



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 02:40 PM UTC

PDB ID : 7D3V / pdb_00007d3v
BMRB ID : 36387
Title : Non-specific and specific interactions work cooperatively to promote cytidine deamination catalyzed by APOBEC3A
Authors : Cao, C.Y.; Liu, Y.P.; Lan, W.X.
Deposited on : 2020-09-21

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

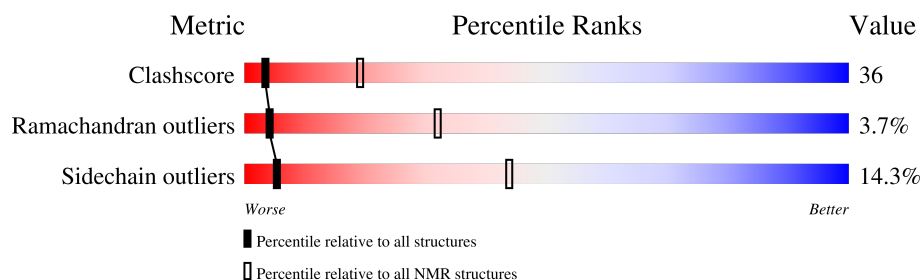
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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	199	44% 44% 10% . .
1	B	199	57% 30% 7% . 6%
2	C	10	80% 20%
2	D	10	30% 70%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:6-A:199, B:204-B:246, B:250-B:300, B:305-B:398 (382)	0.95	5

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

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

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

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

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6978 atoms, of which 3326 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA dC->dU-editing enzyme APOBEC-3A.

Mol	Chain	Residues	Atoms						Trace
1	A	199	Total	C	H	N	O	S	0
			3172	1029	1546	295	293	9	
1	B	199	Total	C	H	N	O	S	0
			3172	1029	1546	295	293	9	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	ASN	LEU	engineered mutation	UNP P31941
A	64	SER	CYS	engineered mutation	UNP P31941
A	72	GLN	GLU	engineered mutation	UNP P31941
A	171	GLN	CYS	engineered mutation	UNP P31941
B	262	ASN	LEU	engineered mutation	UNP P31941
B	263	SER	CYS	engineered mutation	UNP P31941
B	271	GLN	GLU	engineered mutation	UNP P31941
B	370	GLN	CYS	engineered mutation	UNP P31941

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						Trace
2	C	10	Total	C	H	N	O	P	0
			316	99	117	30	61	9	
2	D	10	Total	C	H	N	O	P	0
			316	99	117	30	61	9	

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

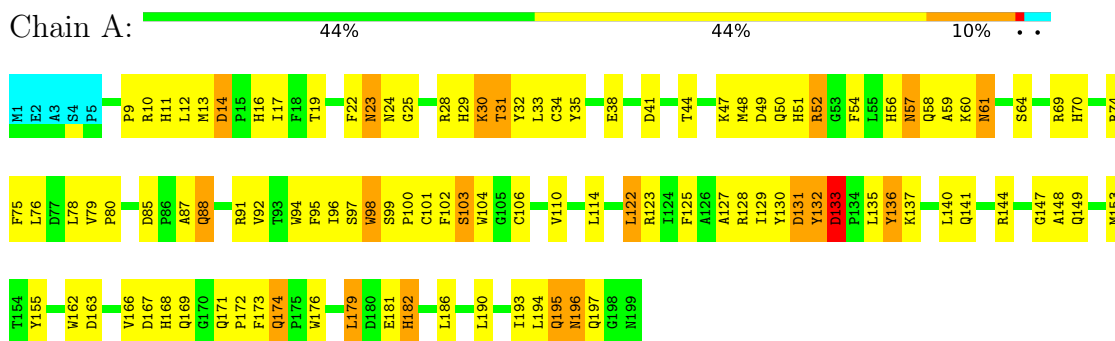
Mol	Chain	Residues	Atoms	
3	A	1	Total	Zn
			1	1
3	B	1	Total	Zn
			1	1

4 Residue-property plots

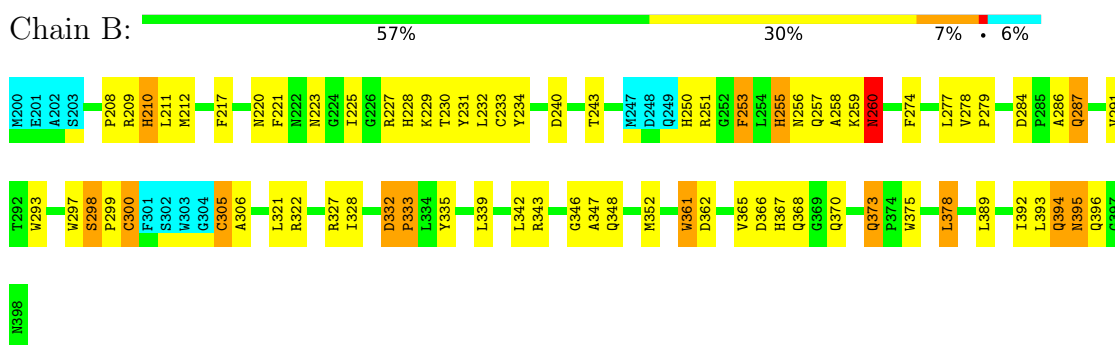
4.1 Average score per residue in the NMR ensemble

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.

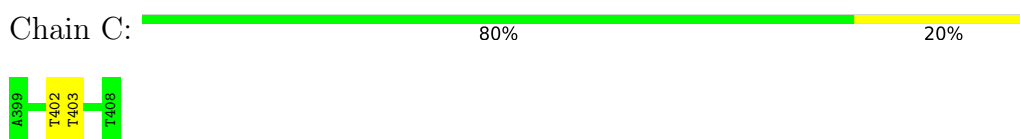
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



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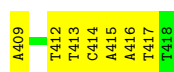


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')





4.2 Scores per residue for each member of the ensemble

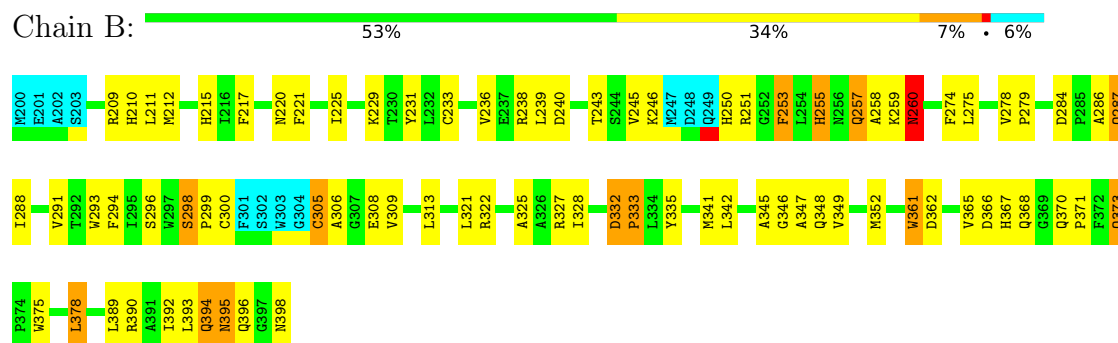
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

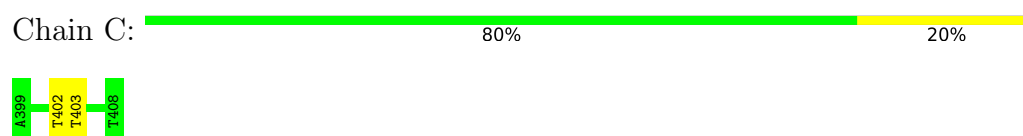
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

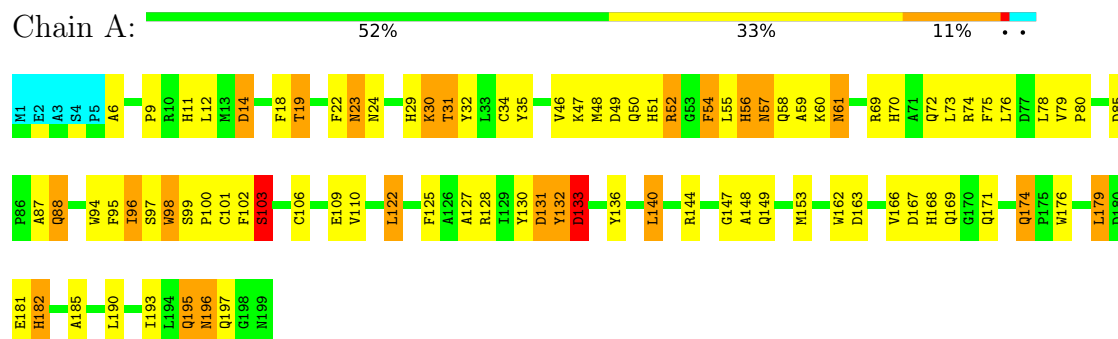


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

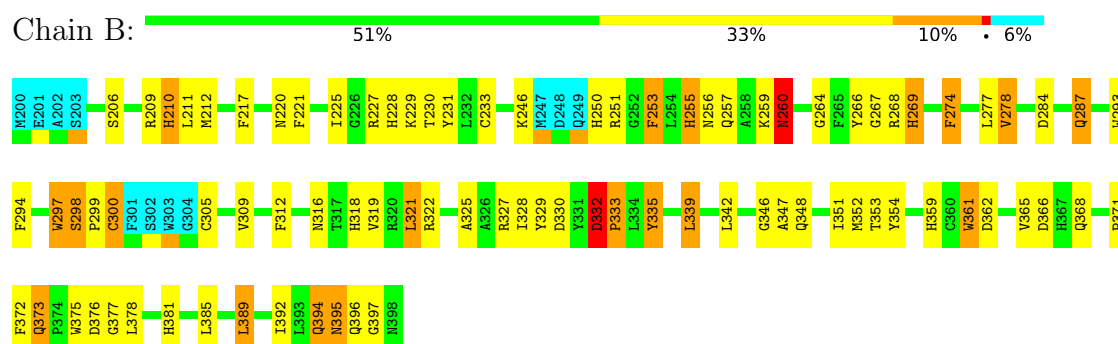


4.2.2 Score per residue for model 2

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



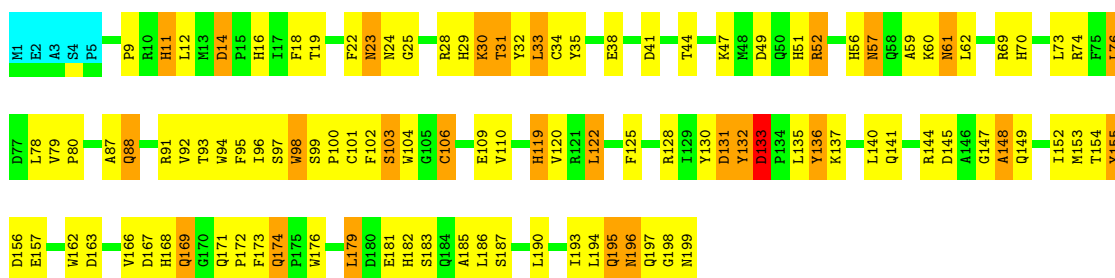
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



4.2.3 Score per residue for model 3

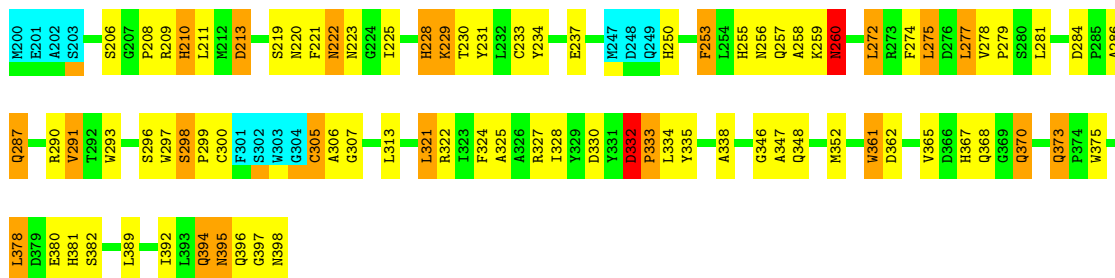
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 52% 31% 11% 6%



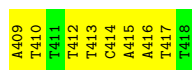
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C: 80% 20%



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

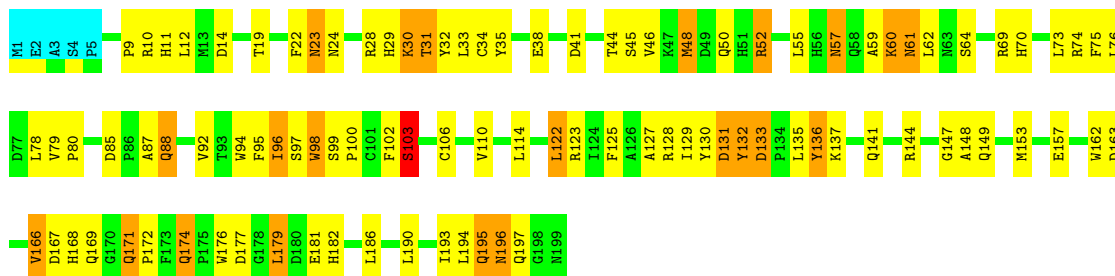
Chain D: 20% 80%



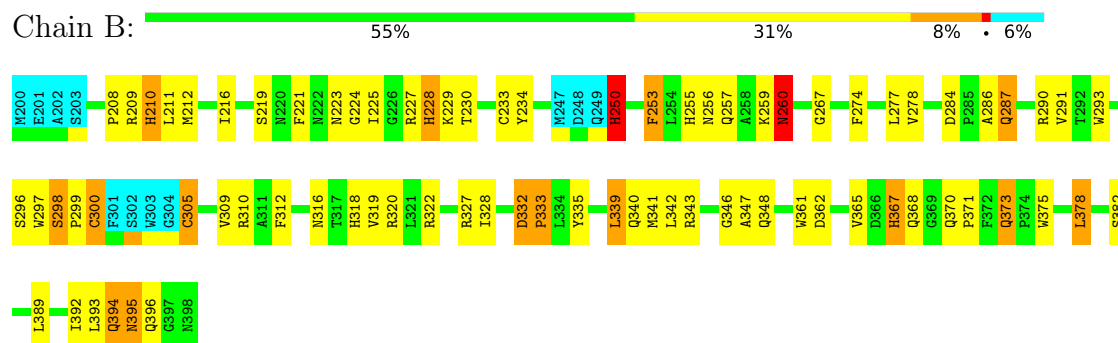
4.2.4 Score per residue for model 4

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

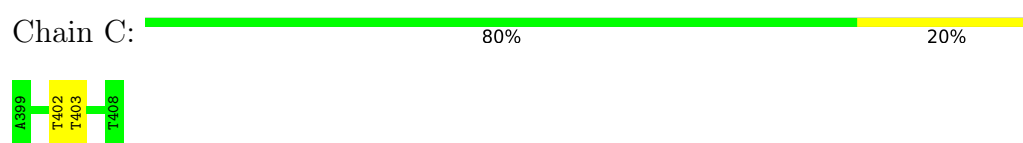
Chain A: 48% 38% 11% 3%



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

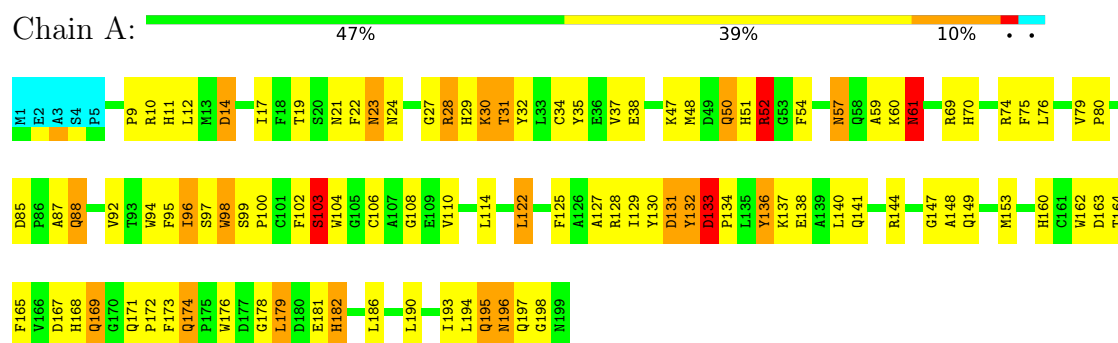


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

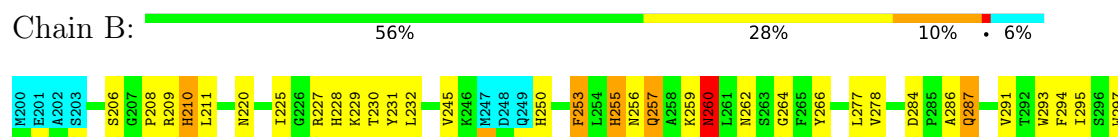


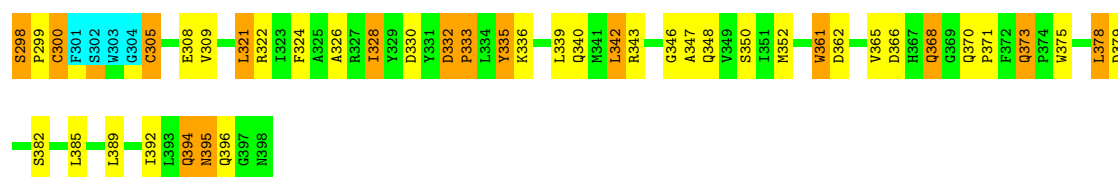
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



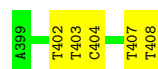
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





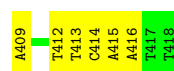
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C: 50% 50%



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

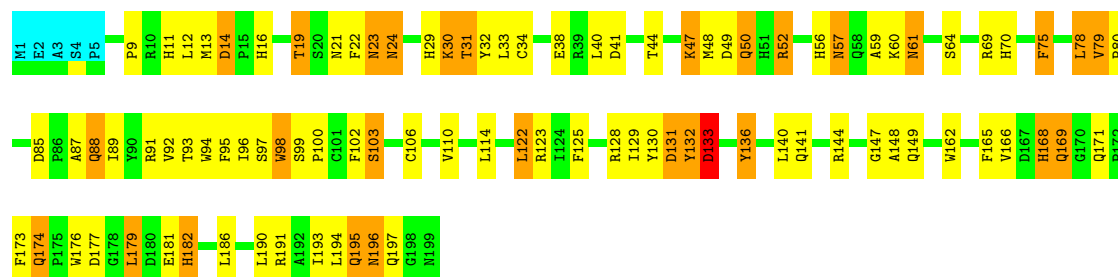
Chain D: 40% 60%



4.2.6 Score per residue for model 6

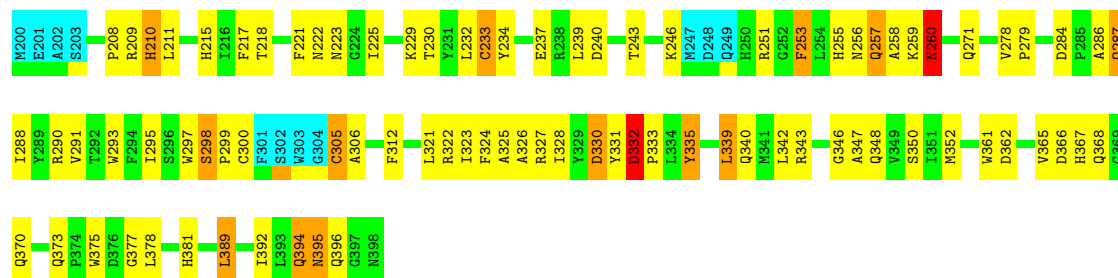
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 50% 33% 14%



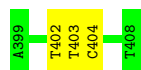
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 51% 36% 7% 6%

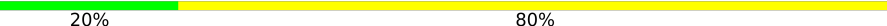


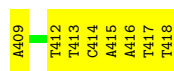
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C:  70% 30%



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

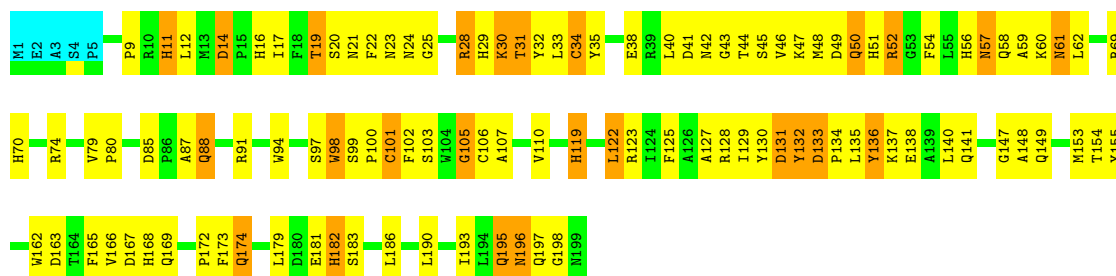
Chain D:  20% 80%



4.2.7 Score per residue for model 7

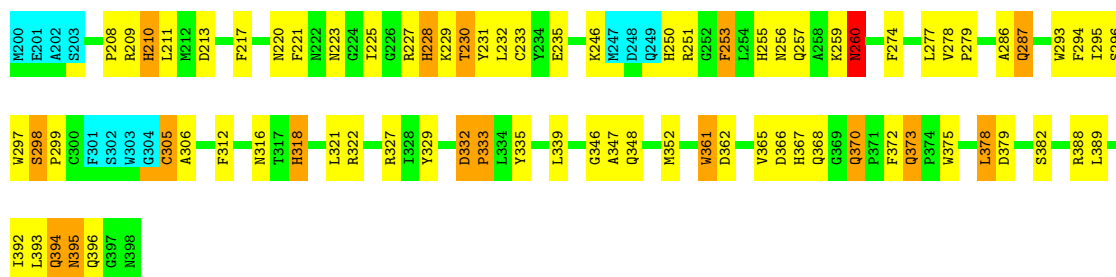
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A:  43% 42% 13% •



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:  56% 30% 8% • 6%

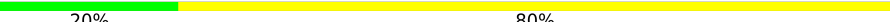


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C:  80% 20%



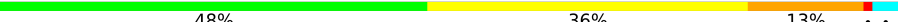
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain D:  20% 80%

A409
T412
T413
C414
A415
A416
T417
T418

4.2.8 Score per residue for model 8

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A:  48% 36% 13% ..

M1 E2 A3 S4 P5 P9 L12 H16 I17 F18 T19 S20 N21 F22 N23 N24 N25 G26 G27 R28 H29 K30 T31 Y32 L33 C34 Y35 F36 V37 E38 M48 D49 G50 H51 R52 G53 F54 N57 G58 A59 R60 N61 L62 N63 S64 G65 P66 R69 H70 R74 F75 V79

P80 A87 Q88 R91 V92 T93 W94 F95 I96 S97 Q98 S99 P100 C101 F102 F103 S103 N104 V104 G105 C106 A107 G108 E109 V110 L114 L122 F125 A126 A127 R128 Y129 D131 Y132 D133 F134 L135 Y136 K137 L140 L143 R144 G147 A148 Q149 M153 E157 F158 M162 D163

T164 F165 V166 D167 H168 Q169 P172 F173 Q174 P175 W176 D177 G178 L179 D180 E181 H182 L190 R191 A192 I193 T194 L194 Q195 N196 Q197 G198 N199

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:  53% 34% 7% 6%

M200 E201 A202 S203 P208 R209 H210 L211 M212 F217 N220 F221 N222 N223 G224 I225 G226 R227 H228 K229 T230 Y231 L232 C233 D240 N241 G242 T243 M247 D248 H250 R251 G252 F253 L254 H255 N256 Q257 A258 K259 S260 L261 S262 G263 G264 F265 Y266 A270 Q271 F274 V278

P279 D284 P285 A286 Q287 T292 W293 V297 S298 P299 G300 F301 S302 S303 W304 G305 E308 V309 R310 L321 R322 I323 F324 R327 Y331 D332 P333 L342 R343 D344 A345 G346 A347 Q348 V349 S350 W361 D362 T363 F364 V365 D366 H367 Q368 F372 Q373 F374 W375 L378

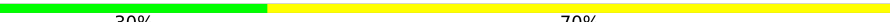
D379 E380 A384 L389 I392 L393 Q394 Q395 Q396 G397 R398

- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C:  30% 70%

A399 T400 T401 P402 T403 A406 T407 T408

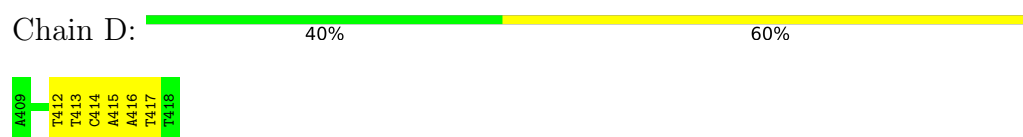
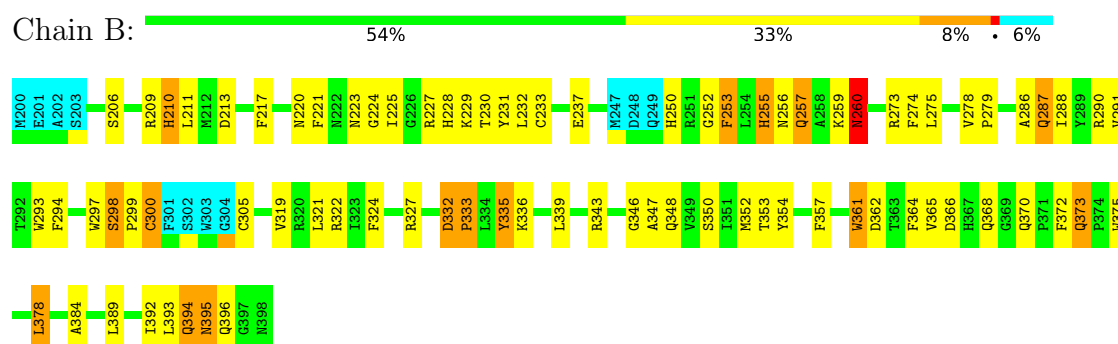
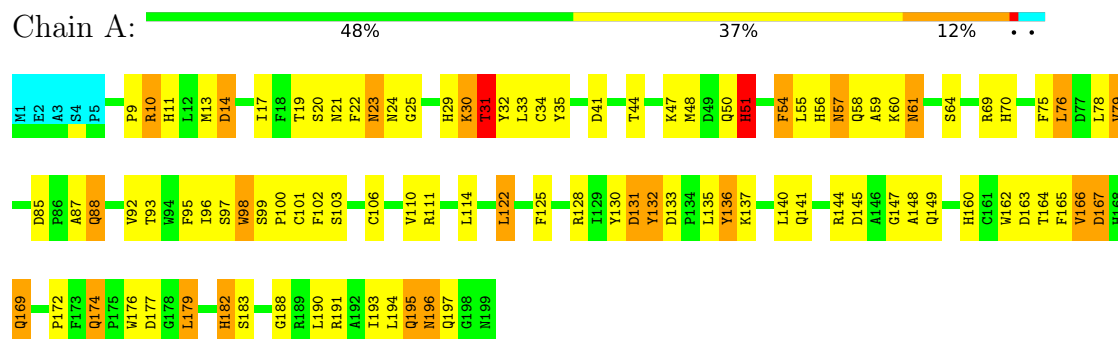
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain D:  30% 70%

A409 T412 T413 C414 A415 A416 T417 T418

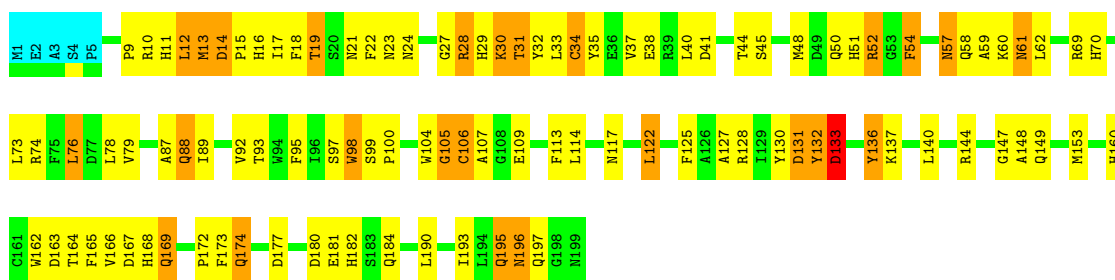
4.2.9 Score per residue for model 9

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





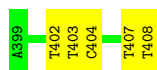
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 46% 39% 10% 6%



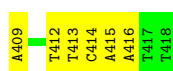
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C: 50% 50%



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

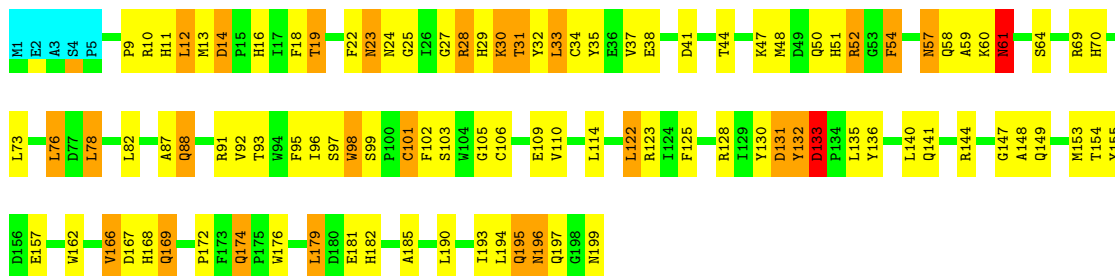
Chain D: 40% 60%



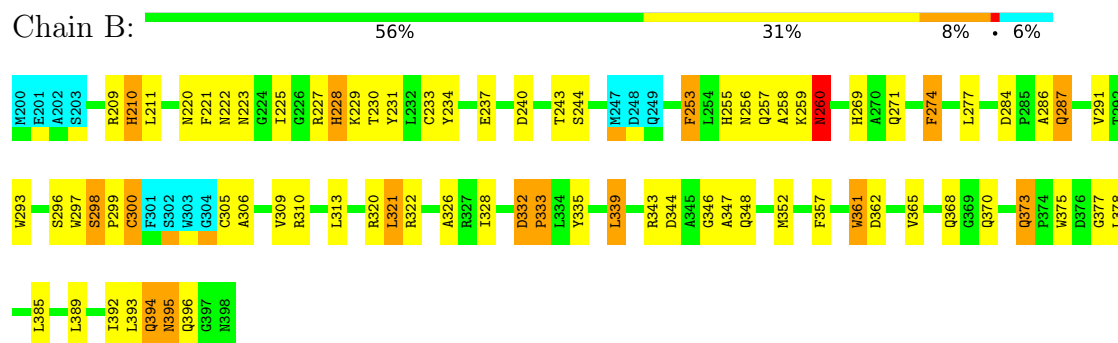
4.2.11 Score per residue for model 11

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

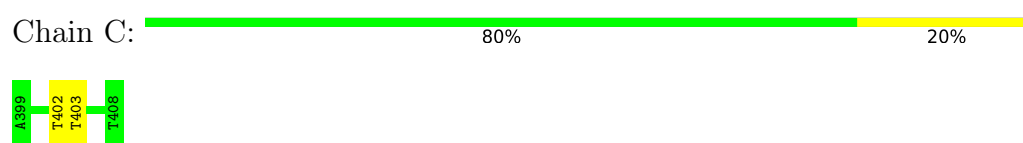
Chain A: 47% 37% 13% 3%



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

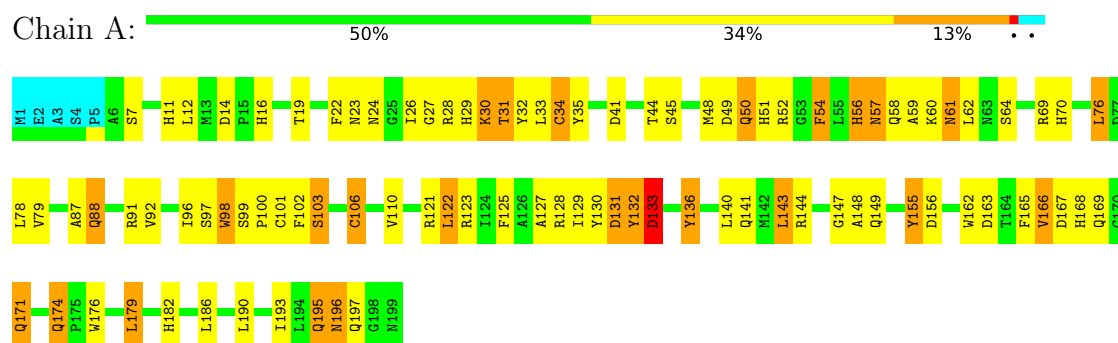


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

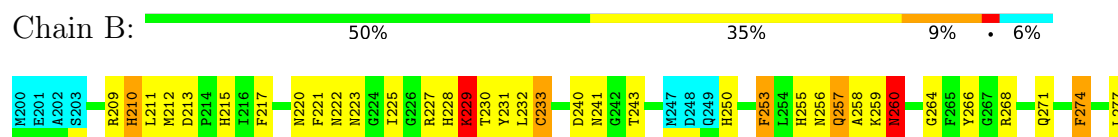


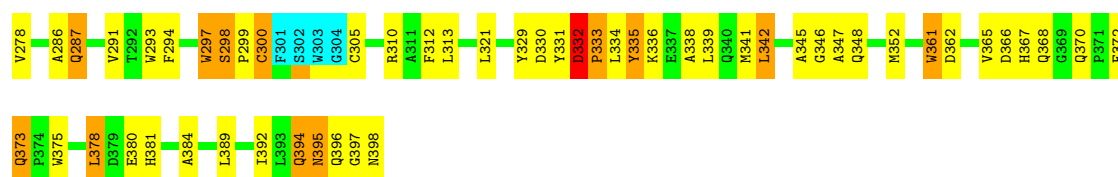
4.2.12 Score per residue for model 12

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





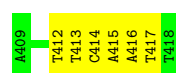
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C: 



