
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	3	0.1
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	5	0.1
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	6	0.1
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	11	0.1
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	12	0.1
(2,457)	1:560:A:CYS:HA	1:561:A:ILE:HG13	17	0.1
(2,445)	1:559:A:ARG:HG2	1:560:A:CYS:H	1	0.1
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	16	0.1
(2,441)	1:559:A:ARG:HA	1:560:A:CYS:HB2	19	0.1
(2,432)	1:559:A:ARG:HA	1:559:A:ARG:HD3	4	0.1
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	6	0.1
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	6	0.1
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	6	0.1
(2,404)	1:556:A:ILE:HD11	1:567:A:LYS:H	10	0.1
(2,404)	1:556:A:ILE:HD12	1:567:A:LYS:H	10	0.1
(2,404)	1:556:A:ILE:HD13	1:567:A:LYS:H	10	0.1
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	4	0.1
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	4	0.1
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	4	0.1
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	6	0.1
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	6	0.1
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	6	0.1
(2,397)	1:556:A:ILE:HD11	1:567:A:LYS:HA	16	0.1
(2,397)	1:556:A:ILE:HD12	1:567:A:LYS:HA	16	0.1
(2,397)	1:556:A:ILE:HD13	1:567:A:LYS:HA	16	0.1
(2,264)	1:550:A:SER:HB2	1:567:A:LYS:H	4	0.1
(2,264)	1:550:A:SER:HB2	1:567:A:LYS:H	7	0.1
(2,264)	1:550:A:SER:HB2	1:567:A:LYS:H	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,264)	1:550:A:SER:HB2	1:567:A:LYS:H	18	0.1
(2,236)	1:550:A:SER:HB2	1:551:A:GLY:H	15	0.1
(2,226)	1:549:A:CYS:H	1:568:A:PHE:HA	14	0.1
(2,226)	1:549:A:CYS:H	1:568:A:PHE:HA	18	0.1
(2,129)	1:547:A:SER:HB2	1:567:A:LYS:HE3	20	0.1
(2,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	10	0.1
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	5	0.1
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	7	0.1
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	9	0.1
(1,1516)	1:602:A:LYS:HB2	1:603:A:LEU:HG	15	0.1
(1,1472)	1:601:A:LEU:HD21	1:601:A:LEU:HA	17	0.1
(1,1472)	1:601:A:LEU:HD22	1:601:A:LEU:HA	17	0.1
(1,1472)	1:601:A:LEU:HD23	1:601:A:LEU:HA	17	0.1
(1,1472)	1:601:A:LEU:HD21	1:601:A:LEU:HA	20	0.1
(1,1472)	1:601:A:LEU:HD22	1:601:A:LEU:HA	20	0.1
(1,1472)	1:601:A:LEU:HD23	1:601:A:LEU:HA	20	0.1
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	7	0.1
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	7	0.1
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	7	0.1
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	9	0.1
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	9	0.1
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	9	0.1
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	10	0.1
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	10	0.1
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	10	0.1
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	11	0.1
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	11	0.1
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	11	0.1
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	14	0.1
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	14	0.1
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	14	0.1
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	15	0.1
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	15	0.1
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	15	0.1
(1,1471)	1:601:A:LEU:HD11	1:601:A:LEU:H	16	0.1
(1,1471)	1:601:A:LEU:HD12	1:601:A:LEU:H	16	0.1
(1,1471)	1:601:A:LEU:HD13	1:601:A:LEU:H	16	0.1
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	4	0.1
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	6	0.1
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	7	0.1
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	11	0.1
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:600:A:PHE:HA	1:604:A:PHE:HA	16	0.1
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	1	0.1
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	5	0.1
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	9	0.1
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	12	0.1
(1,1455)	1:600:A:PHE:HA	1:603:A:LEU:HB3	13	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	3	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	3	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	3	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	6	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	6	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	6	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	10	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	10	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	10	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	11	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	11	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	11	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	12	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	12	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	12	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD21	16	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD22	16	0.1
(1,1416)	1:598:A:ASN:H	1:601:A:LEU:HD23	16	0.1
(1,1415)	1:598:A:ASN:H	1:601:A:LEU:HB2	20	0.1
(1,1396)	1:598:A:ASN:HA	1:598:A:ASN:HD21	10	0.1
(1,1385)	1:597:A:GLN:HB3	1:599:A:CYS:H	20	0.1
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	3	0.1
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	6	0.1
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	12	0.1
(1,1362)	1:596:A:CYS:H	1:598:A:ASN:H	20	0.1
(1,1289)	1:592:A:ASP:HB3	1:593:A:LYS:HB3	8	0.1
(1,1247)	1:590:A:GLN:H	1:591:A:ASN:HB3	2	0.1
(1,1247)	1:590:A:GLN:H	1:591:A:ASN:HB3	4	0.1
(1,1247)	1:590:A:GLN:H	1:591:A:ASN:HB3	18	0.1
(1,1235)	1:590:A:GLN:HG2	1:590:A:GLN:H	20	0.1
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	14	0.1
(1,1166)	1:588:A:LYS:H	1:589:A:GLU:H	15	0.1
(1,1132)	1:587:A:PHE:H	1:588:A:LYS:H	5	0.1
(1,1132)	1:587:A:PHE:H	1:588:A:LYS:H	20	0.1
(1,1123)	1:586:A:THR:HB	1:597:A:GLN:HG3	20	0.1
(1,1099)	1:584:A:LYS:HB3	1:586:A:THR:H	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	2	0.1
(1,1013)	1:581:A:GLN:HG2	1:582:A:LEU:HA	16	0.1
(1,982)	1:581:A:GLN:HB3	1:581:A:GLN:H	5	0.1
(1,982)	1:581:A:GLN:HB3	1:581:A:GLN:H	8	0.1
(1,982)	1:581:A:GLN:HB3	1:581:A:GLN:H	11	0.1
(1,806)	1:574:A:VAL:HA	1:582:A:LEU:HG	4	0.1
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	2	0.1
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	14	0.1
(1,702)	1:570:A:PRO:HB3	1:571:A:GLU:H	15	0.1
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	6	0.1
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	10	0.1
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	12	0.1
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	16	0.1
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	18	0.1
(1,697)	1:570:A:PRO:HA	1:570:A:PRO:HG2	20	0.1
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	2	0.1
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	4	0.1
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	9	0.1
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	16	0.1
(1,656)	1:568:A:PHE:HA	1:572:A:HIS:H	17	0.1
(1,618)	1:566:A:LYS:H	1:566:A:LYS:HE3	11	0.1
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	6	0.1
(1,589)	1:564:A:MET:H	1:565:A:ALA:H	14	0.1
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	8	0.1
(1,495)	1:561:A:ILE:H	1:570:A:PRO:HG2	12	0.1
(1,474)	1:561:A:ILE:HG21	1:563:A:ALA:H	5	0.1
(1,474)	1:561:A:ILE:HG22	1:563:A:ALA:H	5	0.1
(1,474)	1:561:A:ILE:HG23	1:563:A:ALA:H	5	0.1
(1,474)	1:561:A:ILE:HG21	1:563:A:ALA:H	9	0.1
(1,474)	1:561:A:ILE:HG22	1:563:A:ALA:H	9	0.1
(1,474)	1:561:A:ILE:HG23	1:563:A:ALA:H	9	0.1
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	3	0.1
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	5	0.1
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	6	0.1
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	11	0.1
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	12	0.1
(1,443)	1:560:A:CYS:HA	1:561:A:ILE:HG13	17	0.1
(1,431)	1:559:A:ARG:HG2	1:560:A:CYS:H	16	0.1
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	16	0.1
(1,427)	1:559:A:ARG:HA	1:560:A:CYS:HB2	19	0.1
(1,418)	1:559:A:ARG:HA	1:559:A:ARG:HD3	4	0.1
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	6	0.1
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	6	0.1
(1,390)	1:556:A:ILE:HD11	1:567:A:LYS:H	10	0.1
(1,390)	1:556:A:ILE:HD12	1:567:A:LYS:H	10	0.1
(1,390)	1:556:A:ILE:HD13	1:567:A:LYS:H	10	0.1
(1,254)	1:550:A:SER:HB2	1:567:A:LYS:H	4	0.1
(1,254)	1:550:A:SER:HB2	1:567:A:LYS:H	7	0.1
(1,254)	1:550:A:SER:HB2	1:567:A:LYS:H	9	0.1
(1,254)	1:550:A:SER:HB2	1:567:A:LYS:H	18	0.1
(1,230)	1:550:A:SER:HB2	1:551:A:GLY:H	15	0.1
(1,220)	1:549:A:CYS:H	1:568:A:PHE:HA	14	0.1
(1,220)	1:549:A:CYS:H	1:568:A:PHE:HA	18	0.1
(1,152)	1:548:A:LEU:HB2	1:550:A:SER:HA	16	0.1
(1,129)	1:547:A:SER:HB2	1:567:A:LYS:HE3	20	0.1
(1,93)	1:545:A:ARG:HG3	1:546:A:GLY:HA3	10	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found