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

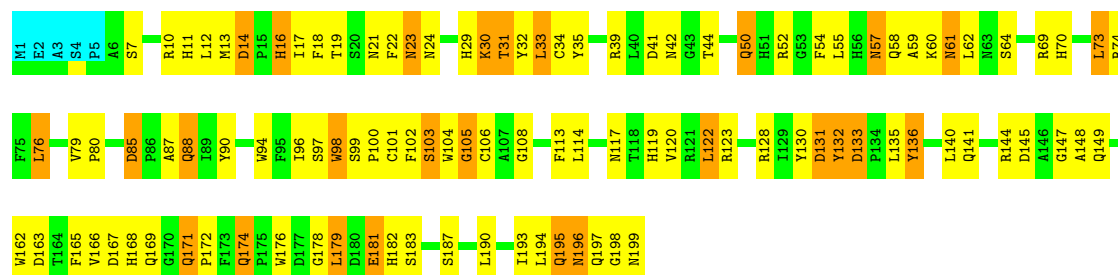
Chain D: 



4.2.13 Score per residue for model 13

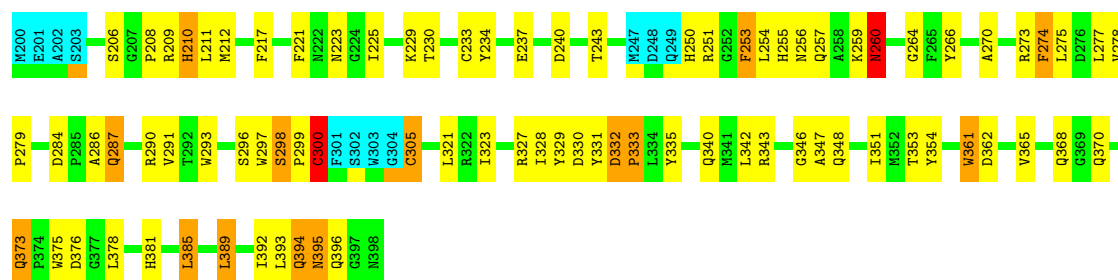
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 

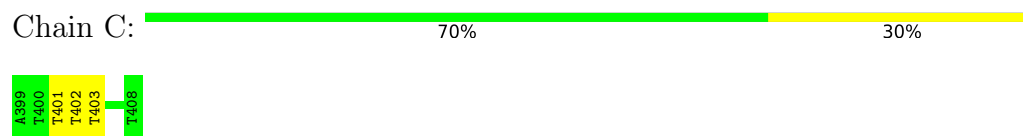


- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

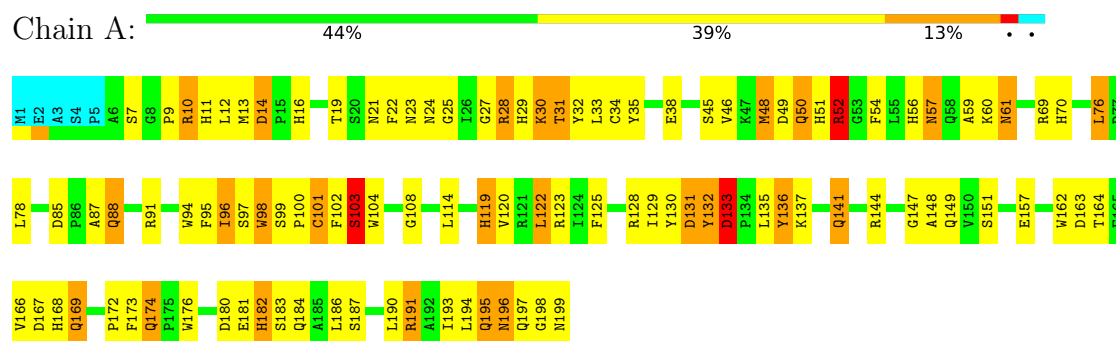


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



4.2.14 Score per residue for model 14

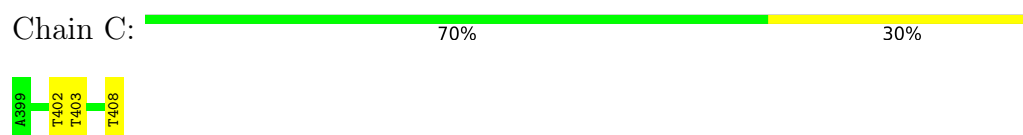
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



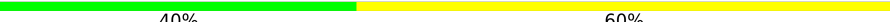
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

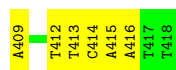


- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain D:  40% 60%



4.2.15 Score per residue for model 15

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A:  49% 37% 10% • •



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:  51% 34% 8% • 6%

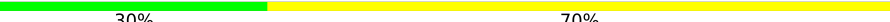


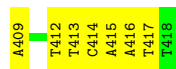
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C:  80% 20%



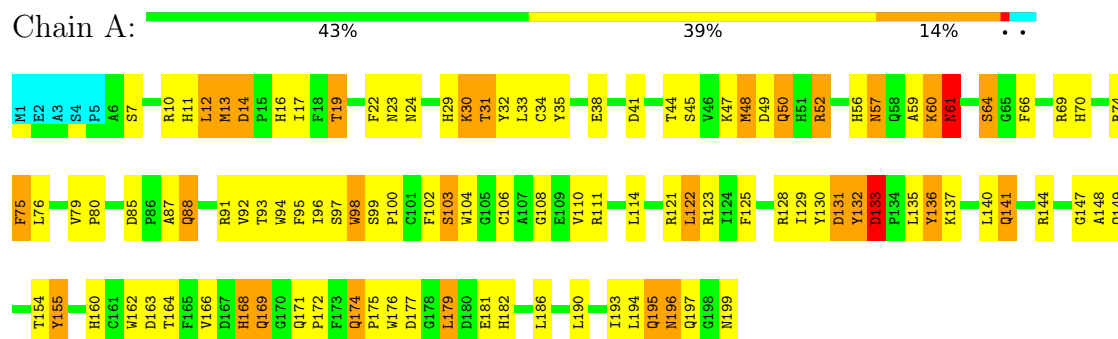
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain D:  30% 70%

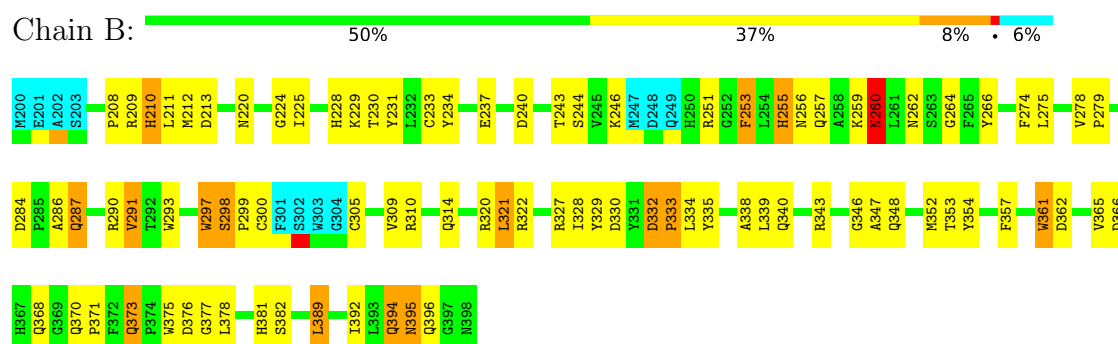


4.2.16 Score per residue for model 16

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



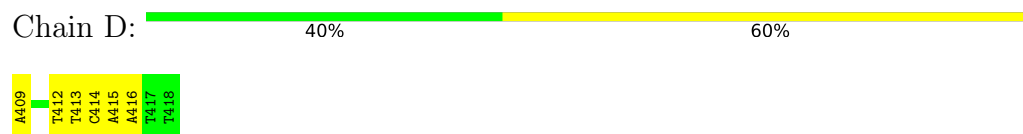
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')



4.2.17 Score per residue for model 17

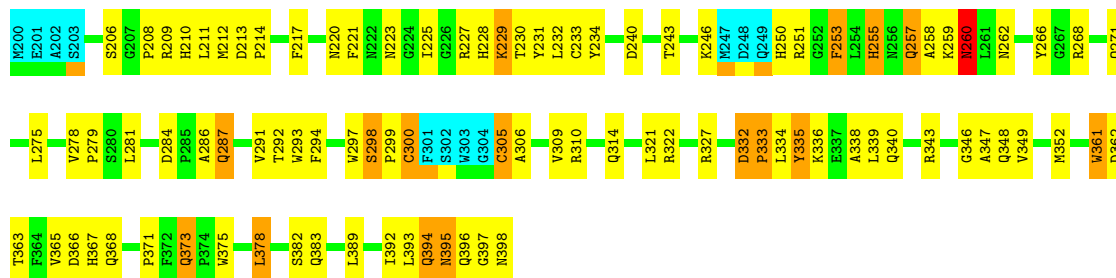
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A





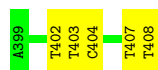
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 47% 39% 8% 6%



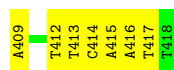
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C: 50% 50%



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

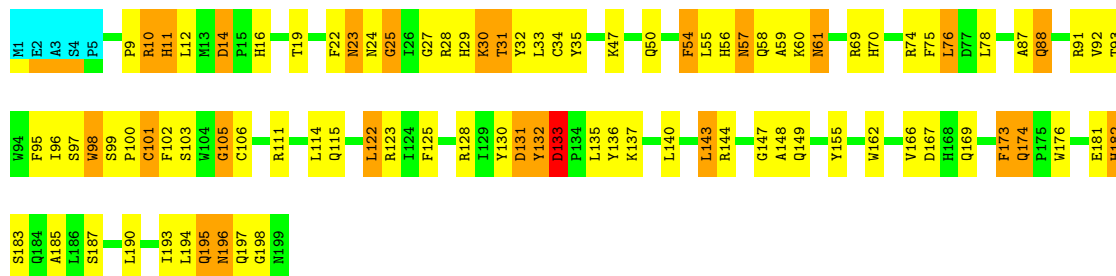
Chain D: 30% 70%



4.2.18 Score per residue for model 18

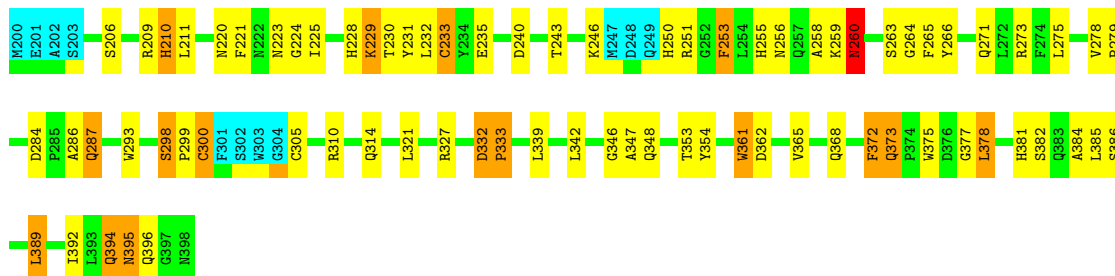
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 51% 34% 12%



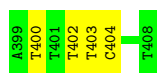
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B:  56% 30% 8% • 6%



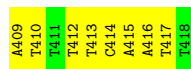
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C:  60% 40%



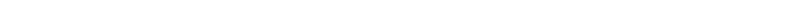
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

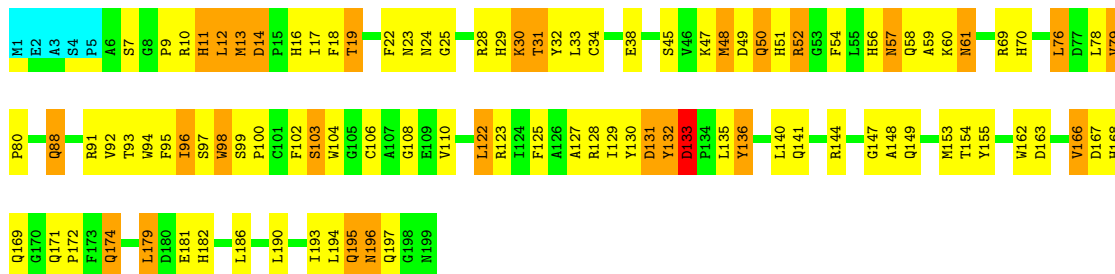
Chain D: 20% 80%



4.2.19 Score per residue for model 19

- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

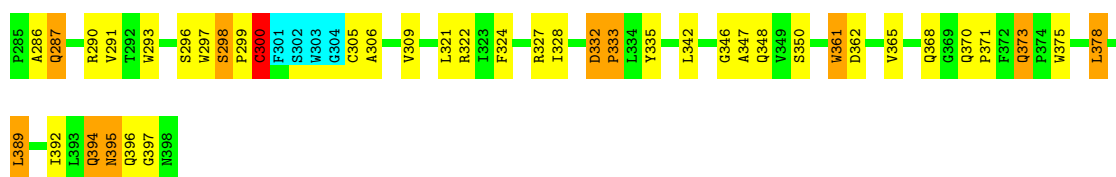
Chain A:  47% 36% 14% . .



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 55% 30% 8% • 6%





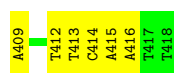
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C: 80% 20%



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

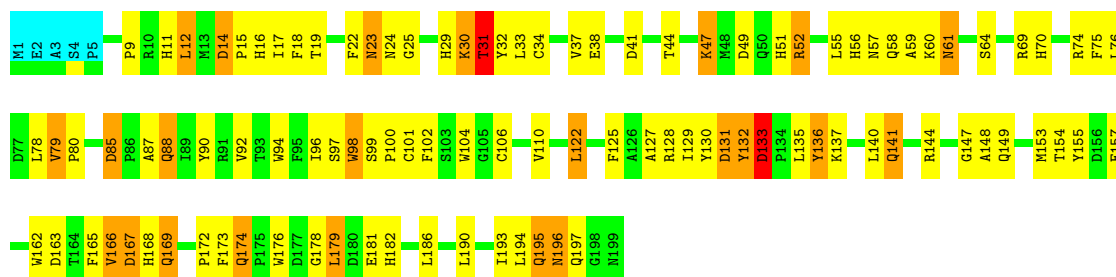
Chain D: 40% 60%



4.2.20 Score per residue for model 20

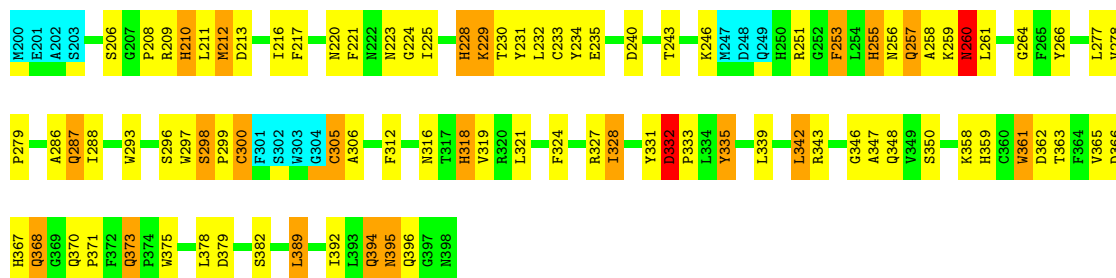
- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain A: 46% 39% 12% ..



- Molecule 1: DNA dC->dU-editing enzyme APOBEC-3A

Chain B: 49% 34% 11% 6%



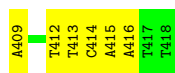
- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain C:  80% 20%



- Molecule 2: DNA (5'-D(*AP*TP*TP*TP*TP*CP*AP*AP*TP*T)-3')

Chain D:  40% 60%



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	
CNS	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	4564
Number of shifts mapped to atoms	4564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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	1.43±0.00	0±0/1638 (0.0± 0.0%)	1.31±0.00	0±0/2218 (0.0± 0.0%)
1	B	1.43±0.00	0±0/1583 (0.0± 0.0%)	1.31±0.01	1±1/2144 (0.1± 0.0%)
2	C	0.61±0.02	0±0/221 (0.0± 0.0%)	0.96±0.01	0±0/339 (0.0± 0.0%)
2	D	0.54±0.01	0±0/221 (0.0± 0.0%)	1.00±0.01	0±0/339 (0.0± 0.0%)
All	All	1.35	4/73260 (0.0%)	1.27	33/100800 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	25	GLY	N-CA	5.05	1.49	1.44	9	3
1	B	278	VAL	CA-CB	5.03	1.57	1.54	19	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	257	GLN	CB-CA-C	-5.67	109.04	115.79	14	18
1	A	75	PHE	CA-CB-CG	-5.39	108.41	113.80	16	5
1	B	274	PHE	CA-CB-CG	-5.28	108.52	113.80	12	8
1	A	70	HIS	CA-CB-CG	-5.11	108.69	113.80	17	1
1	A	11	HIS	CA-CB-CG	-5.04	108.76	113.80	3	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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	1591	1512	1503	142±10
1	B	1538	1471	1462	106±11
2	C	199	117	118	5±2
2	D	199	117	118	23±3
All	All	70580	64340	64020	4855

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:378:LEU:H	1:B:378:LEU:HD22	0.94	1.23	10	12
1:A:179:LEU:HD22	1:A:179:LEU:H	0.93	1.22	3	15
1:B:250:HIS:NE2	1:B:281:LEU:HD21	0.90	1.81	10	1
1:B:361:TRP:CE3	1:B:365:VAL:HG21	0.88	2.03	9	17
1:B:343:ARG:HH11	1:B:393:LEU:HD11	0.88	1.28	17	1
1:A:144:ARG:HE	1:A:194:LEU:HD11	0.88	1.29	16	3
1:A:119:HIS:CD2	1:A:120:VAL:HG23	0.87	2.05	14	3
1:B:296:SER:HG	1:B:297:TRP:CD1	0.87	1.87	19	7
1:B:205:ALA:HB1	1:B:209:ARG:HH22	0.86	1.28	15	1
1:B:298:SER:OG	1:B:339:LEU:HD21	0.85	1.70	12	2
1:A:144:ARG:NE	1:A:194:LEU:HD11	0.85	1.86	16	3
1:B:225:ILE:HD12	2:C:402:DT:OP2	0.85	1.72	1	19
1:A:16:HIS:CG	1:B:258:ALA:HB3	0.85	2.06	20	11
1:A:78:LEU:HD11	1:B:209:ARG:NE	0.85	1.87	3	2
1:B:335:TYR:OH	1:B:392:ILE:HD11	0.85	1.71	3	5
1:B:335:TYR:CE1	1:B:339:LEU:HD11	0.84	2.07	15	1
1:B:246:LYS:HZ3	1:B:251:ARG:HE	0.84	1.15	16	1
1:A:140:LEU:HD23	1:A:193:ILE:HG21	0.83	1.47	6	1
1:A:14:ASP:CG	1:A:17:ILE:HD12	0.83	1.98	19	7
1:A:62:LEU:HD11	2:D:417:DT:OP1	0.83	1.74	12	6
1:A:12:LEU:HD23	1:A:167:ASP:CG	0.83	1.99	3	1
1:A:16:HIS:ND1	1:B:258:ALA:HB3	0.82	1.88	11	6
1:B:205:ALA:HB1	1:B:209:ARG:NH2	0.82	1.90	15	1
1:A:31:THR:HG22	1:A:98:TRP:CZ2	0.79	2.12	14	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:LEU:HD13	1:A:193:ILE:HD13	0.79	1.54	7	11
1:B:343:ARG:NH1	1:B:393:LEU:HD11	0.79	1.92	17	1
1:A:62:LEU:HD21	2:D:417:DT:OP1	0.79	1.78	1	2
1:B:361:TRP:CD1	1:B:362:ASP:N	0.78	2.51	12	20
1:B:293:TRP:CH2	1:B:321:LEU:HD11	0.78	2.14	1	4
1:A:162:TRP:HE1	1:A:168:HIS:CD2	0.78	1.96	16	4
1:B:339:LEU:HD23	1:B:392:ILE:HG21	0.78	1.56	16	4
1:A:31:THR:HG23	1:A:32:TYR:N	0.78	1.94	14	20
1:A:102:PHE:CE2	1:A:135:LEU:HD13	0.77	2.13	14	4
1:A:179:LEU:HD22	1:A:179:LEU:N	0.77	1.95	9	15
1:B:378:LEU:HD22	1:B:378:LEU:N	0.76	1.96	7	12
1:A:14:ASP:OD1	1:A:17:ILE:HD12	0.76	1.80	15	3
1:A:94:TRP:CH2	1:A:122:LEU:HD11	0.76	2.16	20	10
1:B:230:THR:HG23	1:B:256:ASN:OD1	0.75	1.81	13	4
1:A:94:TRP:CE2	1:A:122:LEU:HD21	0.75	2.17	2	10
1:A:78:LEU:HD23	1:A:78:LEU:O	0.75	1.82	4	5
1:B:232:LEU:C	1:B:232:LEU:HD23	0.74	2.08	8	10
1:A:14:ASP:OD2	1:A:17:ILE:HD12	0.74	1.83	1	4
1:A:144:ARG:HH11	1:A:194:LEU:HD11	0.74	1.41	3	1
1:A:96:ILE:HD12	1:A:96:ILE:H	0.74	1.43	5	1
1:A:57:ASN:H	1:A:57:ASN:ND2	0.73	1.81	17	10
1:A:33:LEU:O	1:A:33:LEU:HD23	0.73	1.84	10	8
1:B:335:TYR:CD1	1:B:336:LYS:N	0.73	2.57	5	3
1:A:135:LEU:C	1:A:135:LEU:HD12	0.72	2.08	17	2
1:A:140:LEU:HD13	1:A:193:ILE:HG21	0.72	1.61	19	3
1:B:305:CYS:O	1:B:309:VAL:HG23	0.72	1.85	10	9
1:A:129:ILE:HD11	1:A:186:LEU:CD1	0.72	2.14	16	9
1:B:293:TRP:CZ2	1:B:321:LEU:HD21	0.71	2.20	5	5
1:A:48:MET:HE3	1:A:51:HIS:CE1	0.71	2.20	19	3
1:B:220:ASN:ND2	1:B:231:TYR:CZ	0.71	2.59	5	5
1:A:140:LEU:HD23	1:A:140:LEU:C	0.71	2.10	11	3
1:A:102:PHE:CD1	1:A:135:LEU:HD13	0.71	2.21	9	2
1:A:57:ASN:N	1:A:57:ASN:ND2	0.71	2.39	3	9
1:A:102:PHE:CE1	1:A:135:LEU:HD13	0.71	2.20	15	3
1:A:162:TRP:NE1	1:A:168:HIS:CD2	0.71	2.59	6	4
1:B:220:ASN:ND2	1:B:231:TYR:CE2	0.70	2.59	8	2
1:A:16:HIS:CD2	1:B:258:ALA:HB3	0.70	2.21	20	1
1:A:182:HIS:ND1	1:A:183:SER:N	0.70	2.38	14	4
1:B:335:TYR:CD2	1:B:336:LYS:N	0.70	2.60	12	3
1:A:91:ARG:NE	1:A:121:ARG:NH1	0.70	2.40	16	1
1:A:144:ARG:NH1	1:A:194:LEU:HD11	0.70	2.02	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:PHE:CE2	1:A:32:TYR:CZ	0.70	2.80	10	1
1:A:179:LEU:H	1:A:179:LEU:CD2	0.70	1.99	12	15
1:B:230:THR:HG22	1:B:256:ASN:OD1	0.70	1.87	3	1
1:A:31:THR:HG22	1:A:98:TRP:CH2	0.70	2.22	9	20
1:B:361:TRP:CZ2	1:B:367:HIS:CD2	0.70	2.80	12	4
1:B:220:ASN:ND2	1:B:231:TYR:CG	0.70	2.59	11	2
1:B:220:ASN:ND2	1:B:231:TYR:CE1	0.70	2.60	17	5
1:B:225:ILE:N	2:C:403:DT:H72	0.69	2.02	11	13
1:A:95:PHE:CE1	1:A:125:PHE:CD1	0.69	2.80	11	5
1:A:95:PHE:CE1	1:A:125:PHE:CD2	0.69	2.80	1	3
1:B:246:LYS:NZ	1:B:251:ARG:NH1	0.69	2.41	7	6
1:A:10:ARG:NH2	1:B:277:LEU:HD11	0.69	2.02	5	1
1:B:231:TYR:CE2	1:B:255:HIS:CD2	0.69	2.81	7	3
1:A:91:ARG:NH1	1:A:123:ARG:NH2	0.69	2.40	19	5
1:B:312:PHE:CZ	1:B:316:ASN:ND2	0.69	2.61	4	5
1:B:253:PHE:O	1:B:254:LEU:HD12	0.69	1.88	13	1
1:A:162:TRP:CE3	1:A:166:VAL:HG21	0.69	2.22	18	1
1:B:217:PHE:CE1	1:B:221:PHE:CE1	0.69	2.81	1	3
1:A:95:PHE:CE2	1:A:125:PHE:CD2	0.69	2.81	18	5
1:A:48:MET:SD	1:A:48:MET:N	0.69	2.65	1	3
1:A:56:HIS:ND1	1:A:56:HIS:N	0.69	2.40	2	2
1:A:57:ASN:ND2	1:A:57:ASN:N	0.69	2.41	10	10
1:B:320:ARG:NH2	1:B:322:ARG:HE	0.69	1.86	4	1
1:B:343:ARG:NH1	1:B:396:GLN:NE2	0.69	2.41	6	4
1:B:231:TYR:CZ	1:B:255:HIS:NE2	0.69	2.60	3	2
1:B:294:PHE:CE1	1:B:324:PHE:CD1	0.69	2.81	9	1
1:A:106:CYS:O	1:A:110:VAL:HG23	0.69	1.88	2	14
1:A:162:TRP:NE1	1:A:168:HIS:NE2	0.68	2.41	2	2
1:B:305:CYS:SG	1:B:306:ALA:N	0.68	2.66	7	7
1:B:361:TRP:NE1	1:B:367:HIS:CD2	0.68	2.61	6	5
1:A:136:TYR:CG	1:A:137:LYS:N	0.68	2.61	10	12
1:B:361:TRP:CZ2	1:B:365:VAL:HG11	0.68	2.24	9	2
1:B:231:TYR:CE2	1:B:255:HIS:CG	0.68	2.81	18	1
1:B:255:HIS:ND1	1:B:255:HIS:N	0.68	2.40	1	7
1:B:231:TYR:CE1	1:B:255:HIS:CE1	0.68	2.81	12	1
1:B:246:LYS:HZ3	1:B:251:ARG:HH12	0.68	1.30	7	1
1:B:253:PHE:CE2	1:B:364:PHE:CE1	0.68	2.81	10	1
1:B:231:TYR:CD1	1:B:255:HIS:ND1	0.68	2.62	12	1
1:B:378:LEU:H	1:B:378:LEU:CD2	0.68	2.01	10	12
1:A:54:PHE:CZ	1:A:56:HIS:CE1	0.68	2.81	14	2
1:A:131:ASP:O	1:A:132:TYR:CB	0.68	2.42	8	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:PHE:CE2	1:A:125:PHE:CD1	0.68	2.82	6	3
1:B:217:PHE:CE2	1:B:221:PHE:CE2	0.68	2.82	12	5
1:B:361:TRP:NE1	1:B:367:HIS:NE2	0.68	2.41	12	6
1:B:212:MET:SD	1:B:253:PHE:CE2	0.68	2.87	2	1
1:A:96:ILE:HD12	1:A:96:ILE:N	0.68	2.03	5	1
1:B:312:PHE:CE2	1:B:316:ASN:ND2	0.67	2.61	2	3
1:B:253:PHE:CD1	1:B:253:PHE:C	0.67	2.71	12	5
1:B:367:HIS:ND1	1:B:370:GLN:NE2	0.67	2.42	7	1
1:A:11:HIS:CG	1:A:11:HIS:O	0.67	2.47	5	6
1:B:253:PHE:C	1:B:253:PHE:CD2	0.67	2.70	9	10
1:B:367:HIS:CE1	1:B:370:GLN:NE2	0.67	2.62	7	1
1:A:144:ARG:HE	1:A:194:LEU:HD21	0.67	1.49	6	2
1:A:33:LEU:C	1:A:33:LEU:HD23	0.67	2.14	7	3
1:B:294:PHE:CE1	1:B:352:MET:SD	0.67	2.88	7	1
1:B:217:PHE:CZ	1:B:221:PHE:CZ	0.67	2.83	1	2
1:A:144:ARG:NH2	1:A:197:GLN:NE2	0.67	2.42	8	4
1:A:162:TRP:CZ2	1:A:168:HIS:CD2	0.67	2.83	11	2
1:B:255:HIS:CD2	1:B:257:GLN:H	0.67	2.08	12	2
1:B:250:HIS:CD2	1:B:281:LEU:HD21	0.67	2.24	10	1
1:A:140:LEU:HD22	1:A:193:ILE:HG21	0.67	1.66	11	1
1:A:97:SER:O	1:A:128:ARG:N	0.67	2.28	6	20
1:A:119:HIS:NE2	1:A:120:VAL:HG23	0.67	2.05	13	3
1:B:217:PHE:CE2	1:B:221:PHE:CE1	0.67	2.83	19	2
1:B:255:HIS:CE1	1:B:257:GLN:NE2	0.67	2.63	15	4
1:B:255:HIS:CE1	1:B:257:GLN:H	0.66	2.07	7	1
1:B:246:LYS:HZ3	1:B:251:ARG:NE	0.66	1.87	16	1
1:A:34:CYS:SG	1:A:165:PHE:CE1	0.66	2.88	5	5
1:B:255:HIS:H	1:B:255:HIS:CD2	0.66	2.06	2	1
1:A:98:TRP:CZ3	2:D:414:DC:C2	0.66	2.83	12	20
1:B:294:PHE:CD2	1:B:352:MET:SD	0.66	2.88	1	3
1:A:11:HIS:ND1	1:B:210:HIS:O	0.66	2.29	3	6
1:B:220:ASN:ND2	1:B:231:TYR:CD2	0.66	2.63	2	2
1:B:326:ALA:HB2	1:B:352:MET:CE	0.66	2.21	6	3
1:A:182:HIS:CE1	2:D:409:DA:C6	0.66	2.84	3	13
1:B:320:ARG:NH1	1:B:322:ARG:NH1	0.66	2.43	11	1
1:B:361:TRP:O	1:B:365:VAL:HG23	0.66	1.90	11	20
1:B:233:CYS:SG	1:B:364:PHE:CZ	0.66	2.88	9	1
1:B:294:PHE:CE2	1:B:352:MET:SD	0.66	2.89	12	3
1:A:102:PHE:CZ	1:A:135:LEU:HD13	0.66	2.25	14	2
1:A:28:ARG:HH11	1:A:31:THR:N	0.66	1.89	3	1
1:A:94:TRP:CZ2	1:A:122:LEU:HD21	0.66	2.26	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ILE:HD11	1:A:186:LEU:HD13	0.66	1.67	7	9
1:A:127:ALA:HB2	1:A:153:MET:CE	0.66	2.21	5	2
1:B:340:GLN:NE2	1:B:392:ILE:HG22	0.66	2.06	5	2
1:A:34:CYS:SG	1:A:165:PHE:CZ	0.66	2.88	13	9
1:B:290:ARG:NE	1:B:322:ARG:NH2	0.66	2.44	10	1
1:A:10:ARG:HH12	1:B:273:ARG:NH1	0.66	1.89	18	2
1:B:378:LEU:HD12	1:B:378:LEU:N	0.66	2.06	2	8
1:B:312:PHE:CE1	1:B:316:ASN:ND2	0.65	2.64	15	2
1:B:255:HIS:CD2	1:B:256:ASN:N	0.65	2.64	7	1
1:B:230:THR:HG22	1:B:256:ASN:CG	0.65	2.16	9	1
1:B:361:TRP:HE1	1:B:367:HIS:CD2	0.65	2.08	6	2
1:A:125:PHE:CD1	1:A:153:MET:SD	0.65	2.89	7	1
1:B:294:PHE:CD1	1:B:352:MET:SD	0.65	2.89	7	1
1:A:135:LEU:HD12	1:A:136:TYR:N	0.65	2.05	9	3
1:B:290:ARG:NH1	1:B:322:ARG:HH21	0.65	1.89	19	1
1:A:182:HIS:NE2	2:D:409:DA:N6	0.65	2.44	19	2
1:A:125:PHE:CD2	1:A:153:MET:SD	0.65	2.89	3	1
1:B:343:ARG:HH12	1:B:396:GLN:NE2	0.65	1.88	13	1
1:B:335:TYR:CZ	1:B:339:LEU:HD11	0.65	2.26	15	1
1:B:287:GLN:HE21	1:B:287:GLN:N	0.65	1.89	14	19
1:A:182:HIS:CE1	2:D:409:DA:N6	0.65	2.65	11	4
1:A:144:ARG:NH2	1:A:197:GLN:HE22	0.65	1.90	19	3
1:B:340:GLN:HE22	1:B:343:ARG:NH2	0.65	1.90	13	1
1:B:373:GLN:H	1:B:373:GLN:NE2	0.65	1.90	11	3
1:A:11:HIS:CD2	1:B:212:MET:SD	0.65	2.90	12	2
1:B:298:SER:N	1:B:299:PRO:CD	0.65	2.60	5	20
1:A:182:HIS:NE2	2:D:409:DA:C6	0.65	2.64	8	3
1:B:320:ARG:CZ	1:B:348:GLN:NE2	0.65	2.60	14	1
1:B:373:GLN:HE21	1:B:373:GLN:N	0.65	1.90	2	5
1:A:102:PHE:CD2	1:A:135:LEU:HD13	0.65	2.27	17	1
1:B:332:ASP:H	1:B:333:PRO:CD	0.64	2.04	12	14
1:A:54:PHE:CE1	1:A:56:HIS:NE2	0.64	2.65	14	1
1:A:193:ILE:O	1:A:196:ASN:ND2	0.64	2.31	16	20
1:A:50:GLN:NE2	1:A:52:ARG:NH1	0.64	2.46	7	1
1:B:228:HIS:ND1	1:B:228:HIS:N	0.64	2.43	11	1
1:A:12:LEU:HD13	1:A:167:ASP:CG	0.64	2.17	18	2
1:B:321:LEU:C	1:B:321:LEU:HD23	0.64	2.18	19	12
1:B:224:GLY:C	2:C:403:DT:H73	0.64	2.18	9	1
1:A:45:SER:CB	1:A:91:ARG:NH1	0.64	2.61	17	1
1:A:58:GLN:HE21	1:A:60:LYS:N	0.64	1.90	19	1
1:A:88:GLN:HE21	1:A:88:GLN:N	0.64	1.90	8	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:255:HIS:CD2	1:B:256:ASN:H	0.64	2.10	7	1
1:B:228:HIS:NE2	1:B:259:LYS:NZ	0.64	2.45	20	1
1:A:144:ARG:NH1	1:A:197:GLN:NE2	0.64	2.46	10	1
1:A:29:HIS:NE2	2:D:415:DA:N7	0.64	2.46	12	18
1:A:144:ARG:CZ	1:A:197:GLN:NE2	0.64	2.60	2	4
1:B:255:HIS:N	1:B:255:HIS:CD2	0.64	2.66	10	2
1:B:300:CYS:SG	1:B:300:CYS:O	0.64	2.56	15	10
1:A:33:LEU:HD23	1:A:33:LEU:C	0.64	2.18	19	8
1:B:271:GLN:NE2	1:B:293:TRP:CE3	0.64	2.66	12	1
1:A:28:ARG:NH1	1:A:128:ARG:HE	0.64	1.90	19	1
1:B:392:ILE:O	1:B:395:ASN:ND2	0.64	2.31	1	20
1:A:174:GLN:NE2	1:A:174:GLN:N	0.63	2.46	18	8
1:B:361:TRP:HE1	1:B:367:HIS:CE1	0.63	2.10	6	1
1:B:255:HIS:CE1	1:B:257:GLN:CG	0.63	2.81	8	3
1:A:11:HIS:CE1	1:B:212:MET:SD	0.63	2.91	20	1
1:A:174:GLN:H	1:A:174:GLN:NE2	0.63	1.90	2	2
1:B:231:TYR:CZ	1:B:255:HIS:CD2	0.63	2.86	18	2
1:B:343:ARG:HH11	1:B:396:GLN:NE2	0.63	1.90	6	2
1:B:297:TRP:HE1	1:B:327:ARG:NH1	0.63	1.92	8	1
1:B:343:ARG:CZ	1:B:396:GLN:NE2	0.63	2.61	5	2
1:B:310:ARG:NH1	1:B:341:MET:SD	0.63	2.71	12	1
1:A:141:GLN:HE22	1:A:193:ILE:HG22	0.63	1.53	14	1
1:A:144:ARG:CZ	1:A:197:GLN:HE21	0.63	2.07	10	4
1:A:140:LEU:HD23	1:A:140:LEU:O	0.63	1.93	12	3
1:B:222:ASN:ND2	2:C:403:DT:C2	0.63	2.67	19	3
1:B:251:ARG:NH2	1:B:363:THR:HG23	0.63	2.07	8	2
1:A:54:PHE:O	1:A:54:PHE:CD1	0.63	2.51	12	3
1:A:58:GLN:NE2	1:A:60:LYS:H	0.63	1.91	19	1
1:A:11:HIS:ND1	1:B:253:PHE:CE2	0.63	2.67	1	1
1:A:54:PHE:CZ	1:A:56:HIS:NE2	0.63	2.66	14	2
1:B:253:PHE:CZ	1:B:255:HIS:ND1	0.63	2.67	16	2
1:B:246:LYS:HZ3	1:B:251:ARG:HH11	0.63	1.36	20	1
1:A:29:HIS:CE1	2:D:414:DC:OP1	0.63	2.52	17	11
1:A:57:ASN:HD22	1:A:58:GLN:N	0.63	1.91	18	7
1:A:50:GLN:NE2	1:A:52:ARG:CZ	0.62	2.62	4	1
1:A:48:MET:SD	1:A:51:HIS:CE1	0.62	2.91	10	3
1:B:290:ARG:CZ	1:B:322:ARG:NH1	0.62	2.62	4	1
1:A:87:ALA:C	1:A:88:GLN:NE2	0.62	2.58	13	18
1:A:54:PHE:CD1	1:A:54:PHE:C	0.62	2.76	18	7
1:B:220:ASN:ND2	1:B:231:TYR:CD1	0.62	2.67	16	2
1:A:52:ARG:O	1:B:209:ARG:N	0.62	2.32	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:MET:CE	1:A:51:HIS:CE1	0.62	2.82	5	5
1:B:225:ILE:N	2:C:403:DT:H73	0.62	2.09	9	2
1:A:69:ARG:NH1	1:A:104:TRP:HE1	0.62	1.92	20	2
1:A:29:HIS:O	2:D:415:DA:OP2	0.62	2.18	18	20
1:A:135:LEU:HD12	1:A:135:LEU:C	0.62	2.19	9	1
1:B:290:ARG:HE	1:B:322:ARG:NH2	0.62	1.92	10	1
1:B:367:HIS:CG	1:B:367:HIS:O	0.62	2.53	1	4
1:A:168:HIS:ND1	1:A:168:HIS:O	0.62	2.32	6	2
1:B:361:TRP:CE2	1:B:367:HIS:CD2	0.62	2.88	12	4
1:A:162:TRP:HE1	1:A:168:HIS:CE1	0.62	2.12	5	2
1:A:54:PHE:O	1:A:54:PHE:CD2	0.62	2.52	10	3
1:B:231:TYR:CE1	1:B:255:HIS:ND1	0.62	2.68	12	1
1:B:297:TRP:N	1:B:297:TRP:CD1	0.62	2.67	16	1
1:A:162:TRP:O	1:A:166:VAL:N	0.62	2.33	6	19
1:A:92:VAL:HG13	1:A:92:VAL:O	0.62	1.95	12	15
2:D:418:DT:H73	2:D:418:DT:OP2	0.62	1.95	6	1
1:A:144:ARG:NH1	1:A:197:GLN:HE21	0.62	1.93	10	1
1:A:11:HIS:CD2	1:B:212:MET:CG	0.62	2.83	19	1
1:A:127:ALA:HB2	1:A:153:MET:SD	0.61	2.35	2	6
1:A:60:LYS:NZ	2:D:416:DA:N7	0.61	2.46	10	2
1:A:174:GLN:N	1:A:174:GLN:HE21	0.61	1.91	3	7
1:B:321:LEU:HD23	1:B:322:ARG:N	0.61	2.09	9	8
1:B:367:HIS:O	1:B:367:HIS:ND1	0.61	2.33	12	5
1:A:136:TYR:C	1:A:136:TYR:CD2	0.61	2.79	20	7
1:B:343:ARG:CZ	1:B:396:GLN:HE21	0.61	2.08	5	1
1:A:172:PRO:O	1:A:174:GLN:NE2	0.61	2.34	3	15
1:B:209:ARG:C	1:B:211:LEU:H	0.61	2.04	12	20
1:A:9:PRO:O	1:B:210:HIS:CE1	0.61	2.53	5	8
1:B:246:LYS:NZ	1:B:251:ARG:HH12	0.61	1.93	6	2
1:A:174:GLN:CD	1:A:174:GLN:H	0.61	2.03	12	1
1:A:31:THR:N	1:A:57:ASN:OD1	0.61	2.33	20	19
1:B:367:HIS:CE1	1:B:370:GLN:O	0.61	2.54	12	5
1:A:91:ARG:HH11	1:A:123:ARG:NH2	0.61	1.94	6	2
1:B:286:ALA:C	1:B:287:GLN:NE2	0.61	2.59	9	19
1:A:19:THR:O	1:A:23:ASN:N	0.61	2.34	3	17
1:A:10:ARG:HH11	1:B:273:ARG:NH1	0.61	1.93	9	1
1:A:54:PHE:CD2	1:A:54:PHE:C	0.61	2.77	11	4
1:B:259:LYS:O	1:B:260:ASN:ND2	0.61	2.34	8	20
1:B:223:ASN:C	1:B:327:ARG:NH2	0.61	2.59	9	3
1:B:371:PRO:O	1:B:373:GLN:NE2	0.61	2.34	15	10
1:A:30:LYS:C	1:A:57:ASN:HD21	0.61	2.04	10	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:TYR:CD1	1:A:35:TYR:C	0.61	2.79	10	5
1:A:14:ASP:N	1:A:14:ASP:OD2	0.61	2.33	20	4
1:A:58:GLN:HE21	1:A:60:LYS:H	0.61	1.38	19	1
1:A:136:TYR:CD1	1:A:136:TYR:C	0.61	2.78	12	11
1:B:220:ASN:CG	1:B:231:TYR:CE2	0.61	2.79	12	4
1:A:54:PHE:CD2	1:A:54:PHE:O	0.61	2.54	11	1
1:B:318:HIS:CD2	1:B:319:VAL:HG23	0.61	2.31	20	4
1:B:321:LEU:HD23	1:B:321:LEU:C	0.61	2.21	9	1
1:A:10:ARG:NE	1:B:234:TYR:OH	0.61	2.34	19	2
1:A:57:ASN:HD22	1:A:58:GLN:H	0.60	1.38	12	7
1:B:212:MET:SD	1:B:253:PHE:CE1	0.60	2.94	10	1
1:A:181:GLU:OE2	1:A:182:HIS:CE1	0.60	2.54	13	1
1:A:38:GLU:N	1:A:38:GLU:OE1	0.60	2.35	3	1
1:B:223:ASN:O	1:B:327:ARG:NE	0.60	2.34	7	1
1:A:140:LEU:HD22	1:A:144:ARG:HH22	0.60	1.55	20	2
1:A:14:ASP:OD1	1:A:14:ASP:N	0.60	2.33	13	13
1:A:55:LEU:HD22	1:A:74:ARG:HH21	0.60	1.56	4	4
1:B:342:LEU:O	1:B:346:GLY:N	0.60	2.33	8	7
1:B:367:HIS:ND1	1:B:370:GLN:O	0.60	2.34	6	6
1:A:144:ARG:CZ	1:A:197:GLN:HE22	0.60	2.09	4	1
1:B:237:GLU:OE2	1:B:290:ARG:NH1	0.60	2.35	16	2
1:B:367:HIS:O	1:B:367:HIS:CG	0.60	2.54	12	2
1:A:155:TYR:CE2	1:A:156:ASP:OD1	0.60	2.54	12	2
1:B:210:HIS:CD2	1:B:210:HIS:O	0.60	2.53	7	1
1:B:255:HIS:CE1	1:B:257:GLN:CD	0.60	2.79	9	3
1:A:56:HIS:O	1:A:56:HIS:CD2	0.60	2.54	18	2
1:A:56:HIS:H	1:A:74:ARG:HH11	0.60	1.39	3	1
1:B:220:ASN:OD1	1:B:231:TYR:CE2	0.60	2.54	20	4
1:A:100:PRO:O	1:A:130:TYR:CD2	0.60	2.54	8	18
1:B:324:PHE:CE2	1:B:350:SER:OG	0.60	2.55	6	4
1:A:60:LYS:O	1:B:215:HIS:NE2	0.60	2.34	1	3
1:A:60:LYS:O	1:A:61:ASN:CB	0.60	2.48	12	20
1:A:141:GLN:OE1	1:A:197:GLN:NE2	0.60	2.35	1	4
1:B:229:LYS:O	1:B:231:TYR:CE2	0.60	2.55	2	5
1:B:230:THR:N	1:B:256:ASN:OD1	0.60	2.34	19	6
1:A:88:GLN:NE2	1:A:88:GLN:N	0.60	2.49	7	7
1:B:373:GLN:CD	1:B:373:GLN:H	0.60	2.05	13	4
1:A:125:PHE:CE2	1:A:157:GLU:OE1	0.60	2.55	14	3
1:B:229:LYS:O	1:B:231:TYR:CD1	0.60	2.55	17	4
1:B:229:LYS:NZ	2:C:403:DT:O4	0.60	2.33	19	2
1:A:25:GLY:O	1:A:128:ARG:NH2	0.60	2.35	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:HIS:CG	1:B:213:ASP:OD1	0.60	2.55	16	3
1:A:61:ASN:ND2	1:A:64:SER:H	0.60	1.95	11	1
1:A:11:HIS:O	1:A:11:HIS:CD2	0.60	2.55	3	3
1:B:220:ASN:CG	1:B:231:TYR:CG	0.60	2.80	16	2
1:B:296:SER:OG	1:B:297:TRP:CD1	0.60	2.54	4	5
1:B:340:GLN:OE1	1:B:343:ARG:NH1	0.60	2.35	13	3
1:B:250:HIS:O	1:B:250:HIS:ND1	0.60	2.35	10	1
1:A:111:ARG:NH2	1:A:115:GLN:OE1	0.60	2.35	18	3
1:B:230:THR:O	1:B:256:ASN:ND2	0.59	2.35	2	1
1:A:21:ASN:O	1:A:28:ARG:NH2	0.59	2.35	10	2
1:A:61:ASN:ND2	1:A:64:SER:OG	0.59	2.34	15	3
1:B:223:ASN:O	1:B:327:ARG:NH2	0.59	2.35	17	3
1:A:49:ASP:OD2	1:A:51:HIS:NE2	0.59	2.35	7	1
1:A:121:ARG:NE	1:A:123:ARG:HE	0.59	1.95	16	1
1:B:290:ARG:NH1	1:B:322:ARG:NH2	0.59	2.50	19	1
1:A:11:HIS:CE1	1:B:253:PHE:CE1	0.59	2.89	20	1
1:A:60:LYS:O	1:A:61:ASN:CG	0.59	2.45	3	13
1:A:74:ARG:NH1	1:B:366:ASP:OD2	0.59	2.35	5	6
1:A:97:SER:OG	1:A:98:TRP:CE2	0.59	2.55	12	8
1:B:253:PHE:CD2	1:B:253:PHE:O	0.59	2.56	17	9
1:B:373:GLN:NE2	1:B:373:GLN:N	0.59	2.49	7	12
1:B:362:ASP:OD2	1:B:367:HIS:NE2	0.59	2.35	6	1
1:A:54:PHE:C	1:A:54:PHE:CD2	0.59	2.80	7	2
1:A:60:LYS:O	1:B:215:HIS:CE1	0.59	2.55	12	1
1:A:54:PHE:CD1	1:A:54:PHE:O	0.59	2.55	18	1
1:A:58:GLN:NE2	2:D:416:DA:N6	0.59	2.50	20	1
1:A:69:ARG:O	1:A:70:HIS:CD2	0.59	2.56	7	20
1:B:253:PHE:CD1	1:B:253:PHE:O	0.59	2.55	19	5
1:B:361:TRP:NE1	1:B:362:ASP:OD1	0.59	2.35	3	5
1:B:368:GLN:N	1:B:368:GLN:CD	0.59	2.60	5	2
1:A:180:ASP:OD1	1:A:184:GLN:NE2	0.59	2.35	14	2
1:B:378:LEU:N	1:B:378:LEU:CD1	0.59	2.65	2	8
1:A:50:GLN:CD	1:A:52:ARG:NH1	0.59	2.61	4	2
1:A:56:HIS:O	1:A:56:HIS:ND1	0.59	2.35	12	3
1:B:232:LEU:HD23	1:B:233:CYS:N	0.59	2.13	12	4
1:A:49:ASP:OD2	1:A:51:HIS:CE1	0.59	2.56	7	1
1:B:227:ARG:C	1:B:228:HIS:CG	0.59	2.80	11	1
1:A:48:MET:CG	1:A:49:ASP:H	0.59	2.11	14	1
1:A:38:GLU:CD	1:A:91:ARG:NH1	0.59	2.60	15	1
1:A:9:PRO:O	1:B:210:HIS:NE2	0.59	2.36	8	6
1:B:229:LYS:O	1:B:231:TYR:CD2	0.59	2.55	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:297:TRP:CZ2	1:B:330:ASP:OD1	0.59	2.55	2	1
1:A:101:CYS:O	1:A:101:CYS:SG	0.59	2.60	7	9
1:B:228:HIS:O	1:B:230:THR:N	0.59	2.35	12	6
1:B:320:ARG:NH2	1:B:322:ARG:NE	0.59	2.50	4	1
1:B:361:TRP:CD2	1:B:365:VAL:HG21	0.59	2.32	9	2
1:A:50:GLN:O	1:A:51:HIS:ND1	0.59	2.36	15	2
1:B:310:ARG:NH2	1:B:314:GLN:OE1	0.59	2.35	15	4
1:B:220:ASN:OD1	1:B:231:TYR:CD1	0.59	2.56	1	3
1:A:168:HIS:ND1	1:A:171:GLN:O	0.59	2.36	2	2
1:A:14:ASP:OD1	1:B:255:HIS:CE1	0.59	2.56	5	1
1:A:21:ASN:ND2	1:A:31:THR:OG1	0.59	2.35	13	4
1:B:229:LYS:O	1:B:255:HIS:CE1	0.59	2.55	13	2
1:A:121:ARG:NH2	1:A:123:ARG:HH11	0.59	1.96	17	2
1:B:343:ARG:CZ	1:B:396:GLN:HE22	0.59	2.11	20	1
1:A:11:HIS:O	1:A:11:HIS:CG	0.59	2.55	3	5
1:A:24:ASN:OD1	1:A:176:TRP:CD1	0.59	2.55	8	4
1:A:155:TYR:C	1:A:155:TYR:CD1	0.59	2.79	12	2
1:A:102:PHE:CE1	1:A:135:LEU:HD21	0.59	2.33	19	2
1:B:271:GLN:OE1	1:B:293:TRP:CZ3	0.59	2.56	15	2
1:B:297:TRP:CD1	1:B:330:ASP:OD1	0.59	2.56	12	1
1:A:181:GLU:OE2	1:A:182:HIS:NE2	0.59	2.36	13	1
1:B:246:LYS:NZ	1:B:251:ARG:HH11	0.59	1.93	20	4
1:B:361:TRP:O	1:B:365:VAL:CG2	0.59	2.51	2	19
1:B:297:TRP:CD1	1:B:299:PRO:O	0.59	2.56	5	1
1:B:220:ASN:OD1	1:B:231:TYR:CZ	0.59	2.55	7	2
1:A:51:HIS:N	1:B:206:SER:O	0.59	2.35	9	1
1:A:141:GLN:OE1	1:A:144:ARG:NH1	0.59	2.35	17	1
1:A:33:LEU:HD13	1:A:96:ILE:HG23	0.59	1.75	8	6
1:A:125:PHE:CZ	1:A:157:GLU:OE1	0.59	2.56	8	4
1:B:223:ASN:O	1:B:327:ARG:NH1	0.59	2.34	7	3
1:A:25:GLY:O	1:A:128:ARG:NH1	0.59	2.36	11	7
1:A:56:HIS:H	1:A:74:ARG:NH1	0.59	1.96	3	1
1:A:167:ASP:OD2	1:A:169:GLN:NE2	0.59	2.36	11	2
1:B:229:LYS:O	1:B:231:TYR:CZ	0.59	2.56	9	1
1:A:11:HIS:CD2	1:B:253:PHE:CE2	0.59	2.90	11	1
1:B:237:GLU:OE1	1:B:290:ARG:NH1	0.58	2.35	6	1
1:B:297:TRP:CD2	1:B:330:ASP:OD1	0.58	2.56	6	1
1:B:230:THR:OG1	1:B:256:ASN:ND2	0.58	2.36	13	1
1:B:297:TRP:CD1	1:B:297:TRP:H	0.58	2.16	16	1
1:A:18:PHE:CE2	1:A:22:PHE:CE2	0.58	2.91	2	1
1:B:220:ASN:OD1	1:B:231:TYR:CE1	0.58	2.56	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLN:O	1:A:51:HIS:CG	0.58	2.56	15	2
1:B:230:THR:O	1:B:255:HIS:ND1	0.58	2.36	13	2
1:B:235:GLU:OE2	1:B:251:ARG:NH2	0.58	2.36	18	1
1:B:324:PHE:CE1	1:B:350:SER:OG	0.58	2.55	19	1
1:B:225:ILE:HD11	1:B:327:ARG:HH12	0.58	1.58	2	1
1:B:291:VAL:CG2	1:B:293:TRP:NE1	0.58	2.66	3	12
1:A:169:GLN:CD	1:A:169:GLN:N	0.58	2.61	10	3
1:B:293:TRP:CZ2	1:B:321:LEU:HD11	0.58	2.33	18	4
1:A:10:ARG:O	1:A:12:LEU:HD23	0.58	1.98	14	3
1:A:166:VAL:HG12	1:A:168:HIS:CD2	0.58	2.33	11	1
1:A:39:ARG:NH2	1:A:90:TYR:OH	0.58	2.36	15	2
1:B:255:HIS:CD2	1:B:255:HIS:N	0.58	2.69	2	1
1:B:320:ARG:NH1	1:B:348:GLN:OE1	0.58	2.36	4	1
1:A:60:LYS:NZ	2:D:416:DA:C5	0.58	2.70	5	1
1:B:215:HIS:C	1:B:215:HIS:ND1	0.58	2.60	15	1
1:A:49:ASP:O	1:A:50:GLN:CB	0.58	2.51	16	2
1:A:22:PHE:O	1:A:24:ASN:ND2	0.58	2.37	9	10
1:A:102:PHE:O	1:A:103:SER:CB	0.58	2.51	12	11
1:B:332:ASP:N	1:B:333:PRO:CD	0.58	2.66	12	17
1:B:373:GLN:H	1:B:373:GLN:CD	0.58	2.05	14	2
1:B:362:ASP:N	1:B:362:ASP:OD1	0.58	2.36	20	1
1:A:21:ASN:OD1	1:A:28:ARG:NH2	0.58	2.36	1	5
1:A:35:TYR:OH	1:B:209:ARG:NE	0.58	2.37	10	2
1:B:326:ALA:HB2	1:B:352:MET:SD	0.58	2.38	11	1
1:A:24:ASN:OD1	1:A:176:TRP:NE1	0.58	2.36	1	9
1:A:88:GLN:O	1:A:119:HIS:ND1	0.58	2.36	7	4
1:A:173:PHE:C	1:A:174:GLN:NE2	0.58	2.61	3	1
1:B:297:TRP:CG	1:B:330:ASP:OD1	0.58	2.56	12	2
1:B:310:ARG:NH1	1:B:344:ASP:OD2	0.58	2.37	8	2
1:A:78:LEU:HD12	1:B:209:ARG:NH2	0.58	2.13	9	1
1:A:18:PHE:CD1	1:A:32:TYR:OH	0.58	2.55	10	2
1:B:296:SER:OG	1:B:297:TRP:CE2	0.58	2.55	10	1
1:B:361:TRP:NE1	1:B:362:ASP:OD2	0.58	2.37	18	3
1:A:181:GLU:OE1	1:A:182:HIS:N	0.58	2.36	13	1
1:A:94:TRP:CD2	1:A:122:LEU:HD21	0.58	2.34	5	9
1:A:162:TRP:CD1	1:A:162:TRP:C	0.58	2.82	16	19
1:A:195:GLN:CA	1:A:195:GLN:HE21	0.58	2.12	5	20
1:B:225:ILE:HD11	1:B:327:ARG:NH1	0.58	2.12	2	1
1:A:168:HIS:CD2	1:A:171:GLN:O	0.58	2.57	6	2
1:A:48:MET:HE3	1:A:51:HIS:CG	0.58	2.34	12	1
1:A:125:PHE:CZ	1:A:127:ALA:HB2	0.58	2.34	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:THR:CG2	1:A:32:TYR:N	0.58	2.66	8	13
1:B:227:ARG:O	1:B:228:HIS:CB	0.58	2.51	19	8
1:A:35:TYR:C	1:A:35:TYR:CD2	0.58	2.82	5	3
1:A:174:GLN:H	1:A:174:GLN:CD	0.58	2.06	2	2
1:A:103:SER:OG	1:A:106:CYS:N	0.58	2.36	11	3
1:A:61:ASN:ND2	1:A:61:ASN:C	0.58	2.61	11	1
1:A:56:HIS:CD2	1:B:213:ASP:OD1	0.58	2.56	12	1
1:B:298:SER:OG	1:B:325:ALA:HB2	0.57	1.99	15	5
1:B:346:GLY:O	1:B:348:GLN:N	0.57	2.37	2	20
1:A:144:ARG:NE	1:A:194:LEU:HD22	0.57	2.13	19	3
1:A:11:HIS:ND1	1:A:11:HIS:O	0.57	2.37	14	3
1:B:209:ARG:HH12	1:B:368:GLN:HE22	0.57	1.41	14	1
1:A:72:GLN:HE21	1:A:96:ILE:CD1	0.57	2.12	2	2
1:B:362:ASP:N	1:B:362:ASP:OD2	0.57	2.35	2	1
1:B:297:TRP:CH2	1:B:327:ARG:NH2	0.57	2.72	3	1
1:B:297:TRP:NE1	1:B:299:PRO:O	0.57	2.37	5	1
1:B:232:LEU:HD11	1:B:271:GLN:NE2	0.57	2.13	15	2
1:A:12:LEU:HD23	1:A:12:LEU:H	0.57	1.58	14	2
1:A:40:LEU:HD21	1:A:43:GLY:H	0.57	1.60	7	1
1:A:130:TYR:O	1:A:130:TYR:CD2	0.57	2.57	12	7
1:A:22:PHE:C	1:A:24:ASN:H	0.57	2.08	13	19
1:A:69:ARG:NE	1:A:103:SER:OG	0.57	2.38	1	2
1:B:346:GLY:C	1:B:348:GLN:H	0.57	2.08	8	20
1:B:220:ASN:O	1:B:327:ARG:NH1	0.57	2.38	3	1
1:B:361:TRP:HE1	1:B:367:HIS:HE2	0.57	1.39	20	1
1:B:225:ILE:CD1	1:B:327:ARG:HH12	0.57	2.12	2	1
1:A:21:ASN:OD1	1:A:28:ARG:NH1	0.57	2.37	8	1
1:B:340:GLN:OE1	1:B:396:GLN:NE2	0.57	2.38	10	2
1:B:394:GLN:HE21	1:B:394:GLN:CA	0.57	2.12	4	20
1:A:25:GLY:N	1:A:128:ARG:HH12	0.57	1.97	11	1
1:A:56:HIS:CE1	1:B:213:ASP:OD2	0.57	2.58	3	1
1:A:96:ILE:N	1:A:96:ILE:CD1	0.57	2.67	5	1
1:A:162:TRP:HE1	1:A:168:HIS:CG	0.57	2.16	6	2
1:B:229:LYS:NZ	2:C:404:DC:O2	0.57	2.38	6	1
1:A:51:HIS:NE2	1:A:82:LEU:HD22	0.57	2.15	17	1
1:A:7:SER:HG	1:A:50:GLN:CD	0.57	2.07	19	1
1:A:144:ARG:NH2	1:A:197:GLN:OE1	0.57	2.38	19	1
1:A:12:LEU:N	1:A:12:LEU:HD22	0.57	2.14	2	1
1:A:12:LEU:CD1	1:A:12:LEU:N	0.57	2.68	3	1
1:A:141:GLN:NE2	1:A:196:ASN:HD21	0.57	1.98	7	1
1:B:229:LYS:N	1:B:256:ASN:OD1	0.57	2.38	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:362:ASP:OD1	1:B:367:HIS:CE1	0.57	2.58	12	1
1:A:174:GLN:NE2	1:A:174:GLN:H	0.57	1.98	18	1
1:A:91:ARG:NH1	1:A:123:ARG:HH21	0.57	1.98	18	2
1:B:320:ARG:NH1	1:B:322:ARG:HH11	0.57	1.98	11	1
1:B:217:PHE:CE1	1:B:221:PHE:CE2	0.57	2.93	20	2
1:B:209:ARG:O	1:B:211:LEU:N	0.56	2.36	7	17
1:A:52:ARG:O	1:B:208:PRO:CB	0.56	2.53	5	7
1:A:182:HIS:ND1	2:D:409:DA:N6	0.56	2.52	16	4
1:A:34:CYS:SG	1:A:165:PHE:CE2	0.56	2.96	6	2
1:A:111:ARG:NH1	1:A:145:ASP:OD2	0.56	2.37	9	1
1:B:253:PHE:O	1:B:253:PHE:CD2	0.56	2.58	13	1
1:A:181:GLU:CD	2:D:409:DA:N7	0.56	2.63	18	17
1:A:167:ASP:OD1	1:A:169:GLN:NE2	0.56	2.38	20	3
1:A:59:ALA:O	2:D:416:DA:P	0.56	2.64	20	12
1:A:131:ASP:OD1	2:D:413:DT:N3	0.56	2.37	11	15
1:A:132:TYR:CG	1:A:133:ASP:N	0.56	2.73	2	20
1:B:220:ASN:CG	1:B:231:TYR:CD2	0.56	2.84	2	2
1:A:196:ASN:ND2	1:A:197:GLN:H	0.56	1.98	3	5
1:B:228:HIS:C	1:B:230:THR:N	0.56	2.62	12	10
1:B:231:TYR:OH	1:B:255:HIS:CE1	0.56	2.58	3	1
1:A:125:PHE:CE1	1:A:157:GLU:OE1	0.56	2.59	4	2
1:A:40:LEU:CD2	1:A:43:GLY:H	0.56	2.14	7	1
1:B:220:ASN:CG	1:B:231:TYR:CZ	0.56	2.83	12	3
1:A:141:GLN:CD	1:A:197:GLN:NE2	0.56	2.63	11	1
1:A:121:ARG:CG	1:A:149:GLN:HE22	0.56	2.14	12	1
1:A:114:LEU:CD1	1:A:146:ALA:HB1	0.56	2.29	17	1
1:A:27:GLY:O	1:A:28:ARG:NE	0.56	2.38	18	7
1:A:88:GLN:N	1:A:88:GLN:CD	0.56	2.63	7	1
1:A:130:TYR:CD2	1:A:130:TYR:O	0.56	2.58	7	12
1:B:298:SER:H	1:B:299:PRO:CD	0.56	2.14	16	9
1:B:353:THR:HG22	1:B:354:TYR:N	0.56	2.16	2	5
1:A:60:LYS:O	1:A:61:ASN:ND2	0.56	2.39	3	1
1:B:231:TYR:CZ	1:B:255:HIS:CE1	0.56	2.94	12	2
1:A:95:PHE:CE2	1:A:125:PHE:CG	0.56	2.94	18	5
1:A:140:LEU:CD2	1:A:193:ILE:HD13	0.56	2.31	6	1
1:B:271:GLN:CD	1:B:293:TRP:CZ3	0.56	2.84	12	1
1:B:343:ARG:NH1	1:B:396:GLN:CD	0.56	2.63	13	1
1:B:268:ARG:HE	1:B:272:LEU:HD22	0.56	1.60	14	1
1:B:287:GLN:N	1:B:287:GLN:NE2	0.56	2.53	6	16
1:A:24:ASN:OD1	1:A:176:TRP:CE2	0.56	2.58	3	3
1:B:275:LEU:O	1:B:278:VAL:HG13	0.56	2.01	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:PHE:CE2	1:A:157:GLU:OE2	0.56	2.59	3	1
1:B:292:THR:OG1	1:B:322:ARG:NH1	0.56	2.39	8	2
1:A:165:PHE:CE1	1:B:210:HIS:NE2	0.56	2.73	12	1
1:A:69:ARG:CZ	1:A:104:TRP:HE1	0.56	2.14	13	2
1:A:56:HIS:CE1	1:A:58:GLN:O	0.56	2.59	18	1
1:B:223:ASN:O	1:B:327:ARG:CZ	0.56	2.54	17	2
1:A:168:HIS:NE2	1:A:171:GLN:OE1	0.56	2.39	3	1
1:B:224:GLY:O	1:B:327:ARG:NH2	0.56	2.39	16	6
1:A:56:HIS:HD1	1:B:213:ASP:CG	0.56	2.09	9	1
1:B:264:GLY:O	1:B:266:TYR:CD1	0.56	2.59	2	5
1:A:10:ARG:CZ	1:A:12:LEU:HD12	0.56	2.31	18	1
1:B:235:GLU:OE1	1:B:251:ARG:NH1	0.56	2.39	18	1
1:A:144:ARG:NE	1:A:194:LEU:HD21	0.55	2.16	6	3
1:B:235:GLU:CD	1:B:251:ARG:HH22	0.55	2.09	7	3
1:B:361:TRP:CH2	1:B:365:VAL:HG11	0.55	2.35	9	4
1:B:367:HIS:ND1	1:B:367:HIS:C	0.55	2.64	12	4
1:A:41:ASP:N	1:A:44:THR:O	0.55	2.39	13	12
1:A:181:GLU:OE1	2:D:409:DA:C6	0.55	2.59	8	6
1:B:343:ARG:NH1	1:B:396:GLN:HE21	0.55	1.98	6	1
1:A:91:ARG:NE	1:A:121:ARG:HH11	0.55	1.99	16	1
1:A:155:TYR:CD2	1:A:155:TYR:C	0.55	2.81	16	2
1:A:21:ASN:OD1	1:A:28:ARG:CZ	0.55	2.54	8	3
1:B:339:LEU:HD13	1:B:339:LEU:O	0.55	2.01	11	4
1:A:51:HIS:O	1:A:52:ARG:C	0.55	2.50	14	7
1:A:104:TRP:CD1	1:A:104:TRP:H	0.55	2.17	3	2
1:A:181:GLU:OE2	2:D:409:DA:N6	0.55	2.39	13	7
1:B:262:ASN:ND2	2:C:408:DT:OP1	0.55	2.39	16	3
1:A:78:LEU:HD11	1:B:209:ARG:CD	0.55	2.31	12	1
1:A:144:ARG:HH21	1:A:197:GLN:HE22	0.55	1.42	14	1
1:A:143:LEU:O	1:A:147:GLY:N	0.55	2.36	17	1
1:A:153:MET:SD	1:A:157:GLU:OE2	0.55	2.64	20	1
1:A:16:HIS:NE2	1:B:260:ASN:ND2	0.55	2.54	13	2
1:A:113:PHE:CE2	1:A:117:ASN:OD1	0.55	2.59	10	2
1:B:343:ARG:NE	1:B:393:LEU:HD11	0.55	2.16	14	1
1:A:88:GLN:HE21	1:A:88:GLN:CA	0.55	2.14	7	1
1:A:143:LEU:HD13	1:A:143:LEU:O	0.55	2.02	18	3
1:A:140:LEU:HD22	1:A:144:ARG:NH2	0.55	2.16	20	2
1:A:95:PHE:CE1	1:A:125:PHE:CG	0.55	2.95	11	3
1:A:61:ASN:HD21	1:A:64:SER:H	0.55	1.44	11	1
1:B:271:GLN:OE1	1:B:293:TRP:CH2	0.55	2.59	12	1
1:A:38:GLU:OE2	1:A:91:ARG:NH1	0.55	2.40	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:TRP:CZ2	2:D:414:DC:O4'	0.55	2.59	8	18
1:A:147:GLY:C	1:A:149:GLN:H	0.55	2.09	6	20
1:A:182:HIS:CE1	2:D:409:DA:C5	0.55	2.95	1	9
1:B:250:HIS:CE1	1:B:281:LEU:HD22	0.55	2.37	3	1
1:A:52:ARG:CZ	1:A:164:THR:HG23	0.55	2.32	8	1
1:A:141:GLN:OE1	1:A:196:ASN:ND2	0.55	2.40	19	3
1:A:181:GLU:OE1	2:D:409:DA:N6	0.55	2.40	8	8
1:A:173:PHE:CD1	1:A:173:PHE:C	0.55	2.85	5	3
1:B:232:LEU:C	1:B:232:LEU:CD2	0.55	2.80	20	10
1:B:271:GLN:OE1	1:B:305:CYS:SG	0.55	2.64	10	5
1:A:45:SER:CB	1:A:91:ARG:HH21	0.55	2.14	12	1
1:B:320:ARG:CZ	1:B:348:GLN:HE22	0.55	2.14	14	1
1:A:167:ASP:O	1:A:167:ASP:OD2	0.55	2.25	4	7
1:B:246:LYS:HZ2	1:B:251:ARG:NH1	0.55	2.00	17	3
1:A:56:HIS:N	1:A:74:ARG:HH11	0.55	2.00	3	1
1:A:174:GLN:N	1:A:174:GLN:NE2	0.55	2.54	3	2
1:B:367:HIS:ND1	1:B:370:GLN:CD	0.55	2.64	7	2
1:B:373:GLN:N	1:B:373:GLN:CD	0.55	2.64	7	3
1:B:335:TYR:CE1	1:B:392:ILE:HD11	0.55	2.36	11	1
1:B:250:HIS:CD2	1:B:281:LEU:CD2	0.55	2.89	17	1
1:A:31:THR:O	1:A:57:ASN:ND2	0.55	2.39	15	14
1:A:88:GLN:N	1:A:88:GLN:NE2	0.55	2.55	5	13
1:A:98:TRP:CD2	2:D:414:DC:C6	0.55	2.94	19	20
1:B:293:TRP:CZ3	1:B:321:LEU:HD11	0.55	2.37	9	3
1:B:305:CYS:O	1:B:309:VAL:CG2	0.55	2.55	1	3
1:B:229:LYS:O	1:B:231:TYR:CE1	0.55	2.60	16	5
1:B:230:THR:O	1:B:255:HIS:CE1	0.55	2.60	13	2
1:A:111:ARG:CZ	1:A:115:GLN:OE1	0.55	2.55	15	3
1:A:162:TRP:CD1	1:A:163:ASP:N	0.55	2.74	5	15
1:B:296:SER:OG	1:B:297:TRP:NE1	0.55	2.40	4	3
1:A:56:HIS:N	1:A:56:HIS:CD2	0.55	2.75	17	1
1:A:144:ARG:NH2	1:A:193:ILE:HG21	0.55	2.16	20	1
1:B:246:LYS:HZ3	1:B:251:ARG:NH1	0.54	2.00	1	2
1:B:291:VAL:CG2	1:B:293:TRP:HE1	0.54	2.14	14	13
1:A:106:CYS:O	1:A:110:VAL:CG2	0.54	2.56	7	6
1:A:122:LEU:HD13	1:A:123:ARG:N	0.54	2.17	11	5
1:A:38:GLU:OE1	1:A:91:ARG:NH1	0.54	2.39	7	2
1:A:125:PHE:CE1	1:A:153:MET:SD	0.54	3.00	7	1
1:A:104:TRP:CD1	1:A:104:TRP:N	0.54	2.73	15	1
1:B:235:GLU:OE1	1:B:251:ARG:CZ	0.54	2.55	18	1
1:A:132:TYR:O	1:A:133:ASP:O	0.54	2.24	1	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:395:ASN:ND2	1:B:396:GLN:N	0.54	2.55	19	20
1:B:278:VAL:HG21	1:B:312:PHE:CZ	0.54	2.38	7	7
1:B:227:ARG:O	1:B:228:HIS:C	0.54	2.48	12	2
1:A:10:ARG:HH12	1:B:273:ARG:CZ	0.54	2.15	13	1
1:A:35:TYR:OH	1:B:209:ARG:CB	0.54	2.56	4	4
1:A:78:LEU:O	1:A:78:LEU:HD13	0.54	2.02	6	1
1:A:25:GLY:O	1:A:28:ARG:NH1	0.54	2.39	19	1
1:A:16:HIS:CB	1:B:258:ALA:HB3	0.54	2.32	1	8
1:A:57:ASN:N	1:A:57:ASN:HD22	0.54	2.00	3	13
1:B:321:LEU:HD13	1:B:322:ARG:N	0.54	2.17	5	5
1:A:61:ASN:CG	1:A:61:ASN:O	0.54	2.50	13	4
1:A:173:PHE:CE2	1:A:174:GLN:O	0.54	2.61	10	3
1:A:59:ALA:O	2:D:416:DA:OP2	0.54	2.25	9	18
1:A:62:LEU:HD11	2:D:417:DT:P	0.54	2.42	1	2
1:B:228:HIS:C	1:B:230:THR:H	0.54	2.09	12	4
1:A:132:TYR:O	1:A:133:ASP:C	0.54	2.49	7	20
1:B:220:ASN:ND2	1:B:220:ASN:O	0.54	2.40	2	1
1:B:278:VAL:N	1:B:279:PRO:HD2	0.54	2.16	19	5
1:B:271:GLN:NE2	1:B:300:CYS:SG	0.54	2.80	10	1
1:A:10:ARG:O	1:A:12:LEU:N	0.54	2.39	18	3
1:A:176:TRP:O	1:A:179:LEU:CD2	0.54	2.56	12	14
1:B:275:LEU:O	1:B:279:PRO:CD	0.54	2.56	19	9
1:B:381:HIS:NE2	2:C:401:DT:O4	0.54	2.41	2	3
1:A:56:HIS:N	1:A:56:HIS:ND1	0.54	2.56	3	1
1:A:103:SER:OG	1:A:106:CYS:CB	0.54	2.56	11	3
1:B:221:PHE:O	1:B:223:ASN:ND2	0.54	2.40	4	3
1:A:61:ASN:O	1:A:61:ASN:CG	0.54	2.51	4	2
1:B:229:LYS:CA	1:B:256:ASN:OD1	0.54	2.55	7	2
1:A:121:ARG:HH21	1:A:123:ARG:HH11	0.54	1.46	17	1
1:B:306:ALA:HB1	1:B:341:MET:SD	0.54	2.43	1	1
1:A:114:LEU:HD21	1:A:122:LEU:HB2	0.54	1.80	11	10
1:A:27:GLY:O	1:A:28:ARG:CZ	0.54	2.56	10	3
1:B:342:LEU:HD13	1:B:342:LEU:O	0.54	2.02	10	3
1:B:287:GLN:NE2	1:B:287:GLN:N	0.54	2.56	4	4
1:B:343:ARG:NH2	1:B:396:GLN:HE22	0.54	2.00	9	1
1:B:212:MET:SD	1:B:253:PHE:CD1	0.54	3.01	10	1
1:B:267:GLY:O	1:B:268:ARG:C	0.54	2.51	14	1
1:A:24:ASN:C	1:A:128:ARG:NH1	0.53	2.66	2	1
1:A:154:THR:HG22	1:A:155:TYR:N	0.53	2.18	19	7
1:B:237:GLU:CD	1:B:237:GLU:N	0.53	2.65	3	1
1:B:343:ARG:NH2	1:B:396:GLN:NE2	0.53	2.56	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:HIS:HD1	1:A:56:HIS:H	0.53	1.46	6	1
1:A:181:GLU:OE2	1:A:182:HIS:CD2	0.53	2.61	13	1
1:A:52:ARG:NH2	1:A:164:THR:HG23	0.53	2.18	1	2
1:B:253:PHE:CD2	1:B:253:PHE:C	0.53	2.85	1	2
1:A:19:THR:O	1:A:23:ASN:CG	0.53	2.51	15	6
1:A:76:LEU:HD13	1:A:76:LEU:O	0.53	2.02	15	11
1:A:57:ASN:ND2	1:A:57:ASN:H	0.53	2.01	14	9
1:B:217:PHE:CE1	1:B:221:PHE:CZ	0.53	2.96	1	1
1:A:140:LEU:HG	1:A:193:ILE:HG21	0.53	1.80	2	1
1:B:230:THR:CG2	1:B:256:ASN:OD1	0.53	2.56	5	1
1:A:181:GLU:OE1	2:D:409:DA:C5	0.53	2.62	8	1
1:A:50:GLN:OE1	1:A:52:ARG:NH1	0.53	2.41	7	2
1:A:60:LYS:C	1:A:61:ASN:CG	0.53	2.76	16	3
1:B:235:GLU:CD	1:B:251:ARG:NH2	0.53	2.66	18	4
1:B:343:ARG:HE	1:B:393:LEU:HD11	0.53	1.62	8	1
1:A:10:ARG:HH11	1:B:273:ARG:HH11	0.53	1.44	9	1
1:A:135:LEU:C	1:A:135:LEU:CD1	0.53	2.80	17	3
1:B:320:ARG:NH1	1:B:348:GLN:NE2	0.53	2.56	14	1
1:A:102:PHE:CD1	1:A:135:LEU:HD23	0.53	2.39	1	1
1:A:195:GLN:CA	1:A:195:GLN:NE2	0.53	2.72	12	19
1:A:30:LYS:C	1:A:57:ASN:ND2	0.53	2.66	17	10
1:B:297:TRP:CE2	1:B:330:ASP:OD2	0.53	2.61	2	1
1:B:220:ASN:CG	1:B:231:TYR:CE1	0.53	2.87	3	4
1:B:236:VAL:HG21	1:B:250:HIS:CE1	0.53	2.38	10	1
1:A:181:GLU:OE2	2:D:409:DA:C5	0.53	2.62	13	1
1:A:181:GLU:OE1	1:A:181:GLU:C	0.53	2.51	13	1
1:A:104:TRP:O	1:A:108:GLY:N	0.53	2.40	16	7
1:A:167:ASP:CG	1:A:167:ASP:O	0.53	2.52	3	4
1:A:33:LEU:HD23	1:A:33:LEU:O	0.53	2.03	16	2
1:A:180:ASP:CG	1:A:184:GLN:HE21	0.53	2.11	14	2
1:A:140:LEU:C	1:A:140:LEU:CD2	0.53	2.82	11	1
1:B:395:ASN:ND2	1:B:396:GLN:H	0.53	2.00	19	2
1:B:228:HIS:CE1	1:B:259:LYS:NZ	0.53	2.77	20	1
1:B:343:ARG:NE	1:B:396:GLN:HE22	0.53	2.00	20	1
1:A:9:PRO:C	1:A:11:HIS:H	0.53	2.12	14	13
1:A:196:ASN:ND2	1:A:197:GLN:N	0.53	2.57	3	19
1:B:293:TRP:CH2	1:B:321:LEU:HD21	0.53	2.38	5	1
1:B:293:TRP:CE2	1:B:321:LEU:HD11	0.53	2.39	8	4
1:B:328:ILE:CG2	1:B:335:TYR:CE1	0.53	2.92	1	2
1:B:375:TRP:O	1:B:378:LEU:CD2	0.53	2.57	8	12
1:A:174:GLN:CD	1:A:174:GLN:N	0.53	2.66	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:162:TRP:O	1:A:166:VAL:O	0.53	2.27	6	2
1:A:12:LEU:H	1:A:12:LEU:HD23	0.53	1.63	11	2
1:B:271:GLN:OE1	1:B:309:VAL:HG21	0.53	2.04	19	1
1:A:17:ILE:CD1	1:A:17:ILE:N	0.53	2.72	20	1
1:A:147:GLY:O	1:A:149:GLN:N	0.53	2.40	6	20
1:B:373:GLN:N	1:B:373:GLN:NE2	0.53	2.56	2	4
1:B:221:PHE:C	1:B:223:ASN:H	0.53	2.11	3	4
1:A:181:GLU:OE2	2:D:409:DA:N7	0.53	2.42	20	3
1:B:322:ARG:HH11	1:B:350:SER:CB	0.53	2.16	9	2
1:B:335:TYR:CE2	1:B:339:LEU:HD12	0.53	2.39	9	3
1:B:234:TYR:C	1:B:234:TYR:CD2	0.53	2.87	6	2
1:B:228:HIS:O	1:B:229:LYS:C	0.52	2.52	17	9
1:A:60:LYS:CE	2:D:417:DT:O4	0.52	2.56	9	5
1:A:144:ARG:NE	1:A:194:LEU:CD2	0.52	2.72	6	3
1:A:140:LEU:HD22	1:A:193:ILE:CG2	0.52	2.34	11	1
1:B:291:VAL:HG13	1:B:291:VAL:O	0.52	2.04	1	3
1:B:375:TRP:NE1	1:B:378:LEU:HD11	0.52	2.20	14	4
1:B:220:ASN:ND2	1:B:231:TYR:CB	0.52	2.72	11	2
1:B:394:GLN:CA	1:B:394:GLN:NE2	0.52	2.73	1	20
1:B:361:TRP:CG	1:B:362:ASP:N	0.52	2.77	12	4
1:B:367:HIS:CE1	1:B:370:GLN:HE22	0.52	2.20	7	1
1:A:15:PRO:CG	1:A:168:HIS:NE2	0.52	2.73	20	4
1:A:140:LEU:CD1	1:A:193:ILE:HD13	0.52	2.35	1	6
1:A:97:SER:HG	1:A:98:TRP:CD1	0.52	2.23	2	3
1:B:225:ILE:O	2:C:403:DT:C7	0.52	2.57	7	10
1:B:339:LEU:HD13	1:B:392:ILE:CD1	0.52	2.35	15	3
1:A:18:PHE:CD2	1:A:32:TYR:OH	0.52	2.62	13	1
1:A:33:LEU:HD12	1:A:34:CYS:N	0.52	2.19	13	1
1:B:335:TYR:CD1	1:B:335:TYR:C	0.52	2.85	20	2
1:B:228:HIS:CE1	1:B:259:LYS:HZ2	0.52	2.20	20	1
1:A:131:ASP:OD1	2:D:413:DT:C2	0.52	2.62	14	13
1:B:328:ILE:CG2	1:B:335:TYR:OH	0.52	2.58	3	3
1:B:229:LYS:O	1:B:230:THR:C	0.52	2.51	19	2
1:B:212:MET:O	1:B:366:ASP:N	0.52	2.42	12	1
1:A:38:GLU:OE2	1:A:91:ARG:CZ	0.52	2.58	15	1
1:A:31:THR:O	1:A:57:ASN:OD1	0.52	2.28	6	6
1:B:228:HIS:C	1:B:256:ASN:OD1	0.52	2.53	2	1
1:B:274:PHE:CE1	1:B:277:LEU:HD23	0.52	2.39	4	2
1:B:339:LEU:HD13	1:B:392:ILE:HD13	0.52	1.82	17	4
1:A:105:GLY:O	1:A:106:CYS:C	0.52	2.51	13	3
1:B:331:TYR:O	1:B:332:ASP:O	0.52	2.28	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:LEU:HD21	1:B:209:ARG:NH2	0.52	2.19	9	1
1:A:27:GLY:H	1:A:128:ARG:HH12	0.52	1.46	10	1
1:B:240:ASP:N	1:B:243:THR:O	0.52	2.41	17	11
1:B:268:ARG:O	1:B:269:HIS:O	0.52	2.27	2	1
1:B:210:HIS:C	1:B:210:HIS:CD2	0.52	2.88	8	3
1:A:49:ASP:O	1:A:50:GLN:O	0.52	2.28	7	3
1:B:232:LEU:HD11	1:B:271:GLN:HE21	0.52	1.65	8	1
1:A:58:GLN:O	1:A:58:GLN:CG	0.52	2.58	17	3
1:A:61:ASN:OD1	1:A:61:ASN:O	0.52	2.27	12	1
1:A:48:MET:HE2	1:A:51:HIS:ND1	0.52	2.20	15	1
1:A:50:GLN:O	1:B:206:SER:O	0.52	2.28	2	4
1:A:168:HIS:CD2	1:A:168:HIS:H	0.52	2.24	5	2
1:A:195:GLN:NE2	1:A:195:GLN:CA	0.52	2.73	2	1
1:A:64:SER:O	1:A:66:PHE:CD2	0.52	2.63	8	2
1:A:121:ARG:HH21	1:A:149:GLN:NE2	0.52	2.01	12	1
1:A:55:LEU:HD22	1:A:74:ARG:CD	0.52	2.35	13	2
1:A:52:ARG:NH1	1:A:164:THR:O	0.52	2.43	14	1
1:B:220:ASN:CG	1:B:231:TYR:CD1	0.51	2.88	3	4
1:A:96:ILE:HD12	1:A:98:TRP:O	0.51	2.05	19	7
1:A:18:PHE:CZ	1:A:22:PHE:CD1	0.51	2.98	15	2
1:B:332:ASP:N	1:B:332:ASP:OD2	0.51	2.43	18	1
1:A:28:ARG:NH1	1:A:128:ARG:NE	0.51	2.58	19	1
1:B:359:HIS:O	1:B:362:ASP:OD1	0.51	2.28	20	1
1:A:140:LEU:HD13	1:A:140:LEU:O	0.51	2.06	2	1
1:B:277:LEU:HD13	1:B:277:LEU:O	0.51	2.05	19	2
1:B:255:HIS:CE1	1:B:257:GLN:HE21	0.51	2.23	1	2
1:B:393:LEU:HD22	1:B:393:LEU:N	0.51	2.20	11	8
1:A:73:LEU:CD1	1:A:109:GLU:OE1	0.51	2.58	10	2
1:A:134:PRO:O	1:A:138:GLU:OE1	0.51	2.28	7	1
1:B:274:PHE:CE2	1:B:277:LEU:HD23	0.51	2.40	11	2
1:A:62:LEU:CD1	2:D:417:DT:OP1	0.51	2.58	8	2
1:A:57:ASN:HD22	1:A:57:ASN:N	0.51	2.04	18	2
1:A:12:LEU:N	1:A:12:LEU:CD2	0.51	2.73	2	1
1:B:329:TYR:O	1:B:330:ASP:OD1	0.51	2.28	16	2
1:B:218:THR:O	1:B:222:ASN:CG	0.51	2.54	6	1
1:B:375:TRP:CD1	1:B:378:LEU:CD1	0.51	2.94	14	4
1:B:388:ARG:O	1:B:392:ILE:HD12	0.51	2.05	7	1
1:B:362:ASP:OD1	1:B:367:HIS:NE2	0.51	2.43	12	1
1:A:181:GLU:CD	1:A:182:HIS:N	0.51	2.69	13	1
1:A:74:ARG:HH12	1:B:366:ASP:CG	0.51	2.12	5	4
1:B:255:HIS:CE1	1:B:257:GLN:N	0.51	2.78	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:340:GLN:NE2	1:B:343:ARG:NH2	0.51	2.59	13	1
1:A:59:ALA:O	2:D:416:DA:OP1	0.51	2.29	8	8
1:A:49:ASP:O	1:A:50:GLN:CD	0.51	2.54	8	1
1:B:328:ILE:HG21	1:B:335:TYR:OH	0.51	2.06	19	4
1:A:25:GLY:O	1:A:128:ARG:CZ	0.51	2.58	11	2
1:B:232:LEU:HD23	1:B:232:LEU:O	0.51	2.05	14	1
1:B:320:ARG:NH1	1:B:348:GLN:HE21	0.51	2.04	14	1
1:A:49:ASP:CG	1:A:52:ARG:HH11	0.51	2.13	2	1
1:A:28:ARG:HH22	1:A:128:ARG:HH11	0.51	1.49	11	1
1:A:12:LEU:HD22	1:A:167:ASP:OD1	0.51	2.06	14	1
1:B:320:ARG:NE	1:B:348:GLN:HE22	0.51	2.03	14	1
1:A:22:PHE:C	1:A:24:ASN:N	0.51	2.68	8	19
1:A:59:ALA:C	2:D:416:DA:OP2	0.51	2.54	4	17
1:A:88:GLN:N	1:A:88:GLN:HE21	0.51	2.04	20	2
1:A:194:LEU:HD13	1:A:197:GLN:NE2	0.51	2.21	9	1
1:A:22:PHE:O	1:A:176:TRP:CZ2	0.51	2.64	20	2
1:A:30:LYS:O	1:A:31:THR:O	0.51	2.29	20	19
1:A:24:ASN:C	1:A:128:ARG:HH12	0.51	2.14	2	1
1:B:212:MET:SD	1:B:253:PHE:CZ	0.51	3.04	2	1
1:B:335:TYR:OH	1:B:392:ILE:CD1	0.51	2.55	2	1
1:A:78:LEU:CD1	1:B:209:ARG:NH2	0.51	2.74	9	1
1:A:24:ASN:OD1	1:A:176:TRP:CG	0.51	2.63	13	1
1:B:358:LYS:O	1:B:362:ASP:OD1	0.51	2.29	20	1
1:A:30:LYS:C	1:A:57:ASN:OD1	0.50	2.55	11	15
1:B:217:PHE:CZ	1:B:221:PHE:CE1	0.50	2.99	2	2
1:B:297:TRP:CH2	1:B:327:ARG:NH1	0.50	2.78	4	1
1:A:194:LEU:N	1:A:194:LEU:CD2	0.50	2.75	4	7
1:B:274:PHE:CE1	1:B:293:TRP:NE1	0.50	2.79	7	2
1:A:38:GLU:OE2	1:A:45:SER:C	0.50	2.54	14	2
1:A:173:PHE:C	1:A:173:PHE:CD2	0.50	2.84	7	1
1:A:194:LEU:CD1	1:A:197:GLN:NE2	0.50	2.74	9	1
1:A:180:ASP:CG	1:A:184:GLN:NE2	0.50	2.70	14	2
1:B:237:GLU:OE1	1:B:244:SER:C	0.50	2.54	11	2
1:A:58:GLN:NE2	2:D:416:DA:H62	0.50	2.04	20	1
1:B:361:TRP:CD1	1:B:362:ASP:OD1	0.50	2.64	4	4
1:B:332:ASP:OD1	1:B:332:ASP:N	0.50	2.44	6	1
1:B:343:ARG:HH22	1:B:396:GLN:HE22	0.50	1.49	9	1
1:A:11:HIS:NE2	1:B:212:MET:SD	0.50	2.85	12	1
1:B:234:TYR:CD1	1:B:274:PHE:CE2	0.50	2.99	16	1
1:B:250:HIS:CD2	1:B:281:LEU:HD22	0.50	2.41	17	1
1:A:88:GLN:O	1:A:119:HIS:CE1	0.50	2.65	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:366:ASP:CG	1:B:366:ASP:O	0.50	2.55	6	5
1:A:61:ASN:HD21	1:A:64:SER:N	0.50	2.04	11	1
1:B:331:TYR:O	1:B:335:TYR:CB	0.50	2.60	13	3
1:A:38:GLU:OE1	1:A:45:SER:C	0.50	2.55	16	2
1:B:320:ARG:NH2	1:B:322:ARG:HH11	0.50	2.04	16	1
2:D:412:DT:H3'	2:D:412:DT:O2	0.50	2.07	8	14
2:D:412:DT:O2	2:D:412:DT:C3'	0.50	2.59	8	20
1:A:61:ASN:C	1:A:61:ASN:OD1	0.50	2.52	6	3
1:B:229:LYS:C	1:B:256:ASN:OD1	0.50	2.54	12	2
1:B:393:LEU:N	1:B:393:LEU:CD2	0.50	2.75	11	9
1:B:228:HIS:CD2	1:B:259:LYS:CE	0.50	2.95	2	1
1:B:359:HIS:O	1:B:362:ASP:OD2	0.50	2.30	2	1
1:A:38:GLU:OE1	1:A:91:ARG:O	0.50	2.30	3	1
1:A:49:ASP:O	1:B:206:SER:O	0.50	2.30	20	3
1:A:33:LEU:C	1:A:33:LEU:CD2	0.50	2.85	12	8
1:A:173:PHE:CD2	1:A:174:GLN:N	0.50	2.80	14	4
1:A:38:GLU:N	1:A:38:GLU:CD	0.50	2.70	8	1
1:A:182:HIS:CD2	2:D:409:DA:N6	0.50	2.80	8	1
1:A:106:CYS:SG	1:A:107:ALA:N	0.50	2.81	10	1
1:A:103:SER:OG	1:A:104:TRP:N	0.50	2.42	13	1
1:B:373:GLN:N	1:B:373:GLN:HE21	0.50	2.03	19	1
1:A:23:ASN:CG	1:A:23:ASN:O	0.50	2.55	1	3
1:A:185:ALA:HB1	2:D:410:DT:O4	0.50	2.06	18	5
1:A:165:PHE:CD1	1:B:210:HIS:CE1	0.50	3.00	12	1
1:A:73:LEU:HD13	1:A:73:LEU:O	0.50	2.07	13	1
1:B:232:LEU:CD1	1:B:271:GLN:NE2	0.50	2.75	15	1
1:B:209:ARG:C	1:B:211:LEU:N	0.50	2.70	7	16
1:B:234:TYR:CD1	1:B:234:TYR:C	0.50	2.89	4	4
1:B:259:LYS:C	2:C:407:DT:OP1	0.50	2.55	10	5
1:B:343:ARG:NE	1:B:393:LEU:HD22	0.50	2.22	9	1
1:A:173:PHE:CD2	1:A:173:PHE:C	0.50	2.87	10	4
1:B:209:ARG:NH1	1:B:368:GLN:HE22	0.50	2.04	14	1
1:A:45:SER:CB	1:A:91:ARG:HH11	0.50	2.19	17	1
1:A:70:HIS:CD2	2:D:414:DC:C2	0.50	3.00	9	20
1:A:31:THR:O	1:A:57:ASN:CG	0.50	2.55	3	5
1:A:55:LEU:HD21	1:B:209:ARG:NE	0.50	2.22	2	1
1:B:255:HIS:CG	1:B:256:ASN:N	0.50	2.80	7	2
1:B:384:ALA:CB	2:C:400:DT:P	0.50	3.00	18	4
1:B:329:TYR:O	1:B:330:ASP:OD2	0.50	2.29	12	2
1:A:61:ASN:OD1	1:A:66:PHE:O	0.50	2.30	16	1
1:B:222:ASN:OD1	1:B:222:ASN:C	0.50	2.55	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:272:LEU:HD13	1:B:272:LEU:O	0.49	2.07	3	1
1:A:182:HIS:ND1	1:A:182:HIS:C	0.49	2.70	14	2
1:A:91:ARG:CZ	1:A:123:ARG:NH2	0.49	2.75	14	1
1:B:335:TYR:CZ	1:B:339:LEU:HD22	0.49	2.42	16	1
1:A:98:TRP:CE3	2:D:414:DC:C2	0.49	3.01	14	18
1:A:102:PHE:O	1:A:103:SER:OG	0.49	2.30	3	7
1:A:134:PRO:C	1:A:136:TYR:N	0.49	2.68	1	1
1:B:275:LEU:HD13	1:B:275:LEU:O	0.49	2.07	3	1
1:A:61:ASN:HD21	1:A:64:SER:CB	0.49	2.20	9	2
1:A:40:LEU:HD23	1:A:40:LEU:C	0.49	2.32	7	1
1:A:177:ASP:O	1:A:177:ASP:OD2	0.49	2.30	10	1
1:B:335:TYR:CG	1:B:336:LYS:N	0.49	2.79	17	2
1:A:61:ASN:OD1	1:A:61:ASN:N	0.49	2.43	16	1
1:A:121:ARG:CZ	1:A:123:ARG:HH11	0.49	2.20	16	1
1:A:153:MET:SD	1:A:158:PHE:CZ	0.49	3.06	17	1
1:A:9:PRO:O	1:A:11:HIS:N	0.49	2.43	9	6
1:B:343:ARG:HH22	1:B:395:ASN:HD21	0.49	1.50	4	1
1:A:37:VAL:C	1:A:38:GLU:CD	0.49	2.80	11	2
1:A:13:MET:SD	1:B:210:HIS:CD2	0.49	3.05	9	1
1:A:11:HIS:CD2	1:B:253:PHE:CZ	0.49	3.01	15	1
1:A:18:PHE:CZ	1:A:22:PHE:CE1	0.49	3.00	15	1
1:B:378:LEU:N	1:B:378:LEU:CD2	0.49	2.70	18	5
1:A:11:HIS:CD2	1:A:11:HIS:C	0.49	2.87	3	2
1:A:20:SER:O	1:A:23:ASN:CG	0.49	2.56	7	1
1:A:50:GLN:O	1:A:51:HIS:CB	0.49	2.60	15	2
1:A:125:PHE:CE1	1:A:157:GLU:OE2	0.49	2.65	1	1
1:B:234:TYR:CD1	1:B:274:PHE:CE1	0.49	3.00	3	1
1:B:397:GLY:O	1:B:398:ASN:C	0.49	2.56	3	2
1:A:178:GLY:O	1:A:182:HIS:ND1	0.49	2.45	13	1
1:A:48:MET:CG	1:A:49:ASP:N	0.49	2.75	14	1
1:B:264:GLY:O	1:B:266:TYR:CD2	0.49	2.66	16	2
2:D:412:DT:O2	2:D:412:DT:H3'	0.49	2.08	13	6
1:A:56:HIS:ND1	1:B:213:ASP:CG	0.49	2.71	9	1
1:B:335:TYR:CE1	1:B:339:LEU:HD12	0.49	2.42	12	2
1:A:196:ASN:O	1:A:199:ASN:OD1	0.49	2.30	15	1
1:B:232:LEU:HD12	1:B:233:CYS:N	0.49	2.23	18	1
1:A:141:GLN:CD	1:A:196:ASN:OD1	0.49	2.56	1	9
1:A:122:LEU:O	1:A:149:GLN:OE1	0.49	2.30	12	3
1:B:219:SER:O	1:B:222:ASN:CG	0.49	2.56	3	1
1:B:210:HIS:O	1:B:210:HIS:CG	0.49	2.65	13	3
1:B:240:ASP:O	1:B:241:ASN:C	0.49	2.56	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:CD1	1:A:109:GLU:OE2	0.49	2.61	17	2
1:A:23:ASN:OD1	1:A:23:ASN:O	0.49	2.31	14	2
1:B:290:ARG:HH11	1:B:322:ARG:HH21	0.49	1.47	19	1
1:A:125:PHE:CE2	1:A:127:ALA:HB2	0.49	2.43	20	1
1:A:141:GLN:CD	1:A:196:ASN:CG	0.49	2.81	20	1
1:A:88:GLN:NE2	1:A:88:GLN:CA	0.49	2.76	7	6
1:A:38:GLU:OE2	1:A:91:ARG:O	0.49	2.31	8	1
1:A:141:GLN:OE1	1:A:196:ASN:OD1	0.49	2.31	19	4
1:A:14:ASP:OD2	1:A:14:ASP:N	0.49	2.45	16	1
1:A:173:PHE:O	1:A:173:PHE:CG	0.49	2.64	18	1
1:B:366:ASP:O	1:B:366:ASP:CG	0.49	2.55	20	1
1:A:22:PHE:O	1:A:24:ASN:N	0.49	2.46	6	14
1:A:75:PHE:C	1:A:75:PHE:CD2	0.49	2.90	4	1
1:B:219:SER:C	1:B:229:LYS:NZ	0.49	2.71	4	1
1:A:21:ASN:ND2	1:A:32:TYR:CE1	0.49	2.81	13	1
1:A:24:ASN:OD1	1:A:176:TRP:CZ2	0.48	2.66	3	1
1:A:52:ARG:O	1:B:208:PRO:CA	0.48	2.61	7	10
1:A:50:GLN:CD	1:A:52:ARG:CZ	0.48	2.85	4	1
1:A:29:HIS:CD2	2:D:415:DA:OP2	0.48	2.66	12	2
1:B:340:GLN:OE1	1:B:396:GLN:OE1	0.48	2.31	6	1
1:A:100:PRO:HB3	1:A:140:LEU:HD21	0.48	1.85	20	2
1:A:7:SER:OG	1:B:207:GLY:CA	0.48	2.61	14	1
1:A:58:GLN:CD	1:A:58:GLN:O	0.48	2.56	19	1
1:A:194:LEU:N	1:A:194:LEU:HD22	0.48	2.24	4	6
1:A:12:LEU:HD23	1:A:167:ASP:OD2	0.48	2.08	3	1
1:A:19:THR:O	1:A:23:ASN:OD1	0.48	2.31	19	4
1:A:49:ASP:O	1:A:50:GLN:OE1	0.48	2.32	8	1
1:A:173:PHE:O	1:A:173:PHE:CD2	0.48	2.67	18	1
1:B:246:LYS:HZ2	1:B:251:ARG:HH11	0.48	1.52	18	1
1:B:275:LEU:HD13	1:B:308:GLU:HG2	0.48	1.86	1	1
1:B:221:PHE:C	1:B:223:ASN:N	0.48	2.70	19	8
1:B:250:HIS:O	1:B:250:HIS:CG	0.48	2.66	10	1
1:B:328:ILE:HG23	1:B:335:TYR:CZ	0.48	2.43	16	1
1:A:60:LYS:O	1:B:215:HIS:CD2	0.48	2.67	1	1
1:A:100:PRO:HG2	1:A:130:TYR:O	0.48	2.08	1	13
1:B:361:TRP:O	1:B:365:VAL:CB	0.48	2.62	20	13
1:A:93:THR:CG2	1:A:95:PHE:CE2	0.48	2.97	11	4
1:B:225:ILE:N	2:C:403:DT:C7	0.48	2.76	11	9
1:B:340:GLN:OE1	1:B:395:ASN:ND2	0.48	2.47	5	1
1:B:321:LEU:C	1:B:321:LEU:CD2	0.48	2.87	19	4
1:A:179:LEU:N	1:A:179:LEU:HD12	0.48	2.23	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ASN:OD1	1:A:61:ASN:C	0.48	2.55	13	1
2:D:415:DA:C8	2:D:415:DA:O5'	0.48	2.67	8	13
1:B:264:GLY:O	1:B:266:TYR:CE1	0.48	2.67	13	4
1:B:321:LEU:O	1:B:348:GLN:OE1	0.48	2.31	2	5
1:A:12:LEU:N	1:A:12:LEU:HD12	0.48	2.23	3	1
1:A:60:LYS:O	1:A:61:ASN:HB2	0.48	2.08	6	2
1:A:119:HIS:ND1	1:A:119:HIS:O	0.48	2.47	7	1
1:A:153:MET:CE	1:A:158:PHE:CE1	0.48	2.96	8	1
1:B:211:LEU:N	1:B:211:LEU:HD22	0.48	2.22	9	1
1:B:237:GLU:OE1	1:B:290:ARG:NE	0.48	2.46	9	1
1:B:372:PHE:CE2	1:B:373:GLN:O	0.48	2.67	12	1
1:B:346:GLY:C	1:B:348:GLN:N	0.48	2.72	8	20
1:B:373:GLN:NE2	1:B:373:GLN:CA	0.48	2.76	17	5
1:B:375:TRP:O	1:B:377:GLY:N	0.48	2.46	2	4
1:A:141:GLN:O	1:A:145:ASP:OD1	0.48	2.31	3	2
1:B:324:PHE:CD2	1:B:324:PHE:C	0.48	2.90	3	1
1:A:181:GLU:OE2	2:D:409:DA:C6	0.48	2.66	13	3
1:B:366:ASP:O	1:B:366:ASP:OD1	0.48	2.31	6	3
1:A:50:GLN:C	1:B:206:SER:O	0.48	2.56	9	2
1:B:397:GLY:O	1:B:398:ASN:OD1	0.48	2.31	17	2
1:A:49:ASP:OD2	1:A:49:ASP:N	0.48	2.45	12	1
1:B:254:LEU:HD23	1:B:270:ALA:HB1	0.48	1.83	13	1
1:B:228:HIS:CD2	1:B:259:LYS:NZ	0.48	2.82	14	1
1:B:334:LEU:O	1:B:338:ALA:CB	0.48	2.62	3	4
1:B:367:HIS:ND1	1:B:370:GLN:CB	0.48	2.77	10	2
1:A:23:ASN:O	1:A:23:ASN:CG	0.48	2.57	14	3
1:A:197:GLN:CG	1:A:198:GLY:N	0.48	2.77	5	3
1:B:217:PHE:CE1	1:B:221:PHE:CD1	0.48	3.01	9	1
1:A:55:LEU:HD22	1:A:74:ARG:HD3	0.48	1.86	13	1
1:A:64:SER:O	1:A:66:PHE:CD1	0.48	2.67	16	1
1:A:72:GLN:HE21	1:A:96:ILE:HD12	0.48	1.68	2	1
1:B:339:LEU:HG	1:B:392:ILE:HD13	0.48	1.84	4	3
1:A:198:GLY:O	1:A:199:ASN:OXT	0.48	2.31	13	2
1:B:296:SER:HG	1:B:297:TRP:NE1	0.48	2.06	11	2
1:B:240:ASP:O	1:B:243:THR:N	0.48	2.46	14	3
1:B:237:GLU:OE1	1:B:290:ARG:O	0.48	2.32	13	2
1:A:114:LEU:HD12	1:A:146:ALA:HB1	0.48	1.85	17	1
1:B:278:VAL:HG13	1:B:279:PRO:HD3	0.48	1.86	19	1
1:A:198:GLY:O	1:A:199:ASN:C	0.48	2.56	3	2
1:A:31:THR:HG21	1:A:97:SER:OG	0.48	2.08	17	5
1:A:173:PHE:CD1	1:A:174:GLN:N	0.48	2.82	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ASN:CG	1:A:64:SER:OG	0.48	2.57	6	1
1:B:217:PHE:CE2	1:B:221:PHE:CZ	0.48	3.02	6	2
1:A:16:HIS:NE2	1:B:260:ASN:CG	0.48	2.72	13	1
1:B:253:PHE:CZ	1:B:255:HIS:CE1	0.48	3.02	16	2
1:A:183:SER:O	1:A:187:SER:OG	0.48	2.31	13	4
1:B:395:ASN:O	1:B:398:ASN:O	0.48	2.31	1	1
1:B:389:LEU:O	1:B:389:LEU:HD13	0.48	2.09	2	7
1:B:290:ARG:NH2	1:B:322:ARG:NH1	0.48	2.62	4	1
1:A:10:ARG:NH2	1:B:277:LEU:CD1	0.48	2.76	5	1
1:A:60:LYS:NZ	2:D:417:DT:O4	0.48	2.47	9	2
1:A:60:LYS:NZ	2:D:416:DA:N6	0.48	2.62	16	1
1:A:134:PRO:C	1:A:136:TYR:H	0.47	2.17	1	1
1:A:144:ARG:CZ	1:A:194:LEU:HD21	0.47	2.39	1	2
1:A:183:SER:O	1:A:187:SER:CB	0.47	2.63	3	5
1:B:297:TRP:NE1	1:B:327:ARG:HH11	0.47	2.07	8	1
1:A:35:TYR:OH	1:B:209:ARG:CD	0.47	2.62	10	1
1:B:343:ARG:NH2	1:B:349:VAL:CG2	0.47	2.77	17	1
1:B:263:SER:OG	1:B:265:PHE:CD1	0.47	2.57	18	1
1:A:144:ARG:HH12	1:A:197:GLN:NE2	0.47	2.07	13	1
1:A:69:ARG:HH22	1:A:104:TRP:NE1	0.47	2.06	15	1
1:A:168:HIS:ND1	1:A:168:HIS:N	0.47	2.62	16	1
1:A:33:LEU:HD23	1:A:55:LEU:HD12	0.47	1.86	20	1
1:B:295:ILE:HD12	1:B:297:TRP:O	0.47	2.08	7	1
1:A:177:ASP:OD1	1:A:177:ASP:O	0.47	2.31	9	1
1:A:94:TRP:CZ2	1:A:122:LEU:HD11	0.47	2.44	1	4
1:A:167:ASP:O	1:A:167:ASP:CG	0.47	2.56	1	4
1:B:396:GLN:CG	1:B:397:GLY:N	0.47	2.77	2	4
1:B:223:ASN:O	2:C:402:DT:O4	0.47	2.32	9	5
1:A:37:VAL:O	1:A:38:GLU:CD	0.47	2.57	20	4
1:B:340:GLN:HE21	1:B:392:ILE:HG22	0.47	1.69	5	1
1:B:297:TRP:CE3	1:B:330:ASP:OD1	0.47	2.67	6	1
1:B:372:PHE:O	1:B:372:PHE:CD1	0.47	2.66	18	2
1:B:318:HIS:NE2	1:B:319:VAL:HG23	0.47	2.24	20	1
1:A:144:ARG:HH22	1:A:197:GLN:HE22	0.47	1.50	8	1
1:B:343:ARG:HE	1:B:393:LEU:CD1	0.47	2.22	8	1
1:A:22:PHE:CE2	1:A:32:TYR:OH	0.47	2.67	10	1
1:A:141:GLN:O	1:A:145:ASP:CG	0.47	2.58	1	2
1:B:377:GLY:O	1:B:381:HIS:CG	0.47	2.68	2	4
1:A:38:GLU:OE1	1:A:47:LYS:CG	0.47	2.62	11	2
1:B:323:ILE:CD1	1:B:342:LEU:HD21	0.47	2.39	13	1
1:B:373:GLN:CD	1:B:373:GLN:N	0.47	2.72	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:LEU:CD2	2:D:417:DT:OP1	0.47	2.61	13	3
1:A:196:ASN:CG	1:A:197:GLN:N	0.47	2.73	16	5
1:A:102:PHE:CD1	1:A:135:LEU:CD1	0.47	2.98	4	1
1:B:219:SER:C	1:B:229:LYS:HZ1	0.47	2.17	4	1
1:B:230:THR:OG1	1:B:256:ASN:CG	0.47	2.58	5	3
2:D:418:DT:O5'	2:D:418:DT:H6	0.47	1.93	6	1
1:B:361:TRP:CD1	1:B:362:ASP:OD2	0.47	2.67	16	4
1:B:372:PHE:O	1:B:372:PHE:CG	0.47	2.67	8	2
1:B:332:ASP:OD2	1:B:332:ASP:C	0.47	2.56	9	1
1:A:10:ARG:NH1	1:B:234:TYR:OH	0.47	2.46	10	1
1:A:11:HIS:O	1:A:11:HIS:ND1	0.47	2.48	10	1
1:B:237:GLU:OE1	1:B:237:GLU:N	0.47	2.47	10	2
1:B:215:HIS:ND1	1:B:215:HIS:O	0.47	2.47	15	1
1:A:69:ARG:CZ	1:A:103:SER:OG	0.47	2.63	6	1
1:B:218:THR:O	1:B:222:ASN:OD1	0.47	2.32	6	1
1:A:57:ASN:C	1:A:57:ASN:HD22	0.47	2.16	7	1
1:A:105:GLY:O	1:A:109:GLU:CB	0.47	2.62	11	1
1:A:102:PHE:CE2	1:A:135:LEU:HD23	0.47	2.45	13	1
1:B:232:LEU:HD22	1:B:254:LEU:HD12	0.47	1.86	14	1
1:B:395:ASN:CG	1:B:396:GLN:N	0.47	2.73	19	2
1:A:152:ILE:CD1	1:A:187:SER:OG	0.47	2.63	3	2
1:B:225:ILE:HD13	2:C:402:DT:OP2	0.47	2.10	2	1
1:B:237:GLU:CD	1:B:290:ARG:O	0.47	2.58	3	1
1:A:122:LEU:CD1	1:A:122:LEU:C	0.47	2.88	11	5
1:B:340:GLN:CD	1:B:395:ASN:OD1	0.47	2.58	4	2
1:B:262:ASN:OD1	2:C:408:DT:OP1	0.47	2.33	14	5
1:A:12:LEU:CB	1:A:167:ASP:OD1	0.47	2.63	15	2
1:B:393:LEU:N	1:B:393:LEU:HD22	0.47	2.23	8	1
1:B:211:LEU:N	1:B:211:LEU:CD2	0.47	2.77	9	1
1:A:7:SER:OG	1:A:50:GLN:OE1	0.47	2.30	19	1
1:A:58:GLN:OE1	1:B:215:HIS:CD2	0.47	2.67	19	1
1:A:153:MET:CE	1:A:158:PHE:CE2	0.47	2.97	1	1
1:B:225:ILE:CD1	1:B:327:ARG:NH1	0.47	2.77	2	1
1:B:250:HIS:ND1	1:B:250:HIS:N	0.47	2.63	9	1
1:B:357:PHE:O	1:B:361:TRP:N	0.47	2.46	9	2
1:A:27:GLY:O	1:A:28:ARG:NH1	0.47	2.48	11	1
1:B:224:GLY:O	1:B:327:ARG:CZ	0.47	2.63	16	1
1:B:214:PRO:CG	1:B:367:HIS:NE2	0.47	2.78	17	1
1:A:162:TRP:O	1:A:166:VAL:HG23	0.47	2.10	18	1
1:B:229:LYS:CB	2:C:404:DC:N3	0.47	2.78	18	1
1:B:298:SER:N	1:B:299:PRO:HD2	0.46	2.25	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:313:LEU:HD21	1:B:321:LEU:HB2	0.46	1.86	11	2
1:A:105:GLY:O	1:A:108:GLY:N	0.46	2.48	13	1
1:A:33:LEU:HD12	1:A:96:ILE:CG2	0.46	2.39	16	1
1:A:12:LEU:HD13	1:A:167:ASP:OD2	0.46	2.10	18	1
1:B:378:LEU:O	1:B:382:SER:OG	0.46	2.31	17	4
1:B:379:ASP:O	1:B:382:SER:OG	0.46	2.32	20	4
1:A:132:TYR:CD2	1:A:133:ASP:N	0.46	2.83	19	4
1:A:179:LEU:N	1:A:179:LEU:CD2	0.46	2.70	1	5
1:B:266:TYR:O	1:B:268:ARG:N	0.46	2.48	17	3
1:B:321:LEU:CD1	1:B:321:LEU:C	0.46	2.89	3	5
1:A:50:GLN:CD	1:A:52:ARG:HH11	0.46	2.15	7	1
1:A:62:LEU:N	1:A:62:LEU:CD2	0.46	2.78	10	1
1:A:199:ASN:C	1:A:199:ASN:OD1	0.46	2.58	11	1
1:B:313:LEU:HD13	1:B:345:ALA:HB1	0.46	1.87	12	1
1:A:141:GLN:O	1:A:145:ASP:OD2	0.46	2.34	1	1
1:B:353:THR:HG22	1:B:354:TYR:H	0.46	1.70	13	2
1:B:361:TRP:O	1:B:365:VAL:N	0.46	2.44	17	2
1:A:11:HIS:C	1:B:210:HIS:CE1	0.46	2.94	16	1
1:A:35:TYR:CD2	1:A:35:TYR:C	0.46	2.93	3	7
1:A:60:LYS:CE	2:D:416:DA:C5	0.46	2.99	11	7
1:B:291:VAL:HG22	1:B:293:TRP:NE1	0.46	2.26	14	2
1:A:102:PHE:C	1:A:103:SER:OG	0.46	2.58	2	3
1:B:381:HIS:CE1	2:C:401:DT:O4	0.46	2.69	2	2
1:B:230:THR:OG1	1:B:256:ASN:OD1	0.46	2.33	5	4
1:A:15:PRO:O	1:A:19:THR:OG1	0.46	2.30	15	2
1:A:38:GLU:CD	1:A:91:ARG:HH11	0.46	2.18	15	1
1:B:264:GLY:O	1:B:266:TYR:CE2	0.46	2.69	16	2
1:A:162:TRP:O	1:A:166:VAL:CB	0.46	2.63	2	3
1:B:237:GLU:OE2	1:B:290:ARG:O	0.46	2.33	3	1
1:B:229:LYS:CB	2:C:404:DC:O2	0.46	2.64	9	4
1:A:41:ASP:O	1:A:44:THR:N	0.46	2.46	7	1
1:A:18:PHE:CE1	1:A:32:TYR:OH	0.46	2.55	10	1
1:A:131:ASP:C	2:D:413:DT:O2	0.46	2.58	14	4
1:A:147:GLY:C	1:A:149:GLN:N	0.46	2.73	6	19
1:B:239:LEU:HB2	1:B:288:ILE:HG23	0.46	1.87	1	2
1:B:313:LEU:CD1	1:B:345:ALA:HB1	0.46	2.41	1	1
1:B:340:GLN:OE1	1:B:395:ASN:OD1	0.46	2.34	5	4
1:B:294:PHE:CE2	1:B:324:PHE:CD2	0.46	3.03	5	1
1:B:297:TRP:CZ3	1:B:327:ARG:NH2	0.46	2.84	16	1
1:A:144:ARG:HH22	1:A:196:ASN:HD21	0.46	1.54	17	1
1:B:328:ILE:CG2	1:B:335:TYR:CE2	0.46	2.98	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:320:ARG:HH22	1:B:322:ARG:NE	0.46	2.09	4	1
1:A:168:HIS:ND1	1:A:171:GLN:NE2	0.46	2.64	13	1
1:B:343:ARG:HH21	1:B:393:LEU:HD23	0.46	1.70	13	1
1:B:324:PHE:CD1	1:B:350:SER:O	0.46	2.69	5	1
1:B:328:ILE:HD12	1:B:385:LEU:HD13	0.46	1.88	11	2
1:B:234:TYR:CD2	1:B:234:TYR:C	0.46	2.94	19	1
1:B:328:ILE:CG2	1:B:335:TYR:CZ	0.46	2.98	4	3
1:A:61:ASN:O	1:A:61:ASN:OD1	0.46	2.33	4	1
1:B:297:TRP:HE1	1:B:327:ARG:HH11	0.46	1.52	8	1
1:A:7:SER:CB	1:A:50:GLN:HE22	0.46	2.24	12	1
1:A:61:ASN:OD1	1:A:64:SER:CB	0.46	2.64	12	1
1:A:141:GLN:OE1	1:A:196:ASN:CG	0.46	2.59	16	2
1:A:78:LEU:CD1	1:B:209:ARG:NE	0.46	2.79	18	1
1:A:56:HIS:NE2	1:B:216:ILE:CD1	0.46	2.79	20	1
1:B:328:ILE:HD11	1:B:385:LEU:HD13	0.45	1.88	5	1
1:A:61:ASN:O	1:A:64:SER:OG	0.45	2.32	8	1
1:A:10:ARG:H	1:B:252:GLY:CA	0.45	2.24	9	1
1:A:13:MET:HE1	1:A:32:TYR:CE1	0.45	2.47	11	1
1:B:227:ARG:CB	1:B:228:HIS:CE1	0.45	3.00	11	1
1:B:237:GLU:OE1	1:B:244:SER:O	0.45	2.34	11	1
1:B:293:TRP:CE2	1:B:321:LEU:HD21	0.45	2.47	2	1
1:A:59:ALA:N	2:D:416:DA:OP2	0.45	2.49	3	2
1:A:78:LEU:HD23	1:A:78:LEU:C	0.45	2.34	12	3
1:B:334:LEU:O	1:B:338:ALA:N	0.45	2.43	3	1
1:A:167:ASP:OD2	1:A:167:ASP:C	0.45	2.59	4	1
1:B:234:TYR:CG	1:B:274:PHE:CE2	0.45	3.05	11	1
1:B:261:LEU:N	1:B:261:LEU:HD12	0.45	2.27	20	2
1:A:196:ASN:O	1:A:199:ASN:O	0.45	2.34	16	2
1:B:343:ARG:HH21	1:B:349:VAL:HG21	0.45	1.71	17	1
1:A:98:TRP:CE3	2:D:414:DC:C4	0.45	3.04	11	14
1:A:92:VAL:O	1:A:92:VAL:CG1	0.45	2.63	12	2
1:B:287:GLN:N	1:B:287:GLN:HE21	0.45	2.08	12	1
1:B:332:ASP:H	1:B:333:PRO:HD2	0.45	1.71	13	12
1:B:361:TRP:CD1	1:B:361:TRP:C	0.45	2.91	8	8
1:A:125:PHE:CG	1:A:153:MET:SD	0.45	3.10	3	1
1:A:79:VAL:N	1:A:80:PRO:HD2	0.45	2.26	8	5
1:B:224:GLY:C	1:B:327:ARG:HH22	0.45	2.19	9	3
1:B:224:GLY:O	1:B:327:ARG:NH1	0.45	2.50	16	1
1:A:75:PHE:CE1	1:A:94:TRP:NE1	0.45	2.85	2	1
1:B:255:HIS:CD2	1:B:255:HIS:H	0.45	2.28	5	2
1:A:194:LEU:HD12	1:A:194:LEU:N	0.45	2.27	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:PHE:CD2	1:A:32:TYR:OH	0.45	2.70	15	2
1:A:47:LYS:O	1:A:48:MET:O	0.45	2.34	16	1
1:A:144:ARG:HD3	1:A:194:LEU:HD11	0.45	1.88	1	1
1:B:291:VAL:HG22	1:B:293:TRP:HE1	0.45	1.70	1	1
1:B:220:ASN:ND2	1:B:220:ASN:C	0.45	2.73	2	1
1:B:376:ASP:O	1:B:376:ASP:OD2	0.45	2.35	2	2
1:B:395:ASN:ND2	1:B:395:ASN:C	0.45	2.75	2	6
1:A:144:ARG:NE	1:A:194:LEU:CD1	0.45	2.78	5	2
1:A:78:LEU:CD1	1:B:209:ARG:HH21	0.45	2.25	9	1
1:A:141:GLN:CG	1:A:196:ASN:OD1	0.45	2.64	20	1
1:B:361:TRP:O	1:B:365:VAL:HB	0.45	2.12	20	4
1:A:168:HIS:CD2	1:A:171:GLN:OE1	0.45	2.70	3	1
1:A:93:THR:CG2	1:A:95:PHE:CE1	0.45	3.00	18	5
1:A:105:GLY:O	1:A:107:ALA:N	0.45	2.50	7	1
1:B:283:LEU:HD22	1:B:289:TYR:CG	0.45	2.46	10	1
1:A:136:TYR:OH	1:A:193:ILE:HD11	0.45	2.12	14	1
1:B:261:LEU:N	1:B:261:LEU:CD1	0.45	2.80	15	2
1:B:343:ARG:CD	1:B:396:GLN:NE2	0.45	2.80	20	1
1:B:221:PHE:O	1:B:223:ASN:N	0.45	2.50	3	1
1:A:61:ASN:OD1	1:A:64:SER:OG	0.45	2.31	4	2
1:A:134:PRO:O	1:A:138:GLU:OE2	0.45	2.34	5	1
1:A:69:ARG:NH1	1:A:103:SER:OG	0.45	2.49	6	1
1:B:327:ARG:NH1	1:B:381:HIS:NE2	0.45	2.65	6	1
1:A:199:ASN:OD1	1:A:199:ASN:OXT	0.45	2.35	11	1
1:A:33:LEU:HD12	1:A:33:LEU:C	0.45	2.37	13	1
1:B:375:TRP:NE1	1:B:378:LEU:CD1	0.45	2.80	14	2
1:A:10:ARG:NH1	1:B:273:ARG:NH1	0.45	2.61	18	1
1:A:102:PHE:CE1	1:A:135:LEU:HD22	0.45	2.47	18	1
1:A:17:ILE:N	1:A:17:ILE:HD12	0.45	2.26	20	1
1:A:174:GLN:NE2	1:A:174:GLN:CA	0.45	2.75	3	3
1:B:297:TRP:CD1	1:B:297:TRP:N	0.45	2.85	4	1
1:A:125:PHE:CE1	1:A:127:ALA:HB2	0.45	2.47	12	2
1:B:274:PHE:CD2	1:B:274:PHE:C	0.45	2.95	10	1
1:B:359:HIS:O	1:B:363:THR:OG1	0.45	2.29	10	2
1:B:320:ARG:HH21	1:B:322:ARG:HH11	0.45	1.54	16	1
1:A:134:PRO:O	1:A:136:TYR:N	0.44	2.49	1	1
1:B:210:HIS:CD2	1:B:210:HIS:C	0.44	2.93	2	4
1:B:397:GLY:O	1:B:398:ASN:OXT	0.44	2.34	3	1
1:A:9:PRO:C	1:A:11:HIS:N	0.44	2.76	14	7
1:A:168:HIS:ND1	1:A:171:GLN:CB	0.44	2.80	19	3
1:A:160:HIS:O	1:A:164:THR:OG1	0.44	2.30	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ASP:OD2	1:A:177:ASP:C	0.44	2.59	10	1
1:B:253:PHE:CE2	1:B:364:PHE:CD1	0.44	3.05	10	1
1:B:326:ALA:HB2	1:B:352:MET:HE1	0.44	1.88	14	1
1:B:215:HIS:ND1	1:B:215:HIS:C	0.44	2.72	19	1
1:A:85:ASP:OD1	1:A:90:TYR:OH	0.44	2.35	20	1
1:A:62:LEU:CD1	1:A:62:LEU:N	0.44	2.80	4	1
1:A:62:LEU:N	1:A:62:LEU:HD12	0.44	2.27	4	1
1:B:378:LEU:O	1:B:382:SER:N	0.44	2.43	17	3
1:A:196:ASN:ND2	1:A:196:ASN:C	0.44	2.74	5	3
1:A:173:PHE:CE1	1:A:174:GLN:O	0.44	2.70	6	1
1:B:366:ASP:OD1	1:B:366:ASP:C	0.44	2.60	6	3
1:B:362:ASP:OD1	1:B:367:HIS:O	0.44	2.36	7	1
1:A:56:HIS:CD2	1:A:56:HIS:C	0.44	2.95	9	1
1:B:335:TYR:CZ	1:B:339:LEU:CD1	0.44	2.99	15	1
1:B:343:ARG:NH1	1:B:393:LEU:HD21	0.44	2.26	17	1
1:A:23:ASN:OD1	1:A:23:ASN:C	0.44	2.59	20	1
1:B:366:ASP:OD1	1:B:366:ASP:N	0.44	2.51	1	2
1:B:323:ILE:HD13	1:B:342:LEU:HD21	0.44	1.88	13	2
1:A:41:ASP:O	1:A:42:ASN:C	0.44	2.59	7	2
1:A:10:ARG:NH1	1:B:250:HIS:O	0.44	2.51	10	1
1:B:343:ARG:NH2	1:B:396:GLN:HE21	0.44	2.10	15	1
1:A:131:ASP:O	1:A:132:TYR:HB3	0.44	2.13	2	17
1:B:398:ASN:OD1	1:B:398:ASN:C	0.44	2.60	14	2
1:A:35:TYR:CG	1:A:75:PHE:CE1	0.44	3.05	5	1
1:A:194:LEU:N	1:A:194:LEU:CD1	0.44	2.81	6	1
1:B:230:THR:CB	1:B:256:ASN:OD1	0.44	2.64	8	1
1:A:22:PHE:CZ	1:A:32:TYR:CE1	0.44	3.06	10	1
1:A:102:PHE:C	1:A:103:SER:HG	0.44	2.21	14	1
1:B:253:PHE:CE1	1:B:364:PHE:CD1	0.44	3.05	14	1
1:A:34:CYS:CB	1:A:165:PHE:CZ	0.44	3.00	15	1
1:B:297:TRP:CZ2	1:B:327:ARG:NH2	0.44	2.86	2	1
1:A:56:HIS:HD1	1:A:56:HIS:N	0.44	2.11	6	1
1:A:154:THR:HG22	1:A:155:TYR:H	0.44	1.72	7	2
1:B:367:HIS:CE1	1:B:370:GLN:CD	0.44	2.96	7	1
1:A:168:HIS:CG	1:A:171:GLN:HE21	0.44	2.30	12	1
1:B:294:PHE:CD2	1:B:352:MET:HE3	0.44	2.46	17	1
1:B:321:LEU:HD13	1:B:321:LEU:C	0.44	2.38	3	4
1:B:376:ASP:O	1:B:376:ASP:CG	0.44	2.59	2	2
1:B:246:LYS:HZ1	1:B:251:ARG:NH1	0.44	2.07	6	2
1:A:51:HIS:O	1:A:52:ARG:O	0.44	2.35	14	2
1:B:376:ASP:CG	1:B:376:ASP:O	0.44	2.61	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:398:ASN:OD1	1:B:398:ASN:OXT	0.44	2.36	14	1
1:B:255:HIS:NE2	1:B:257:GLN:CG	0.44	2.81	15	1
1:B:310:ARG:CZ	1:B:314:GLN:OE1	0.44	2.66	17	1
1:B:384:ALA:HB1	2:C:400:DT:OP1	0.44	2.13	18	1
1:B:366:ASP:OD1	1:B:368:GLN:NE2	0.44	2.51	20	1
1:B:297:TRP:CD2	1:B:330:ASP:OD2	0.44	2.71	2	1
1:A:30:LYS:O	1:A:30:LYS:CG	0.44	2.64	3	1
1:A:144:ARG:O	1:A:148:ALA:HB2	0.44	2.11	3	1
1:A:92:VAL:O	1:A:92:VAL:HG13	0.44	2.12	5	1
1:A:95:PHE:CZ	1:A:125:PHE:CD1	0.44	3.05	11	1
1:A:144:ARG:NH2	1:A:197:GLN:CG	0.44	2.80	17	1
1:B:230:THR:HG1	1:B:297:TRP:CD1	0.44	2.30	3	1
1:B:380:GLU:CG	1:B:381:HIS:N	0.44	2.81	12	2
1:A:75:PHE:CZ	1:A:92:VAL:HG21	0.44	2.48	6	3
1:B:361:TRP:CD1	1:B:367:HIS:NE2	0.44	2.86	6	1
1:A:102:PHE:CE1	1:A:135:LEU:CD2	0.44	3.00	19	2
1:B:222:ASN:O	2:C:402:DT:O4	0.44	2.36	11	2
1:A:198:GLY:C	1:A:199:ASN:OXT	0.44	2.61	13	1
1:B:268:ARG:HE	1:B:272:LEU:CD2	0.44	2.24	14	1
1:A:76:LEU:O	1:A:80:PRO:CD	0.43	2.66	16	8
1:B:367:HIS:ND1	1:B:370:GLN:OE1	0.43	2.50	3	1
1:A:91:ARG:HH11	1:A:123:ARG:HH21	0.43	1.56	12	3
1:A:49:ASP:OD1	1:A:49:ASP:N	0.43	2.47	7	1
1:B:267:GLY:O	1:B:268:ARG:O	0.43	2.36	14	1
1:A:141:GLN:CD	1:A:196:ASN:ND2	0.43	2.76	19	1
1:A:69:ARG:CZ	1:A:104:TRP:NE1	0.43	2.81	20	1
1:B:328:ILE:HG23	1:B:335:TYR:CE1	0.43	2.48	1	1
1:B:330:ASP:OD1	1:B:330:ASP:C	0.43	2.60	15	2
1:A:140:LEU:HD23	1:A:193:ILE:HD13	0.43	1.88	6	1
1:B:259:LYS:O	2:C:407:DT:OP1	0.43	2.36	8	1
1:B:343:ARG:NE	1:B:393:LEU:CD2	0.43	2.81	9	1
1:B:352:MET:CE	1:B:357:PHE:CE2	0.43	3.01	9	1
1:A:122:LEU:HD13	1:A:122:LEU:C	0.43	2.37	11	1
1:B:278:VAL:N	1:B:279:PRO:CD	0.43	2.81	19	1
1:A:11:HIS:CE1	1:B:253:PHE:CE2	0.43	3.07	1	1
1:A:162:TRP:O	1:A:166:VAL:HB	0.43	2.13	2	2
1:B:255:HIS:CD2	1:B:257:GLN:CG	0.43	3.01	15	3
1:A:38:GLU:OE2	1:A:45:SER:OG	0.43	2.29	7	1
1:A:24:ASN:HD21	1:A:176:TRP:NE1	0.43	2.11	8	1
1:B:233:CYS:SG	1:B:253:PHE:CE2	0.43	3.11	10	1
1:A:28:ARG:NH2	1:A:128:ARG:HH11	0.43	2.11	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:HIS:NE2	1:A:74:ARG:NH1	0.43	2.65	18	1
1:A:58:GLN:CD	1:A:58:GLN:C	0.43	2.86	19	1
1:B:238:ARG:O	1:B:245:VAL:N	0.43	2.49	1	1
1:B:228:HIS:O	1:B:256:ASN:CB	0.43	2.66	2	1
1:B:295:ILE:CG2	1:B:297:TRP:O	0.43	2.67	5	2
1:A:11:HIS:CD2	1:A:11:HIS:H	0.43	2.32	7	1
1:B:343:ARG:NH1	1:B:396:GLN:CG	0.43	2.81	13	1
1:A:10:ARG:C	1:A:12:LEU:H	0.43	2.22	19	1
1:B:398:ASN:OXT	1:B:398:ASN:OD1	0.43	2.37	1	1
1:A:132:TYR:CD1	1:A:133:ASP:N	0.43	2.85	2	2
1:B:389:LEU:CD1	1:B:389:LEU:C	0.43	2.91	13	7
1:A:130:TYR:CE1	2:D:413:DT:H2"	0.43	2.48	7	8
2:D:418:DT:OP2	2:D:418:DT:C7	0.43	2.65	6	1
1:A:56:HIS:CD2	1:A:58:GLN:O	0.43	2.71	12	2
1:A:198:GLY:O	1:A:199:ASN:O	0.43	2.36	15	1
1:A:50:GLN:CA	1:B:206:SER:O	0.43	2.66	18	1
1:B:361:TRP:CD2	1:B:372:PHE:CB	0.43	3.01	18	1
1:A:183:SER:O	1:A:187:SER:N	0.43	2.48	1	2
1:B:297:TRP:CE2	1:B:330:ASP:OD1	0.43	2.72	2	1
1:A:75:PHE:CE2	1:A:94:TRP:NE1	0.43	2.87	5	1
1:B:340:GLN:HE21	1:B:392:ILE:CG2	0.43	2.27	5	1
1:B:250:HIS:O	1:B:251:ARG:C	0.43	2.61	8	2
1:B:253:PHE:CE2	1:B:255:HIS:CE1	0.43	3.06	16	1
1:B:343:ARG:CZ	1:B:393:LEU:HD21	0.43	2.44	17	1
1:B:296:SER:O	1:B:327:ARG:N	0.43	2.51	1	2
1:B:372:PHE:C	1:B:373:GLN:NE2	0.43	2.77	2	1
1:A:40:LEU:HB2	1:A:89:ILE:HG23	0.43	1.89	15	3
1:A:12:LEU:HD13	1:A:167:ASP:OD1	0.43	2.13	14	1
1:A:75:PHE:CE1	1:A:78:LEU:HD22	0.43	2.48	18	2
1:B:212:MET:SD	1:B:253:PHE:CD2	0.43	3.12	2	1
1:A:93:THR:HG22	1:A:95:PHE:CE2	0.43	2.49	10	2
1:A:138:GLU:OE1	1:A:138:GLU:N	0.43	2.47	7	1
1:B:318:HIS:O	1:B:318:HIS:CG	0.43	2.70	7	1
1:B:210:HIS:CD2	1:B:210:HIS:N	0.43	2.86	11	3
1:B:395:ASN:HD21	1:B:396:GLN:HE21	0.43	1.56	10	1
1:A:10:ARG:CZ	1:B:234:TYR:OH	0.43	2.67	16	1
1:A:153:MET:SD	1:A:158:PHE:CE1	0.43	3.12	17	1
1:B:384:ALA:CB	2:C:400:DT:OP1	0.43	2.66	18	1
1:A:13:MET:O	1:A:14:ASP:C	0.43	2.62	10	4
1:A:168:HIS:CD2	1:A:168:HIS:N	0.43	2.86	2	1
1:A:129:ILE:CD1	1:A:186:LEU:CD1	0.43	2.95	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:HIS:NE2	2:C:406:DA:OP1	0.43	2.52	8	1
1:A:60:LYS:O	1:A:61:ASN:OD1	0.43	2.37	8	1
1:B:220:ASN:ND2	1:B:231:TYR:OH	0.43	2.52	9	1
1:A:14:ASP:OD2	1:A:17:ILE:CD1	0.43	2.67	5	1
1:A:40:LEU:HD23	1:A:41:ASP:N	0.43	2.29	7	1
1:A:16:HIS:HE2	1:B:260:ASN:CG	0.43	2.22	13	1
1:B:250:HIS:NE2	1:B:281:LEU:HD22	0.43	2.29	14	1
1:A:11:HIS:CD2	1:B:253:PHE:CE1	0.43	3.07	15	1
1:A:12:LEU:CD2	1:A:12:LEU:H	0.42	2.27	2	1
1:A:55:LEU:HD21	1:B:209:ARG:HE	0.42	1.73	2	1
1:A:57:ASN:C	1:A:57:ASN:ND2	0.42	2.77	7	1
1:A:62:LEU:N	1:A:62:LEU:HD22	0.42	2.29	10	1
1:A:113:PHE:CE2	1:A:117:ASN:ND2	0.42	2.87	13	1
1:A:198:GLY:O	1:A:199:ASN:OD1	0.42	2.37	14	1
1:B:361:TRP:NE1	1:B:367:HIS:HE2	0.42	2.08	20	1
1:A:65:GLY:O	1:A:67:TYR:CE2	0.42	2.72	1	1
1:A:32:TYR:CD2	1:A:32:TYR:C	0.42	2.97	5	1
1:B:246:LYS:HZ1	1:B:251:ARG:HH12	0.42	1.56	6	1
1:B:335:TYR:CD2	1:B:335:TYR:C	0.42	2.92	6	1
1:A:105:GLY:C	1:A:107:ALA:N	0.42	2.75	7	1
1:A:22:PHE:CZ	1:A:32:TYR:CZ	0.42	3.07	10	1
1:B:351:ILE:HD12	1:B:385:LEU:HD12	0.42	1.90	13	1
1:A:198:GLY:C	1:A:199:ASN:O	0.42	2.62	15	1
1:B:290:ARG:HH11	1:B:322:ARG:NH2	0.42	2.12	19	1
1:B:380:GLU:O	2:C:399:DA:O5'	0.42	2.32	8	1
1:A:76:LEU:CD1	1:A:76:LEU:C	0.42	2.92	12	5
1:B:352:MET:CE	1:B:357:PHE:CE1	0.42	3.02	16	2
1:A:98:TRP:CD2	2:D:414:DC:C5	0.42	3.08	19	1
1:B:254:LEU:CD1	1:B:270:ALA:HB1	0.42	2.45	8	1
1:B:274:PHE:CE2	1:B:293:TRP:NE1	0.42	2.87	9	1
1:B:230:THR:HG23	1:B:297:TRP:CD1	0.42	2.49	10	1
1:A:48:MET:CE	1:A:51:HIS:CG	0.42	3.01	12	1
1:A:144:ARG:HD2	1:A:194:LEU:HD11	0.42	1.90	13	1
1:A:181:GLU:CG	1:A:182:HIS:N	0.42	2.82	13	1
1:A:129:ILE:CG1	1:A:186:LEU:HD22	0.42	2.44	17	2
1:A:177:ASP:O	1:A:177:ASP:CG	0.42	2.63	16	3
1:A:37:VAL:C	1:A:38:GLU:OE1	0.42	2.62	8	1
1:B:230:THR:HG23	1:B:297:TRP:NE1	0.42	2.30	10	1
1:A:78:LEU:HD13	1:B:209:ARG:NH2	0.42	2.28	11	1
1:A:168:HIS:CE1	1:A:171:GLN:HE21	0.42	2.31	12	1
1:A:60:LYS:CE	2:D:416:DA:C6	0.42	3.03	15	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLN:CB	1:B:206:SER:O	0.42	2.67	5	1
1:A:130:TYR:CD2	1:A:130:TYR:C	0.42	2.97	12	2
1:B:331:TYR:C	1:B:332:ASP:O	0.42	2.63	8	1
1:B:329:TYR:O	1:B:329:TYR:CD1	0.42	2.73	16	1
1:A:11:HIS:N	1:A:11:HIS:CD2	0.42	2.88	18	1
1:A:144:ARG:CD	1:A:194:LEU:CD2	0.42	2.97	18	1
1:B:382:SER:O	1:B:386:SER:CB	0.42	2.68	18	1
1:B:384:ALA:HB2	2:C:400:DT:P	0.42	2.55	18	1
1:B:287:GLN:NE2	1:B:287:GLN:CA	0.42	2.83	1	8
1:A:186:LEU:N	1:A:186:LEU:CD1	0.42	2.83	3	1
1:A:27:GLY:H	1:A:128:ARG:HH22	0.42	1.57	5	1
1:B:335:TYR:CE2	1:B:339:LEU:CD1	0.42	3.02	5	1
1:A:119:HIS:O	1:A:119:HIS:CG	0.42	2.69	7	1
1:A:51:HIS:CG	1:A:82:LEU:HD22	0.42	2.50	11	1
1:A:102:PHE:CZ	1:A:135:LEU:CD2	0.42	3.03	11	1
1:A:167:ASP:O	1:A:169:GLN:NE2	0.42	2.53	14	1
1:A:95:PHE:CZ	1:A:125:PHE:CD2	0.42	3.07	18	1
1:B:229:LYS:CG	2:C:404:DC:H42	0.42	2.28	2	1
2:D:415:DA:O5'	2:D:415:DA:C8	0.42	2.73	14	5
1:A:50:GLN:HE22	1:A:52:ARG:NH1	0.42	2.12	7	1
1:B:372:PHE:CD1	1:B:373:GLN:N	0.42	2.87	7	1
1:B:217:PHE:CE2	1:B:221:PHE:CD2	0.42	3.08	10	2
1:B:227:ARG:C	1:B:228:HIS:ND1	0.42	2.77	11	1
1:B:343:ARG:HH21	1:B:393:LEU:CD2	0.42	2.27	13	1
1:B:254:LEU:C	1:B:255:HIS:CD2	0.42	2.98	14	1
1:B:352:MET:HE2	1:B:357:PHE:CE1	0.42	2.50	16	1
1:B:385:LEU:CD1	1:B:385:LEU:N	0.42	2.83	18	1
1:A:18:PHE:CE2	1:A:22:PHE:CE1	0.42	3.08	3	2
1:A:73:LEU:HD13	1:A:109:GLU:OE2	0.42	2.15	3	1
1:B:330:ASP:OD2	1:B:330:ASP:C	0.42	2.60	3	1
1:A:74:ARG:NH1	1:B:366:ASP:CG	0.42	2.77	5	1
1:A:45:SER:O	1:A:45:SER:OG	0.42	2.36	10	1
1:B:361:TRP:CE2	1:B:372:PHE:HB2	0.42	2.50	12	1
1:B:236:VAL:O	1:B:236:VAL:HG23	0.42	2.15	1	1
1:A:28:ARG:NH1	1:A:31:THR:N	0.42	2.64	3	1
1:A:186:LEU:N	1:A:186:LEU:HD12	0.42	2.29	3	1
1:A:97:SER:OG	1:A:98:TRP:CD1	0.42	2.73	6	1
1:B:220:ASN:OD1	1:B:231:TYR:OH	0.42	2.30	7	1
1:A:31:THR:CG2	1:A:98:TRP:CZ2	0.42	2.97	13	1
1:B:339:LEU:C	1:B:339:LEU:CD1	0.41	2.94	2	2
1:B:385:LEU:N	1:B:385:LEU:CD2	0.41	2.82	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:THR:HG23	1:A:32:TYR:H	0.41	1.73	4	1
1:A:178:GLY:H	1:A:179:LEU:HD22	0.41	1.75	8	3
1:A:100:PRO:O	1:A:130:TYR:CG	0.41	2.73	8	5
1:B:324:PHE:CD2	1:B:325:ALA:N	0.41	2.88	3	1
1:B:335:TYR:CZ	1:B:392:ILE:HD11	0.41	2.49	3	1
1:A:191:ARG:O	1:A:195:GLN:N	0.41	2.49	6	1
1:B:229:LYS:NZ	1:B:255:HIS:CE1	0.41	2.88	7	1
1:B:324:PHE:CZ	1:B:350:SER:OG	0.41	2.70	8	1
1:B:343:ARG:NE	1:B:393:LEU:CD1	0.41	2.82	8	1
1:A:16:HIS:HE2	1:B:260:ASN:ND2	0.41	2.12	13	1
1:A:140:LEU:O	1:A:144:ARG:CB	0.41	2.69	13	1
1:A:18:PHE:CE1	1:A:22:PHE:CE1	0.41	3.08	15	1
1:B:353:THR:CG2	1:B:354:TYR:N	0.41	2.83	2	1
1:A:75:PHE:CE1	1:A:79:VAL:HG23	0.41	2.51	9	1
1:A:155:TYR:CD1	1:A:155:TYR:O	0.41	2.74	12	1
1:A:7:SER:OG	1:A:50:GLN:CD	0.41	2.63	13	1
1:A:10:ARG:NH2	1:B:254:LEU:HD11	0.41	2.31	13	1
1:B:288:ILE:HG23	1:B:288:ILE:O	0.41	2.15	20	1
1:A:153:MET:HE2	1:A:158:PHE:CE2	0.41	2.51	1	1
1:B:291:VAL:O	1:B:291:VAL:CG1	0.41	2.68	1	1
1:A:97:SER:OG	1:A:98:TRP:CD2	0.41	2.74	12	3
1:A:140:LEU:CD1	1:A:140:LEU:C	0.41	2.93	2	1
1:A:48:MET:HE3	1:A:51:HIS:ND1	0.41	2.31	8	1
1:A:125:PHE:CD2	1:A:151:SER:O	0.41	2.74	14	1
1:B:297:TRP:CE2	1:B:330:ASP:CG	0.41	2.97	2	1
1:B:223:ASN:H	1:B:327:ARG:HH11	0.41	1.58	3	1
1:A:93:THR:HG22	1:A:95:PHE:CE1	0.41	2.50	6	2
1:B:331:TYR:O	1:B:332:ASP:C	0.41	2.63	8	2
1:A:16:HIS:NE2	1:B:265:PHE:CE1	0.41	2.89	10	1
1:A:60:LYS:NZ	2:D:416:DA:C6	0.41	2.89	16	1
1:A:155:TYR:CE2	1:A:175:PRO:CG	0.41	3.02	16	1
1:B:227:ARG:C	1:B:229:LYS:N	0.41	2.77	2	1
1:B:330:ASP:O	1:B:330:ASP:OD1	0.41	2.39	5	1
1:B:218:THR:O	1:B:222:ASN:N	0.41	2.54	6	1
1:B:332:ASP:CB	1:B:333:PRO:CD	0.41	2.98	6	3
1:A:56:HIS:CE1	1:A:74:ARG:NH2	0.41	2.88	7	1
1:A:22:PHE:CZ	1:A:153:MET:HE1	0.41	2.49	11	1
1:B:229:LYS:CA	1:B:255:HIS:NE2	0.41	2.83	11	1
1:A:144:ARG:HH12	1:A:197:GLN:HE21	0.41	1.56	13	1
1:B:310:ARG:HH11	1:B:344:ASP:CB	0.41	2.28	14	1
1:B:328:ILE:HG22	1:B:335:TYR:OH	0.41	2.15	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:246:LYS:CD	1:B:251:ARG:NH1	0.41	2.84	2	1
1:A:73:LEU:HD12	1:A:76:LEU:HD12	0.41	1.93	4	1
1:B:310:ARG:NH2	1:B:341:MET:O	0.41	2.53	4	1
1:A:16:HIS:CD2	1:B:260:ASN:CG	0.41	2.99	7	1
1:A:104:TRP:CG	1:A:105:GLY:N	0.41	2.88	10	1
1:A:187:SER:O	1:A:191:ARG:CG	0.41	2.68	14	1
1:A:62:LEU:HD13	2:D:417:DT:OP1	0.41	2.16	15	1
1:A:10:ARG:O	1:A:12:LEU:CD2	0.41	2.69	17	1
1:A:72:GLN:NE2	1:A:96:ILE:CD1	0.41	2.83	17	1
1:A:56:HIS:CE1	1:B:216:ILE:HD11	0.41	2.51	19	1
1:B:320:ARG:HH21	1:B:322:ARG:HE	0.41	1.55	4	1
1:B:340:GLN:NE2	1:B:392:ILE:CG2	0.41	2.82	5	1
1:B:262:ASN:CG	2:C:408:DT:OP1	0.41	2.63	8	1
1:A:12:LEU:H	1:A:12:LEU:CD2	0.41	2.26	20	1
1:A:137:LYS:CG	1:A:138:GLU:N	0.41	2.84	1	1
1:A:137:LYS:HG3	1:A:138:GLU:N	0.41	2.31	1	1
1:A:167:ASP:OD1	1:A:167:ASP:C	0.41	2.63	2	1
1:A:76:LEU:C	1:A:76:LEU:CD1	0.41	2.93	3	2
1:B:250:HIS:CE1	1:B:281:LEU:HD13	0.41	2.51	3	1
1:A:31:THR:C	1:A:57:ASN:OD1	0.41	2.63	6	1
1:B:221:PHE:CE2	1:B:294:PHE:CE2	0.41	3.09	7	1
1:A:99:SER:N	1:A:100:PRO:HD2	0.41	2.31	8	1
1:B:232:LEU:CD1	1:B:271:GLN:HE21	0.41	2.28	8	1
1:A:188:GLY:O	1:A:191:ARG:CG	0.41	2.69	9	1
1:A:166:VAL:CG1	1:A:168:HIS:CD2	0.41	3.03	11	1
1:A:181:GLU:CD	1:A:182:HIS:CD2	0.41	2.99	13	1
1:A:119:HIS:NE2	1:A:120:VAL:CG2	0.41	2.80	14	1
1:A:132:TYR:C	1:A:133:ASP:O	0.41	2.65	17	3
1:A:70:HIS:CE1	1:A:101:CYS:SG	0.41	3.13	2	1
1:A:138:GLU:OE2	1:A:138:GLU:N	0.41	2.47	5	1
1:A:17:ILE:O	1:A:20:SER:OG	0.41	2.31	9	1
1:A:195:GLN:HE21	1:A:195:GLN:N	0.41	2.14	12	1
1:B:271:GLN:NE2	1:B:293:TRP:CZ3	0.41	2.88	12	1
1:A:155:TYR:CD2	1:A:155:TYR:O	0.41	2.74	16	1
1:B:216:ILE:O	1:B:219:SER:OG	0.40	2.33	4	1
1:B:329:TYR:O	1:B:329:TYR:CD2	0.40	2.74	7	1
1:A:61:ASN:ND2	1:A:61:ASN:O	0.40	2.54	11	1
1:A:7:SER:OG	1:A:50:GLN:NE2	0.40	2.53	13	1
1:A:85:ASP:O	1:A:119:HIS:CE1	0.40	2.74	13	1
1:A:45:SER:OG	1:A:91:ARG:NH1	0.40	2.53	17	1
1:A:92:VAL:CG2	1:A:94:TRP:HE1	0.40	2.29	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:VAL:HG22	1:A:94:TRP:HE1	0.40	1.75	20	1
1:B:275:LEU:C	1:B:275:LEU:CD1	0.40	2.94	3	1
1:B:330:ASP:OD2	1:B:330:ASP:O	0.40	2.39	3	1
1:A:62:LEU:HD23	2:D:418:DT:C7	0.40	2.46	7	1
1:B:318:HIS:O	1:B:318:HIS:ND1	0.40	2.54	7	1
1:B:393:LEU:CD1	1:B:396:GLN:NE2	0.40	2.85	7	1
1:A:141:GLN:CD	1:A:196:ASN:HD21	0.40	2.24	9	1
1:B:223:ASN:O	2:C:402:DT:C4	0.40	2.74	9	1
1:A:16:HIS:CG	1:B:258:ALA:CB	0.40	3.04	12	1
1:A:38:GLU:OE1	1:A:45:SER:OG	0.40	2.40	19	1
1:B:351:ILE:HD13	1:B:385:LEU:HB3	0.40	1.93	2	1
1:A:28:ARG:NH2	1:A:128:ARG:NH1	0.40	2.69	11	1
1:A:73:LEU:CD1	1:A:73:LEU:C	0.40	2.94	13	1
1:A:195:GLN:C	1:A:197:GLN:N	0.40	2.79	13	1
1:B:234:TYR:CD2	1:B:274:PHE:CE1	0.40	3.09	13	1
1:B:343:ARG:HH12	1:B:396:GLN:HE21	0.40	1.56	13	1
1:A:169:GLN:N	1:A:169:GLN:CD	0.40	2.79	3	1
1:B:225:ILE:C	2:C:403:DT:H73	0.40	2.40	4	1
1:A:38:GLU:OE2	1:A:47:LYS:CG	0.40	2.69	6	1
1:A:102:PHE:CZ	1:A:135:LEU:HD21	0.40	2.52	11	1
1:A:132:TYR:N	2:D:413:DT:O2	0.40	2.54	11	1
1:B:310:ARG:NH1	1:B:341:MET:CG	0.40	2.85	12	1
1:B:220:ASN:OD1	1:B:231:TYR:CB	0.40	2.69	16	1
1:A:15:PRO:HG2	1:A:168:HIS:NE2	0.40	2.32	17	1
1:A:143:LEU:C	1:A:143:LEU:CD1	0.40	2.95	18	1
1:A:40:LEU:HD21	1:A:43:GLY:N	0.40	2.29	7	1
1:B:216:ILE:HG22	1:B:220:ASN:OD1	0.40	2.17	10	1
1:B:342:LEU:O	1:B:342:LEU:CD1	0.40	2.70	10	1
1:A:16:HIS:CE1	1:B:258:ALA:HB3	0.40	2.50	11	1
1:B:234:TYR:CD1	1:B:234:TYR:O	0.40	2.75	11	1
1:B:297:TRP:CZ3	1:B:300:CYS:SG	0.40	3.14	13	1
1:A:121:ARG:CZ	1:A:123:ARG:HE	0.40	2.30	16	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	193/199 (97%)	172±2 (89±1%)	12±2 (6±1%)	9±1 (5±1%)	3	26
1	B	187/199 (94%)	168±2 (90±1%)	14±2 (7±1%)	5±1 (3±1%)	6	40
All	All	7600/7960 (95%)	6804 (90%)	514 (7%)	282 (4%)	4	32

All 30 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	30	LYS	20
1	A	31	THR	20
1	A	61	ASN	20
1	A	132	TYR	20
1	A	148	ALA	20
1	B	210	HIS	20
1	B	260	ASN	20
1	B	347	ALA	20
1	A	133	ASP	18
1	B	333	PRO	17
1	A	103	SER	12
1	A	50	GLN	12
1	A	23	ASN	11
1	A	10	ARG	6
1	B	332	ASP	6
1	B	229	LYS	6
1	B	228	HIS	5
1	A	48	MET	4
1	A	52	ARG	4
1	A	105	GLY	4
1	B	300	CYS	4
1	B	250	HIS	2
1	A	51	HIS	2
1	A	12	LEU	2
1	A	11	HIS	2
1	B	267	GLY	1
1	B	269	HIS	1
1	B	222	ASN	1
1	B	268	ARG	1
1	B	305	CYS	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/171 (98%)	140±3 (84±2%)	27±3 (16±2%)	4	40
1	B	162/171 (95%)	142±2 (87±1%)	20±2 (13±1%)	7	48
All	All	6580/6840 (96%)	5639 (86%)	941 (14%)	5	44

All 115 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	88	GLN	20
1	A	98	TRP	20
1	A	99	SER	20
1	A	122	LEU	20
1	A	131	ASP	20
1	A	169	GLN	20
1	A	174	GLN	20
1	A	190	LEU	20
1	A	195	GLN	20
1	A	196	ASN	20
1	B	260	ASN	20
1	B	287	GLN	20
1	B	298	SER	20
1	B	332	ASP	20
1	B	368	GLN	20
1	B	373	GLN	20
1	B	389	LEU	20
1	B	394	GLN	20
1	B	395	ASN	20
1	A	57	ASN	19
1	A	136	TYR	19
1	A	14	ASP	18
1	B	233	CYS	18
1	B	253	PHE	18
1	B	300	CYS	18
1	B	361	TRP	18
1	A	133	ASP	17
1	A	34	CYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	179	LEU	15
1	B	284	ASP	15
1	A	79	VAL	14
1	A	12	LEU	14
1	A	52	ARG	13
1	B	305	CYS	13
1	A	85	ASP	12
1	A	182	HIS	12
1	B	255	HIS	12
1	B	378	LEU	12
1	B	278	VAL	11
1	A	96	ILE	11
1	A	76	LEU	11
1	A	47	LYS	10
1	B	335	TYR	9
1	B	370	GLN	9
1	A	166	VAL	8
1	A	19	THR	8
1	A	28	ARG	8
1	A	48	MET	7
1	B	212	MET	7
1	A	103	SER	7
1	B	297	TRP	7
1	A	13	MET	7
1	A	54	PHE	6
1	A	78	LEU	6
1	A	168	HIS	6
1	A	101	CYS	5
1	A	46	VAL	5
1	B	277	LEU	5
1	B	321	LEU	5
1	B	213	ASP	5
1	A	61	ASN	4
1	B	339	LEU	4
1	A	33	LEU	4
1	A	60	LYS	4
1	A	171	GLN	4
1	B	328	ILE	4
1	B	342	LEU	4
1	A	167	ASP	3
1	B	390	ARG	3
1	A	106	CYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	119	HIS	3
1	A	155	TYR	3
1	B	318	HIS	3
1	A	143	LEU	3
1	B	372	PHE	3
1	A	141	GLN	3
1	A	56	HIS	2
1	B	291	VAL	2
1	B	250	HIS	2
1	B	367	HIS	2
1	A	191	ARG	2
1	A	31	THR	2
1	A	51	HIS	2
1	A	23	ASN	2
1	B	228	HIS	2
1	A	16	HIS	2
1	B	215	HIS	2
1	A	64	SER	2
1	B	349	VAL	1
1	A	140	LEU	1
1	B	272	LEU	1
1	B	275	LEU	1
1	B	352	MET	1
1	B	245	VAL	1
1	A	24	ASN	1
1	B	330	ASP	1
1	A	11	HIS	1
1	B	230	THR	1
1	B	232	LEU	1
1	A	17	ILE	1
1	A	50	GLN	1
1	B	288	ILE	1
1	B	319	VAL	1
1	A	26	ILE	1
1	B	229	LYS	1
1	A	73	LEU	1
1	A	181	GLU	1
1	B	385	LEU	1
1	A	104	TRP	1
1	A	7	SER	1
1	A	111	ARG	1
1	A	114	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	150	VAL	1
1	B	383	GLN	1
1	A	173	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 77% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *A3A_shifts-2plus2_20200918.txt*

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	4564
Number of shifts mapped to atoms	4564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	21

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	384	0.04 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	350	0.68 ± 0.11	Should be checked
$^{13}\text{C}'$	345	-0.02 ± 0.10	None needed (< 0.5 ppm)
^{15}N	362	-0.31 ± 0.16	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 4403 atoms were assigned a chemical shift out of a possible 5725. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1811/1903 (95%)	749/774 (97%)	709/764 (93%)	353/365 (97%)
Sidechain	2151/2806 (77%)	1539/1813 (85%)	592/852 (69%)	20/141 (14%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	275/640 (43%)	232/313 (74%)	38/280 (14%)	5/47 (11%)
Sugar	140/240 (58%)	140/140 (100%)	0/100 (0%)	0/0 (—%)
Base	26/136 (19%)	26/76 (34%)	0/40 (0%)	0/20 (0%)
Overall	4403/5725 (77%)	2686/3116 (86%)	1339/2036 (66%)	378/573 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 4522 atoms were assigned a chemical shift out of a possible 5916. 0 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1863/1982 (94%)	772/806 (96%)	729/796 (92%)	362/380 (95%)
Sidechain	2207/2896 (76%)	1577/1872 (84%)	610/882 (69%)	20/142 (14%)
Aromatic	286/662 (43%)	238/324 (73%)	42/290 (14%)	6/48 (12%)
Sugar	140/240 (58%)	140/140 (100%)	0/100 (0%)	0/0 (—%)
Base	26/136 (19%)	26/76 (34%)	0/40 (0%)	0/20 (0%)
Overall	4522/5916 (76%)	2753/3218 (86%)	1381/2108 (66%)	388/590 (66%)

7.1.4 Statistically unusual chemical shifts ⓘ

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	44	THR	HG1	5.07	0.08 – 2.19	18.6
1	B	243	THR	HG1	5.07	0.08 – 2.19	18.6
1	A	70	HIS	CE1	118.42	126.08 – 149.12	-8.3
1	B	269	HIS	CE1	118.42	126.08 – 149.12	-8.3
1	A	94	TRP	HE1	5.58	6.88 – 13.28	-7.0
1	B	293	TRP	HE1	5.58	6.88 – 13.28	-7.0
1	A	66	PHE	CD2	124.86	125.53 – 137.61	-5.6
1	B	265	PHE	CD2	124.86	125.53 – 137.61	-5.6
1	A	72	GLN	CB	38.88	20.34 – 37.98	5.5
1	B	271	GLN	CB	38.88	20.34 – 37.98	5.5
1	A	131	ASP	CB	32.21	32.98 – 48.76	-5.5
1	B	330	ASP	CB	32.21	32.98 – 48.76	-5.5
1	A	66	PHE	CD1	124.86	125.33 – 137.83	-5.4
1	B	265	PHE	CD1	124.86	125.33 – 137.83	-5.4
1	B	369	GLY	H	11.62	5.23 – 11.42	5.3
1	A	170	GLY	H	11.61	5.23 – 11.42	5.3
1	B	378	LEU	HG	-0.22	-0.13 – 3.16	-5.2
1	A	179	LEU	HG	-0.21	-0.13 – 3.16	-5.2

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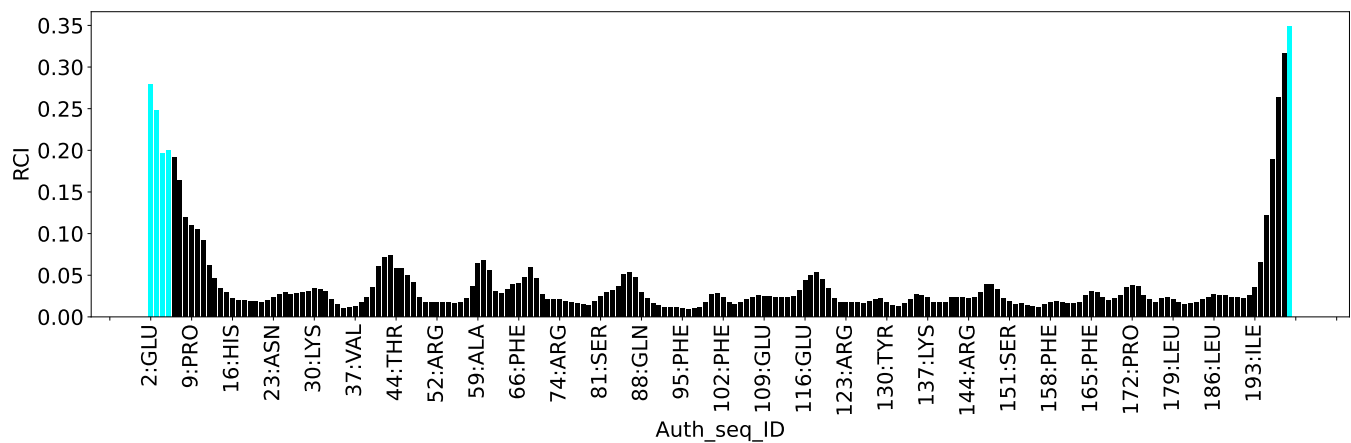
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	97	SER	HB3	2.44	2.49 – 5.20	-5.2
1	B	296	SER	HB3	2.44	2.49 – 5.20	-5.2
1	B	371	PRO	CG	32.94	21.69 – 32.72	5.2

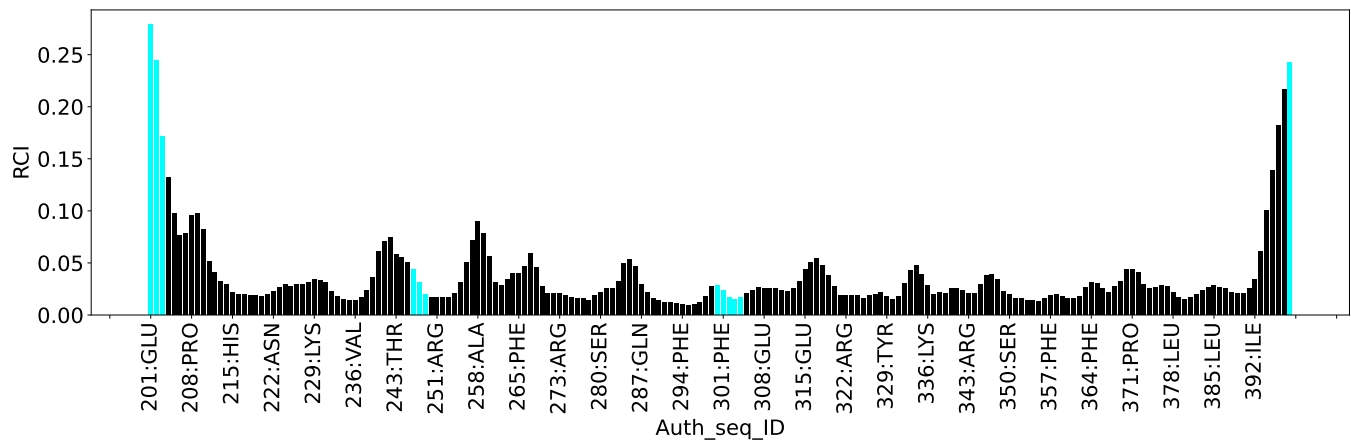
7.1.5 Random Coil Index (RCI) plots

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:



Random coil index (RCI) for chain B:



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	7003
Intra-residue ($ i-j =0$)	3464
Sequential ($ i-j =1$)	1379
Medium range ($ i-j >1$ and $ i-j <5$)	741
Long range ($ i-j \geq 5$)	1316
Inter-chain	103
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	16.7
Number of long range restraints per residue ¹	3.1

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)	118.1	0.2
0.2-0.5 (Medium)	38.5	0.5
>0.5 (Large)	107.7	59.27

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 ⓘ

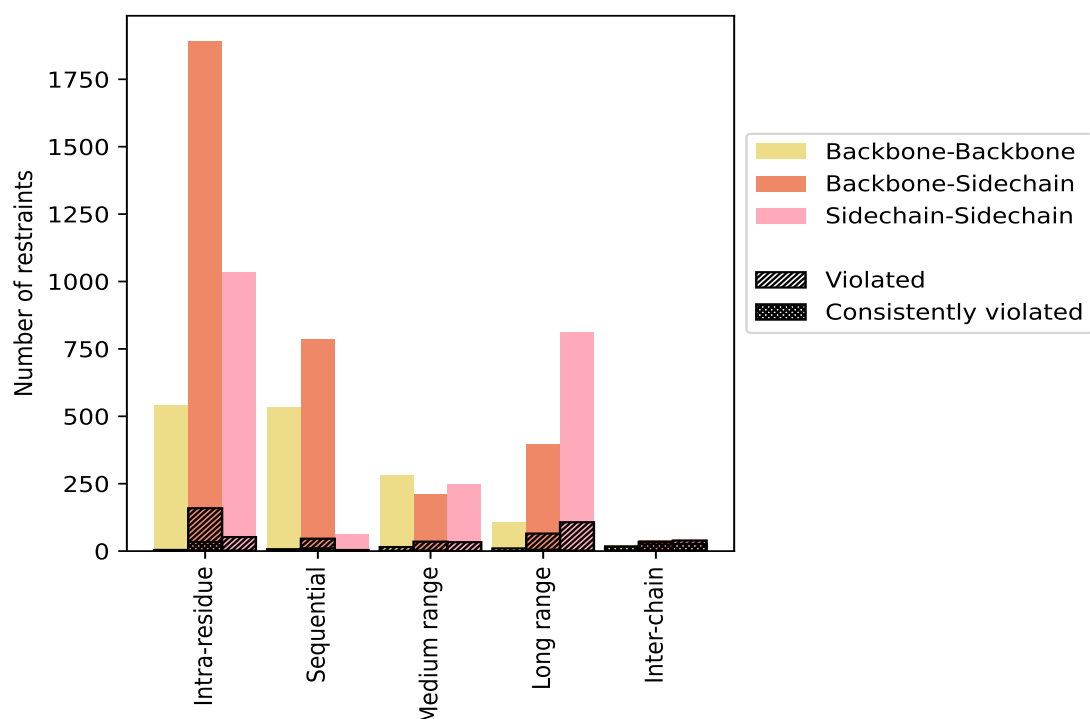
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	3464	49.5	215	6.2	3.1	40	1.2	0.6
Backbone-Backbone	540	7.7	4	0.7	0.1	4	0.7	0.1
Backbone-Sidechain	1891	27.0	159	8.4	2.3	34	1.8	0.5
Sidechain-Sidechain	1033	14.8	52	5.0	0.7	2	0.2	0.0
Sequential ($i-j =1$)	1379	19.7	57	4.1	0.8	12	0.9	0.2
Backbone-Backbone	532	7.6	7	1.3	0.1	2	0.4	0.0
Backbone-Sidechain	785	11.2	46	5.9	0.7	10	1.3	0.1
Sidechain-Sidechain	62	0.9	4	6.5	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	741	10.6	83	11.2	1.2	3	0.4	0.0
Backbone-Backbone	282	4.0	15	5.3	0.2	1	0.4	0.0
Backbone-Sidechain	211	3.0	35	16.6	0.5	2	0.9	0.0
Sidechain-Sidechain	248	3.5	33	13.3	0.5	0	0.0	0.0
Long range ($i-j \geq 5$)	1316	18.8	182	13.8	2.6	7	0.5	0.1
Backbone-Backbone	108	1.5	10	9.3	0.1	0	0.0	0.0
Backbone-Sidechain	397	5.7	65	16.4	0.9	5	1.3	0.1
Sidechain-Sidechain	811	11.6	107	13.2	1.5	2	0.2	0.0
Inter-chain	103	1.5	91	88.3	1.3	75	72.8	1.1
Backbone-Backbone	20	0.3	17	85.0	0.2	16	80.0	0.2
Backbone-Sidechain	39	0.6	35	89.7	0.5	32	82.1	0.5
Sidechain-Sidechain	44	0.6	39	88.6	0.6	27	61.4	0.4
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	7003	100.0	628	9.0	9.0	137	2.0	2.0
Backbone-Backbone	1482	21.2	53	3.6	0.8	23	1.6	0.3
Backbone-Sidechain	3323	47.5	340	10.2	4.9	83	2.5	1.2
Sidechain-Sidechain	2198	31.4	235	10.7	3.4	31	1.4	0.4

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 disulfid 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	98	26	26	52	85	287	5.89	58.17	12.82	0.25
2	96	16	27	56	85	280	6.0	58.88	12.91	0.23
3	92	21	22	57	86	278	6.0	58.94	12.95	0.23
4	102	20	23	54	85	284	5.97	58.95	12.87	0.21
5	91	18	25	42	84	260	6.46	57.57	13.29	0.25
6	101	28	26	48	85	288	5.79	58.96	12.78	0.21
7	110	22	29	60	86	307	5.51	58.8	12.42	0.2
8	98	24	32	53	85	292	5.87	59.27	12.85	0.21
9	90	17	33	41	82	263	6.3	58.77	13.16	0.28
10	92	22	30	39	84	267	6.34	58.65	13.27	0.23

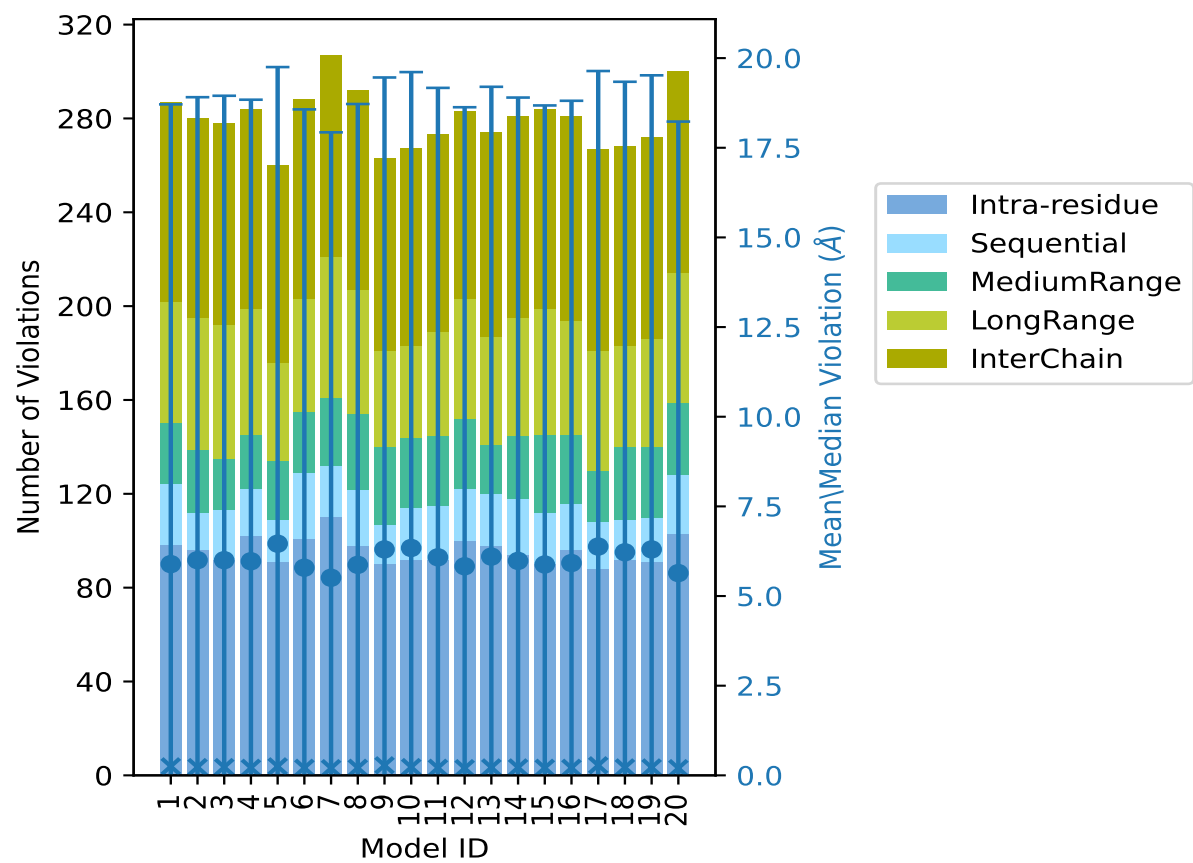
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	92	23	30	44	84	273	6.08	58.47	13.09	0.21
12	100	22	30	51	80	283	5.83	58.32	12.8	0.2
13	98	22	21	46	87	274	6.1	58.93	13.1	0.22
14	94	24	27	50	86	281	5.98	58.61	12.92	0.22
15	90	22	33	54	85	284	5.88	57.58	12.8	0.21
16	96	20	29	49	87	281	5.92	58.88	12.89	0.21
17	88	20	22	51	86	267	6.38	58.88	13.26	0.28
18	92	17	31	43	85	268	6.22	57.55	13.12	0.22
19	91	19	30	46	86	272	6.3	59.23	13.22	0.22
20	103	25	31	55	86	300	5.64	57.67	12.59	0.2

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 ⓘ



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

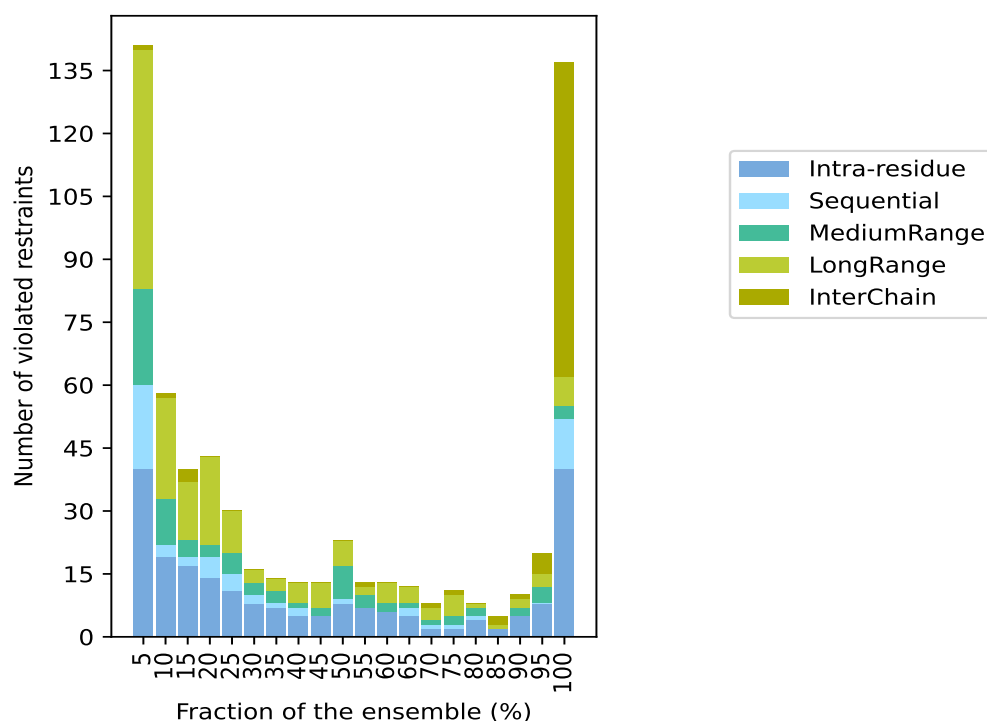
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 6375(IR:3249, SQ:1322, MR:658, LR:1134, IC:12) restraints 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	%
40	20	23	57	1	141	1	5.0
19	3	11	24	1	58	2	10.0
17	2	4	14	3	40	3	15.0
14	5	3	21	0	43	4	20.0
11	4	5	10	0	30	5	25.0
8	2	3	3	0	16	6	30.0
7	1	3	3	0	14	7	35.0
5	2	1	5	0	13	8	40.0
5	0	2	6	0	13	9	45.0
8	1	8	6	0	23	10	50.0
7	0	3	2	1	13	11	55.0
6	0	2	5	0	13	12	60.0
5	2	1	4	0	12	13	65.0
2	1	1	3	1	8	14	70.0
2	1	2	5	1	11	15	75.0
4	1	2	1	0	8	16	80.0
2	0	0	1	2	5	17	85.0
5	0	2	2	1	10	18	90.0
8	0	4	3	5	20	19	95.0
40	12	3	7	75	137	20	100.0

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

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

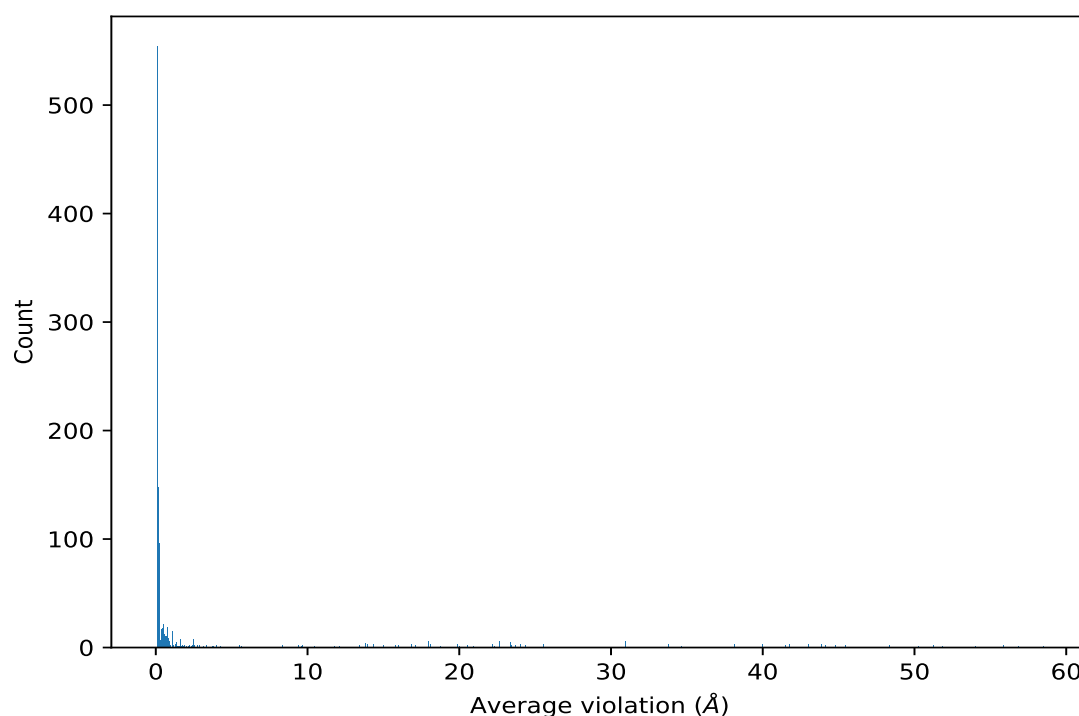
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	20	58.53	0.59	58.78
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	20	56.82	0.59	56.6
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	20	55.87	0.17	55.88
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	20	55.85	0.34	55.96
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	20	54.01	0.35	54.14
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	20	51.82	0.33	51.94
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	20	51.28	0.27	51.24
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	20	51.28	0.27	51.24
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	20	50.3	0.34	50.43
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	20	48.39	0.17	48.41
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	20	48.39	0.17	48.41
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	20	45.46	0.19	45.5
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	20	45.46	0.19	45.5
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	20	44.78	0.2	44.82
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	20	44.78	0.2	44.82
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	20	44.14	0.17	44.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	20	44.14	0.17	44.16
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	20	43.86	0.29	43.94
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	20	43.86	0.29	43.94
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	20	43.86	0.29	43.94
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	20	43.05	0.27	43.12
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	20	43.05	0.27	43.12
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	20	43.05	0.27	43.12
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	20	41.76	0.29	41.84
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	20	41.76	0.29	41.84
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	20	41.76	0.29	41.84
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	20	41.54	0.18	41.51
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	20	41.54	0.18	41.51
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB1	20	39.98	0.29	40.08
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB2	20	39.98	0.29	40.08
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB3	20	39.98	0.29	40.08
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	20	38.13	0.28	38.24
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	20	38.13	0.28	38.24
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	20	38.13	0.28	38.24
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	20	34.62	0.77	34.37
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	20	33.79	0.44	33.94
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	20	33.79	0.44	33.94
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	20	33.79	0.44	33.94
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	20	30.99	0.25	31.04
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	20	30.99	0.25	31.04
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	20	30.99	0.25	31.04
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	20	30.99	0.25	31.04
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	20	30.99	0.25	31.04
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	20	30.99	0.25	31.04
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	20	25.58	0.17	25.58
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	20	25.58	0.17	25.58
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	20	25.58	0.17	25.58
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	20	24.37	1.92	24.84
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	20	24.37	1.92	24.84
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	20	24.0	0.15	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	20	24.0	0.15	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	20	24.0	0.15	24.02
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	20	23.67	0.98	23.48
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	20	23.67	0.98	23.48
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	20	23.44	1.78	23.82
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	20	23.44	1.78	23.82
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	20	23.38	1.65	23.6
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	20	23.37	0.36	23.5

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	20	23.37	0.36	23.5
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	20	23.37	0.36	23.5
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	20	23.37	0.36	23.5
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	20	22.7	0.16	22.74
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	20	22.7	0.16	22.74
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	20	22.7	0.16	22.74
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	20	22.7	0.16	22.74
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	20	22.7	0.16	22.74
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	20	22.7	0.16	22.74
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	20	22.3	1.49	22.66
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	20	22.2	0.75	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	20	22.2	0.75	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	20	22.2	0.75	22.52
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	20	20.91	0.17	20.91
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	20	20.51	0.94	20.21
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	20	20.51	0.94	20.21
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	20	20.02	1.62	20.54
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	20	19.9	0.18	19.93
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	20	19.9	0.18	19.93
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	20	19.9	0.18	19.93
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	20	18.75	0.19	18.74
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	20	18.14	0.15	18.12
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	20	18.14	0.15	18.12
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	20	18.14	0.15	18.12
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	20	17.99	0.16	18.01
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	20	17.99	0.16	18.01
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	20	17.99	0.16	18.01
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	20	17.99	0.16	18.01
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	20	17.99	0.16	18.01
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	20	17.99	0.16	18.01
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	20	17.14	0.19	17.09
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	20	17.14	0.19	17.09
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	20	16.85	1.22	17.28
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	20	16.85	1.22	17.28
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	20	16.85	1.22	17.28
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	20	15.97	0.17	16.02
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	20	15.97	0.17	16.02
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	20	15.82	0.38	15.96
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	20	15.82	0.38	15.96
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	20	15.01	0.56	15.18
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	20	15.01	0.56	15.18
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	20	14.3	0.14	14.3

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	20	14.3	0.14	14.3
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	20	14.3	0.14	14.3
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	20	13.98	0.19	13.97
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	20	13.98	0.19	13.97
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	20	13.98	0.19	13.97
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	20	13.81	0.35	13.96
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	20	13.81	0.35	13.96
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	20	13.81	0.35	13.96
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	20	13.81	0.35	13.96
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	20	13.45	0.15	13.45
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	20	13.45	0.15	13.45
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	20	12.14	0.34	12.24
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	20	11.79	0.27	11.88
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	20	10.47	0.24	10.53
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	20	9.65	0.21	9.63
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	20	9.65	0.21	9.63
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	20	9.59	0.09	9.6
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	20	9.36	0.2	9.35
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	20	9.36	0.2	9.35
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	20	8.35	0.63	8.54
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	20	8.35	0.63	8.54
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	20	5.68	0.67	5.86
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	20	5.51	0.38	5.46
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	20	5.51	0.38	5.46
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	20	4.27	1.13	4.02
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	20	3.95	0.09	3.96
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	20	3.95	0.09	3.96
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	20	3.77	1.19	3.23
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	20	3.74	0.66	3.85
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	20	3.33	1.11	2.92
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	20	3.31	0.62	3.51
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	20	3.16	0.7	3.38
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	20	2.86	1.04	2.55
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	20	2.86	1.04	2.55
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	20	2.8	0.65	2.86
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	20	2.57	0.61	2.7
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	20	2.57	0.61	2.7
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	20	2.55	0.47	2.51
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	20	2.55	0.47	2.51
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	20	2.46	0.53	2.42
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	20	2.46	0.53	2.42
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	20	2.46	0.53	2.42

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	20	2.46	0.53	2.42
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	20	2.45	0.64	2.59
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	20	2.42	0.0	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	20	2.42	0.0	2.42
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	20	2.4	1.53	2.68
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	20	2.21	1.04	1.86
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	20	2.2	0.9	2.02
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	20	2.16	1.16	1.9
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	20	1.89	1.21	1.4
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	20	1.89	1.21	1.4
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	20	1.71	0.52	1.59
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	20	1.44	0.24	1.49
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	20	1.38	0.35	1.53
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	20	1.38	0.35	1.53
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	20	1.37	0.03	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	20	1.37	0.03	1.37
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	20	1.3	1.15	0.7
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	20	1.19	0.13	1.2
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	20	1.19	0.13	1.2
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	20	0.99	0.24	1.04
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	20	0.93	0.21	1.04
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	20	0.93	0.21	1.04
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	20	0.93	0.21	1.04
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	20	0.66	0.01	0.66
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	20	0.66	0.01	0.66
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	20	0.61	0.21	0.57
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	20	0.6	0.09	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	20	0.6	0.09	0.62
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	20	0.56	0.18	0.5
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	20	0.56	0.18	0.5
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	20	0.56	0.18	0.5
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	20	0.48	0.02	0.48
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	20	0.48	0.02	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	20	0.48	0.02	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	20	0.48	0.02	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	20	0.46	0.05	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	20	0.46	0.05	0.46
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	20	0.45	0.01	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	20	0.45	0.01	0.45
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	20	0.43	0.04	0.44
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	20	0.43	0.04	0.44
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	20	0.39	0.2	0.39
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	20	0.36	0.08	0.38
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	20	0.36	0.08	0.38
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	20	0.36	0.08	0.38
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	20	0.3	0.12	0.31
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	20	0.28	0.04	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	20	0.28	0.04	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	20	0.28	0.04	0.28
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	20	0.26	0.07	0.24
(1,6868)	2:404:C:DC:H2''	2:404:C:DC:H5	20	0.25	0.03	0.24
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	20	0.22	0.0	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	20	0.22	0.0	0.22
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	20	0.21	0.06	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	20	0.21	0.06	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	20	0.21	0.06	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	20	0.21	0.01	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	20	0.21	0.01	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	20	0.21	0.01	0.21
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	20	0.2	0.01	0.2
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	20	0.2	0.01	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	20	0.2	0.01	0.21
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	20	0.2	0.0	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	20	0.2	0.0	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	20	0.2	0.01	0.2
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	20	0.19	0.01	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	20	0.19	0.01	0.19
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	20	0.18	0.03	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	20	0.18	0.03	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	20	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	20	0.18	0.0	0.18
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	20	0.17	0.01	0.17
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	20	0.16	0.04	0.15
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	20	0.16	0.04	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	20	0.16	0.04	0.15
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	20	0.16	0.01	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	20	0.16	0.01	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	20	0.16	0.01	0.16
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	20	0.16	0.02	0.16
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	20	0.16	0.02	0.16
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	20	0.14	0.01	0.14
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	20	0.14	0.01	0.14
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	20	0.14	0.01	0.14
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	20	0.13	0.0	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	20	0.13	0.01	0.13
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	20	0.13	0.01	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	20	0.13	0.01	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	20	0.13	0.01	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	20	0.12	0.01	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	20	0.12	0.01	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	20	0.12	0.0	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	20	0.12	0.0	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	20	0.12	0.01	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	20	0.12	0.0	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	20	0.12	0.0	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	20	0.12	0.0	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	20	0.12	0.0	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	20	0.12	0.0	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	20	0.12	0.01	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	20	0.11	0.0	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	20	0.11	0.01	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	20	0.11	0.0	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	20	0.11	0.0	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	20	0.11	0.0	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	20	0.11	0.0	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	20	0.11	0.0	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	20	0.11	0.0	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	20	0.11	0.0	0.11
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	19	2.71	1.25	2.92
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	19	2.71	1.25	2.92
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	19	2.34	0.88	2.54
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	19	2.04	0.82	2.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	19	1.79	0.8	1.85
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	19	1.79	0.8	1.85
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	19	1.54	1.18	1.05
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	19	0.87	0.19	0.93
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	19	0.87	0.19	0.93
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	19	0.87	0.19	0.93
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	19	0.75	0.17	0.76
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	19	0.75	0.17	0.76
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	19	0.75	0.17	0.76
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	19	0.51	0.17	0.54
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	19	0.42	0.1	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	19	0.42	0.1	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	19	0.42	0.1	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	19	0.42	0.1	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	19	0.42	0.1	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	19	0.42	0.1	0.44
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	19	0.36	0.14	0.37
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	19	0.22	0.06	0.2
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	19	0.22	0.06	0.2
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	19	0.22	0.06	0.2
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	19	0.2	0.01	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	19	0.2	0.01	0.2
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	19	0.14	0.02	0.15
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	19	0.12	0.0	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	19	0.12	0.0	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	19	0.12	0.0	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	19	0.12	0.01	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	19	0.12	0.0	0.12
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	19	0.11	0.01	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	19	0.11	0.0	0.11
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	18	1.82	1.57	0.78
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	18	0.82	0.21	0.82
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	18	0.82	0.21	0.82
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	18	0.82	0.21	0.82
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	18	0.63	0.2	0.63
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	18	0.63	0.2	0.63
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	18	0.63	0.2	0.63
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	18	0.52	0.18	0.62
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	18	0.42	0.03	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	18	0.42	0.03	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	18	0.42	0.03	0.42
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	18	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	18	0.16	0.02	0.16
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	18	0.15	0.02	0.15
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	18	0.14	0.01	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	18	0.14	0.01	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	18	0.14	0.01	0.14
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	18	0.12	0.0	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	18	0.12	0.0	0.12
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	17	2.46	0.99	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	17	2.46	0.99	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	17	2.46	0.99	2.62
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	17	1.3	0.58	1.45
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	17	1.3	0.58	1.45
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	17	1.09	0.48	1.06
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	17	1.09	0.48	1.06
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	17	1.09	0.48	1.06
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	17	0.15	0.02	0.14
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	17	0.12	0.0	0.12
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	16	0.66	0.34	0.62
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	16	0.66	0.34	0.62
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	16	0.66	0.34	0.62
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	16	0.15	0.03	0.16
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	16	0.14	0.02	0.13
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	16	0.14	0.02	0.14
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	16	0.14	0.02	0.14
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	16	0.14	0.02	0.14
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	16	0.12	0.01	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	16	0.12	0.0	0.12
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	16	0.11	0.0	0.11
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	16	0.1	0.0	0.1
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	15	1.07	0.05	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	15	1.07	0.05	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	15	1.07	0.05	1.06
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	15	0.63	0.26	0.62
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	15	0.63	0.26	0.62
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	15	0.63	0.26	0.62
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	15	0.62	0.23	0.72
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	15	0.54	0.26	0.47
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	15	0.54	0.26	0.47
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	15	0.54	0.26	0.47
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	15	0.47	0.19	0.49
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	15	0.47	0.19	0.49
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	15	0.47	0.19	0.49

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	15	0.47	0.19	0.49
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	15	0.4	0.04	0.4
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	15	0.4	0.04	0.4
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	15	0.21	0.03	0.21
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	15	0.21	0.03	0.21
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	15	0.2	0.07	0.19
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	15	0.16	0.03	0.16
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	15	0.15	0.02	0.15
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	15	0.15	0.02	0.15
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	15	0.15	0.02	0.15
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	15	0.11	0.0	0.11
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	14	1.65	0.76	1.96
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	14	1.65	0.76	1.96
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	14	0.79	0.27	0.97
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	14	0.79	0.27	0.97
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	14	0.79	0.27	0.97
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	14	0.79	0.27	0.97
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	14	0.79	0.27	0.97
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	14	0.79	0.27	0.97
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	14	0.39	0.2	0.4
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	14	0.39	0.2	0.4
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	14	0.39	0.2	0.4
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	14	0.39	0.2	0.4
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	14	0.39	0.2	0.4
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	14	0.39	0.2	0.4
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	14	0.29	0.1	0.31
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	14	0.22	0.07	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	14	0.22	0.07	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	14	0.22	0.07	0.26
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	14	0.15	0.04	0.15
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	14	0.15	0.04	0.15
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	14	0.15	0.04	0.15
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	14	0.14	0.03	0.13
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	14	0.14	0.03	0.13
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	14	0.14	0.03	0.13
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	14	0.1	0.0	0.1
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	13	0.47	0.24	0.55
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	13	0.47	0.24	0.55
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	13	0.47	0.24	0.55
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	13	0.29	0.0	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	13	0.29	0.0	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	13	0.29	0.0	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	13	0.26	0.17	0.17
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	13	0.19	0.05	0.21
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	13	0.15	0.04	0.15
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	13	0.15	0.03	0.15
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	13	0.15	0.03	0.15
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	13	0.15	0.03	0.15
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	13	0.15	0.02	0.15
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	13	0.15	0.03	0.14
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	13	0.15	0.03	0.14
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	13	0.15	0.03	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	13	0.14	0.01	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	13	0.14	0.01	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	13	0.14	0.01	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	13	0.14	0.01	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	13	0.14	0.01	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	13	0.14	0.01	0.14
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	13	0.12	0.01	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	13	0.12	0.02	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	13	0.12	0.02	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	13	0.12	0.02	0.12
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	13	0.12	0.02	0.11
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	13	0.12	0.02	0.11
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	12	0.36	0.14	0.3
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	12	0.36	0.14	0.3
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	12	0.36	0.14	0.3
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	12	0.34	0.1	0.35
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	12	0.34	0.1	0.35
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	12	0.28	0.1	0.26
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	12	0.28	0.1	0.26
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	12	0.2	0.02	0.2
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	12	0.2	0.02	0.2
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	12	0.17	0.07	0.15
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	12	0.17	0.05	0.16
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	12	0.17	0.04	0.16
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	12	0.15	0.04	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	12	0.15	0.04	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	12	0.15	0.04	0.14
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	12	0.15	0.02	0.15
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	12	0.15	0.02	0.15
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	12	0.15	0.02	0.15
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	12	0.13	0.03	0.12
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	12	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	12	0.11	0.01	0.11
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	12	0.1	0.0	0.1
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	11	0.7	0.0	0.7
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	11	0.37	0.22	0.32
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	11	0.37	0.22	0.32
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	11	0.34	0.11	0.37
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	11	0.34	0.11	0.37
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	11	0.34	0.11	0.37
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	11	0.27	0.09	0.28
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	11	0.27	0.09	0.28
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	11	0.27	0.09	0.28
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	11	0.27	0.09	0.28
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	11	0.27	0.09	0.28
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	11	0.27	0.09	0.28
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	11	0.16	0.04	0.15
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	11	0.16	0.04	0.15
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	11	0.16	0.04	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	11	0.16	0.02	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	11	0.16	0.02	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	11	0.16	0.02	0.15
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	11	0.15	0.03	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	11	0.15	0.03	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	11	0.13	0.03	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	11	0.13	0.03	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	11	0.13	0.03	0.13
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	11	0.12	0.0	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	11	0.12	0.0	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	11	0.12	0.0	0.12
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	11	0.1	0.0	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	11	0.1	0.0	0.1
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	10	1.59	0.01	1.58
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	10	1.09	0.04	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	10	1.09	0.04	1.1
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	10	0.5	0.36	0.34
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	10	0.41	0.24	0.32
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	10	0.4	0.21	0.38
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	10	0.35	0.06	0.36
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	10	0.31	0.15	0.3
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	10	0.29	0.02	0.3
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	10	0.29	0.02	0.3
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	10	0.29	0.02	0.3
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	10	0.2	0.03	0.21
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	10	0.17	0.03	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	10	0.17	0.03	0.16
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	10	0.16	0.04	0.18
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	10	0.16	0.02	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	10	0.16	0.03	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	10	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	10	0.16	0.03	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	10	0.16	0.03	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	10	0.16	0.03	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	10	0.16	0.03	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	10	0.16	0.03	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	10	0.16	0.03	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	10	0.16	0.03	0.16
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	10	0.15	0.03	0.15
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	10	0.15	0.02	0.15
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	10	0.15	0.02	0.15
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	10	0.15	0.02	0.15
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	10	0.15	0.03	0.14
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	10	0.15	0.03	0.14
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	10	0.14	0.03	0.13
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	10	0.14	0.03	0.13
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	10	0.14	0.03	0.13
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	10	0.14	0.03	0.13
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	10	0.14	0.03	0.13
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	10	0.14	0.03	0.13
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	10	0.14	0.01	0.14
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	10	0.14	0.01	0.14
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	10	0.13	0.02	0.13
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	10	0.11	0.01	0.12
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	10	0.11	0.0	0.11
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	10	0.1	0.0	0.1
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	9	0.29	0.07	0.32
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	9	0.23	0.03	0.23
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	9	0.23	0.03	0.23

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	9	0.18	0.03	0.18
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	9	0.18	0.03	0.18
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	9	0.18	0.03	0.18
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	9	0.15	0.03	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	9	0.15	0.03	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	9	0.15	0.03	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	9	0.15	0.03	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	9	0.15	0.03	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	9	0.15	0.03	0.14
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	9	0.15	0.02	0.14
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	9	0.15	0.02	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	9	0.14	0.02	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	9	0.14	0.02	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	9	0.14	0.02	0.14
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	9	0.14	0.02	0.14
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	9	0.13	0.02	0.12
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	9	0.13	0.02	0.12
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	9	0.13	0.02	0.12
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	9	0.12	0.02	0.12
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	9	0.12	0.01	0.12
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	9	0.11	0.0	0.11
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	9	0.1	0.0	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	9	0.1	0.0	0.1
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	8	0.23	0.11	0.18
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	8	0.22	0.04	0.22
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	8	0.22	0.04	0.22
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	8	0.22	0.04	0.22
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	8	0.2	0.05	0.21
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	8	0.2	0.04	0.2
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	8	0.2	0.04	0.2
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	8	0.16	0.04	0.15
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	8	0.16	0.04	0.15
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	8	0.16	0.04	0.15
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	8	0.15	0.03	0.16
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	8	0.14	0.01	0.14
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	8	0.13	0.02	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	8	0.13	0.02	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	8	0.13	0.02	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	8	0.13	0.01	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	8	0.13	0.01	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	8	0.13	0.01	0.13
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	8	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	8	0.12	0.02	0.12
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	8	0.12	0.02	0.12
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	8	0.12	0.01	0.12
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	8	0.11	0.0	0.11
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	8	0.1	0.01	0.1
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	7	0.7	0.03	0.7
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	7	0.17	0.04	0.19
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	7	0.16	0.02	0.17
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	7	0.16	0.04	0.14
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	7	0.16	0.04	0.14
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	7	0.15	0.03	0.15
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	7	0.15	0.03	0.15
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	7	0.13	0.02	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	7	0.13	0.02	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	7	0.13	0.02	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	7	0.13	0.02	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	7	0.13	0.02	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	7	0.13	0.02	0.13
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	7	0.13	0.01	0.14
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	7	0.12	0.0	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	7	0.12	0.01	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	7	0.12	0.01	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	7	0.12	0.01	0.12
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	7	0.12	0.01	0.12
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	7	0.12	0.0	0.12
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	7	0.11	0.01	0.11
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	7	0.1	0.0	0.1
(1,3063)	1:382:B:SER:HB2	1:382:B:SER:H	6	0.7	0.01	0.7
(1,4619)	1:76:A:LEU:HD11	1:94:A:TRP:HZ3	6	0.24	0.1	0.21
(1,4619)	1:76:A:LEU:HD12	1:94:A:TRP:HZ3	6	0.24	0.1	0.21
(1,4619)	1:76:A:LEU:HD13	1:94:A:TRP:HZ3	6	0.24	0.1	0.21
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD21	6	0.22	0.08	0.19
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD22	6	0.22	0.08	0.19
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD23	6	0.22	0.08	0.19
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD21	6	0.22	0.08	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD22	6	0.22	0.08	0.19
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD23	6	0.22	0.08	0.19
(1,3886)	1:36:A:GLU:HA	1:93:A:THR:HB	6	0.22	0.07	0.23
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD11	6	0.19	0.04	0.2
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD12	6	0.19	0.04	0.2
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD13	6	0.19	0.04	0.2
(1,2346)	1:335:B:TYR:HE1	1:335:B:TYR:H	6	0.15	0.03	0.16
(1,2346)	1:335:B:TYR:HE2	1:335:B:TYR:H	6	0.15	0.03	0.16
(1,1708)	1:295:B:ILE:HD11	1:296:B:SER:H	6	0.15	0.03	0.14
(1,1708)	1:295:B:ILE:HD12	1:296:B:SER:H	6	0.15	0.03	0.14
(1,1708)	1:295:B:ILE:HD13	1:296:B:SER:H	6	0.15	0.03	0.14
(1,4968)	1:91:A:ARG:HB3	1:91:A:ARG:H	6	0.14	0.02	0.14
(1,6035)	1:155:A:TYR:HE1	1:155:A:TYR:H	6	0.14	0.03	0.14
(1,6035)	1:155:A:TYR:HE2	1:155:A:TYR:H	6	0.14	0.03	0.14
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD11	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD12	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD13	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD21	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD22	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD23	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD11	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD12	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD13	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD21	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD22	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD23	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD11	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD12	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD13	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD21	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD22	6	0.13	0.02	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD23	6	0.13	0.02	0.12
(1,2901)	1:372:B:PHE:HZ	1:375:B:TRP:H	6	0.13	0.02	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD11	6	0.12	0.01	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD12	6	0.12	0.01	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD13	6	0.12	0.01	0.12
(1,2638)	1:354:B:TYR:HD1	1:355:B:ASP:H	6	0.11	0.01	0.11
(1,2638)	1:354:B:TYR:HD2	1:355:B:ASP:H	6	0.11	0.01	0.11
(1,3456)	1:7:A:SER:HA	1:7:A:SER:HB2	6	0.11	0.0	0.11
(1,6487)	1:184:A:GLN:HE21	1:184:A:GLN:HE22	6	0.1	0.0	0.1
(1,6697)	1:197:A:GLN:HB3	1:197:A:GLN:H	6	0.1	0.0	0.1
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD21	5	0.91	0.18	0.94

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD22	5	0.91	0.18	0.94
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD23	5	0.91	0.18	0.94
(1,319)	1:221:B:PHE:HE1	1:296:B:SER:H	5	0.86	0.39	1.16
(1,319)	1:221:B:PHE:HE2	1:296:B:SER:H	5	0.86	0.39	1.16
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG21	5	0.24	0.08	0.18
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG22	5	0.24	0.08	0.18
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG23	5	0.24	0.08	0.18
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG21	5	0.24	0.08	0.18
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG22	5	0.24	0.08	0.18
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG23	5	0.24	0.08	0.18
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD1	5	0.21	0.09	0.16
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD2	5	0.21	0.09	0.16
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD1	5	0.21	0.09	0.16
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD2	5	0.21	0.09	0.16
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD1	5	0.21	0.09	0.16
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD2	5	0.21	0.09	0.16
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD11	5	0.2	0.02	0.21
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD12	5	0.2	0.02	0.21
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD13	5	0.2	0.02	0.21
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG21	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG22	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG23	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG21	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG22	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG23	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG21	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG22	5	0.2	0.07	0.18
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG23	5	0.2	0.07	0.18
(1,910)	1:254:B:LEU:HD21	1:274:B:PHE:HA	5	0.18	0.08	0.14
(1,910)	1:254:B:LEU:HD22	1:274:B:PHE:HA	5	0.18	0.08	0.14
(1,910)	1:254:B:LEU:HD23	1:274:B:PHE:HA	5	0.18	0.08	0.14
(1,5856)	1:143:A:LEU:HD21	1:146:A:ALA:H	5	0.17	0.04	0.17
(1,5856)	1:143:A:LEU:HD22	1:146:A:ALA:H	5	0.17	0.04	0.17
(1,5856)	1:143:A:LEU:HD23	1:146:A:ALA:H	5	0.17	0.04	0.17
(1,4265)	1:52:A:ARG:HG3	1:53:A:GLY:H	5	0.17	0.02	0.17
(1,6367)	1:176:A:TRP:HB2	1:177:A:ASP:H	5	0.17	0.04	0.17
(1,4015)	1:39:A:ARG:H	1:47:A:LYS:HA	5	0.16	0.04	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD11	5	0.15	0.02	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD12	5	0.15	0.02	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD13	5	0.15	0.02	0.14
(1,3089)	1:383:B:GLN:HA	1:386:B:SER:H	5	0.15	0.04	0.16
(1,1231)	1:275:B:LEU:HD11	1:312:B:PHE:HZ	5	0.13	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1231)	1:275:B:LEU:HD12	1:312:B:PHE:HZ	5	0.13	0.02	0.14
(1,1231)	1:275:B:LEU:HD13	1:312:B:PHE:HZ	5	0.13	0.02	0.14
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD11	5	0.13	0.03	0.13
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD12	5	0.13	0.03	0.13
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD13	5	0.13	0.03	0.13
(1,6348)	1:175:A:PRO:HA	1:179:A:LEU:HG	5	0.13	0.02	0.12
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD21	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD22	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD23	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD21	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD22	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD23	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD21	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD22	5	0.13	0.02	0.13
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD23	5	0.13	0.02	0.13
(1,3086)	1:383:B:GLN:H	1:383:B:GLN:HE21	5	0.12	0.01	0.12
(1,4173)	1:47:A:LYS:HG3	1:47:A:LYS:HD3	5	0.12	0.0	0.12
(1,5446)	1:116:A:GLU:HA	1:116:A:GLU:HB3	5	0.12	0.0	0.12
(1,6687)	1:196:A:ASN:HD22	1:196:A:ASN:H	5	0.12	0.01	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG11	5	0.12	0.0	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG12	5	0.12	0.0	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG13	5	0.12	0.0	0.12
(1,2574)	1:351:B:ILE:HB	1:351:B:ILE:H	5	0.12	0.01	0.12
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD21	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD22	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD23	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD21	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD22	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD23	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD21	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD22	5	0.11	0.01	0.11
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD23	5	0.11	0.01	0.11
(1,2347)	1:335:B:TYR:HD1	1:336:B:LYS:H	5	0.11	0.01	0.11
(1,2347)	1:335:B:TYR:HD2	1:336:B:LYS:H	5	0.11	0.01	0.11
(1,2978)	1:376:B:ASP:HB2	1:376:B:ASP:H	5	0.11	0.0	0.11
(1,138)	1:212:B:MET:HB2	1:212:B:MET:H	5	0.11	0.0	0.11
(1,3689)	1:19:A:THR:HB	1:19:A:THR:H	5	0.1	0.0	0.1
(1,1427)	1:283:B:LEU:HB3	1:283:B:LEU:H	5	0.1	0.0	0.1
(1,2409)	1:340:B:GLN:HE21	1:340:B:GLN:HE22	5	0.1	0.0	0.1
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE1	4	1.65	0.63	1.58
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE2	4	1.65	0.63	1.58
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE3	4	1.65	0.63	1.58

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE1	4	1.65	0.63	1.58
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE2	4	1.65	0.63	1.58
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE3	4	1.65	0.63	1.58
(1,573)	1:237:B:GLU:HG2	1:290:B:ARG:HB3	4	0.98	0.27	1.12
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG21	4	0.64	0.47	0.64
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG22	4	0.64	0.47	0.64
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG23	4	0.64	0.47	0.64
(1,316)	1:221:B:PHE:HD1	1:296:B:SER:H	4	0.53	0.27	0.58
(1,316)	1:221:B:PHE:HD2	1:296:B:SER:H	4	0.53	0.27	0.58
(1,3560)	1:13:A:MET:HE1	1:14:A:ASP:H	4	0.3	0.08	0.3
(1,3560)	1:13:A:MET:HE2	1:14:A:ASP:H	4	0.3	0.08	0.3
(1,3560)	1:13:A:MET:HE3	1:14:A:ASP:H	4	0.3	0.08	0.3
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD21	4	0.19	0.06	0.16
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD22	4	0.19	0.06	0.16
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD23	4	0.19	0.06	0.16
(1,2727)	1:361:B:TRP:HB2	1:361:B:TRP:H	4	0.18	0.04	0.18
(1,6479)	1:184:A:GLN:HB2	1:184:A:GLN:HE21	4	0.18	0.02	0.18
(1,6479)	1:184:A:GLN:HB3	1:184:A:GLN:HE21	4	0.18	0.02	0.18
(1,6056)	1:155:A:TYR:H	1:179:A:LEU:HG	4	0.16	0.03	0.16
(1,3292)	1:396:B:GLN:HA	1:396:B:GLN:HG2	4	0.16	0.01	0.16
(1,1447)	1:283:B:LEU:HD21	1:318:B:HIS:HD2	4	0.15	0.02	0.16
(1,1447)	1:283:B:LEU:HD22	1:318:B:HIS:HD2	4	0.15	0.02	0.16
(1,1447)	1:283:B:LEU:HD23	1:318:B:HIS:HD2	4	0.15	0.02	0.16
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG11	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG12	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG13	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG11	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG12	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG13	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG11	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG12	4	0.14	0.04	0.14
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG13	4	0.14	0.04	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD11	4	0.14	0.02	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD12	4	0.14	0.02	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD13	4	0.14	0.02	0.14
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD11	4	0.14	0.03	0.14
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD12	4	0.14	0.03	0.14
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD13	4	0.14	0.03	0.14
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD11	4	0.14	0.03	0.14
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD12	4	0.14	0.03	0.14
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD13	4	0.14	0.03	0.14
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD11	4	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD12	4	0.14	0.03	0.14
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD13	4	0.14	0.03	0.14
(1,2586)	1:351:B:ILE:HG21	1:352:B:MET:H	4	0.14	0.01	0.14
(1,2586)	1:351:B:ILE:HG22	1:352:B:MET:H	4	0.14	0.01	0.14
(1,2586)	1:351:B:ILE:HG23	1:352:B:MET:H	4	0.14	0.01	0.14
(1,2594)	1:351:B:ILE:HD11	1:352:B:MET:H	4	0.14	0.03	0.14
(1,2594)	1:351:B:ILE:HD12	1:352:B:MET:H	4	0.14	0.03	0.14
(1,2594)	1:351:B:ILE:HD13	1:352:B:MET:H	4	0.14	0.03	0.14
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD11	4	0.14	0.02	0.14
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD12	4	0.14	0.02	0.14
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD13	4	0.14	0.02	0.14
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG11	4	0.13	0.01	0.13
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG12	4	0.13	0.01	0.13
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG13	4	0.13	0.01	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD11	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD12	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD13	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD11	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD12	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD13	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD11	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD12	4	0.13	0.0	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD13	4	0.13	0.0	0.13
(1,5815)	1:141:A:GLN:HE21	1:193:A:ILE:HG21	4	0.13	0.01	0.14
(1,6650)	1:194:A:LEU:HB2	1:195:A:GLN:H	4	0.13	0.02	0.12
(1,2104)	1:318:B:HIS:HE1	1:318:B:HIS:H	4	0.13	0.02	0.12
(1,411)	1:232:B:LEU:HD11	1:274:B:PHE:HZ	4	0.12	0.02	0.12
(1,411)	1:232:B:LEU:HD12	1:274:B:PHE:HZ	4	0.12	0.02	0.12
(1,411)	1:232:B:LEU:HD13	1:274:B:PHE:HZ	4	0.12	0.02	0.12
(1,411)	1:232:B:LEU:HD21	1:274:B:PHE:HZ	4	0.12	0.02	0.12
(1,411)	1:232:B:LEU:HD22	1:274:B:PHE:HZ	4	0.12	0.02	0.12
(1,411)	1:232:B:LEU:HD23	1:274:B:PHE:HZ	4	0.12	0.02	0.12
(1,5800)	1:140:A:LEU:H	1:193:A:ILE:HG22	4	0.12	0.01	0.12
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG11	4	0.12	0.02	0.12
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG12	4	0.12	0.02	0.12
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG13	4	0.12	0.02	0.12
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG11	4	0.12	0.02	0.12
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG12	4	0.12	0.02	0.12
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG13	4	0.12	0.02	0.12
(1,157)	1:212:B:MET:HE1	1:233:B:CYS:HB3	4	0.12	0.02	0.11
(1,157)	1:212:B:MET:HE2	1:233:B:CYS:HB3	4	0.12	0.02	0.11
(1,157)	1:212:B:MET:HE3	1:233:B:CYS:HB3	4	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE1	4	0.12	0.02	0.11
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE2	4	0.12	0.02	0.11
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE1	4	0.12	0.02	0.11
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE2	4	0.12	0.02	0.11
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE1	4	0.12	0.02	0.11
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE2	4	0.12	0.02	0.11
(1,2456)	1:342:B:LEU:HD11	1:347:B:ALA:H	4	0.12	0.01	0.12
(1,2456)	1:342:B:LEU:HD12	1:347:B:ALA:H	4	0.12	0.01	0.12
(1,2456)	1:342:B:LEU:HD13	1:347:B:ALA:H	4	0.12	0.01	0.12
(1,4009)	1:39:A:ARG:HG2	1:88:A:GLN:HB2	4	0.11	0.01	0.11
(1,5103)	1:96:A:ILE:HG21	1:97:A:SER:H	4	0.11	0.01	0.11
(1,5103)	1:96:A:ILE:HG22	1:97:A:SER:H	4	0.11	0.01	0.11
(1,5103)	1:96:A:ILE:HG23	1:97:A:SER:H	4	0.11	0.01	0.11
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG11	4	0.11	0.01	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG12	4	0.11	0.01	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG13	4	0.11	0.01	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG21	4	0.11	0.01	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG22	4	0.11	0.01	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG23	4	0.11	0.01	0.12
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD1	4	0.11	0.01	0.11
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD2	4	0.11	0.01	0.11
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD1	4	0.11	0.01	0.11
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD2	4	0.11	0.01	0.11
(1,4404)	1:62:A:LEU:HB3	1:62:A:LEU:H	4	0.11	0.0	0.11
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD11	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD12	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD13	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD11	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD12	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD13	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD11	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD12	4	0.11	0.01	0.11
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD13	4	0.11	0.01	0.11
(1,2583)	1:351:B:ILE:HD11	1:351:B:ILE:H	4	0.11	0.01	0.11
(1,2583)	1:351:B:ILE:HD12	1:351:B:ILE:H	4	0.11	0.01	0.11
(1,2583)	1:351:B:ILE:HD13	1:351:B:ILE:H	4	0.11	0.01	0.11
(1,76)	1:209:B:ARG:HA	1:209:B:ARG:HB3	4	0.11	0.0	0.11
(1,3077)	1:383:B:GLN:HB2	1:383:B:GLN:HE21	4	0.11	0.0	0.11
(1,3077)	1:383:B:GLN:HB3	1:383:B:GLN:HE21	4	0.11	0.0	0.11
(1,944)	1:256:B:ASN:HD21	1:256:B:ASN:HD22	4	0.1	0.0	0.1
(1,2034)	1:314:B:GLN:HE21	1:314:B:GLN:HE22	4	0.1	0.0	0.1
(1,4347)	1:57:A:ASN:HD21	1:57:A:ASN:HD22	4	0.1	0.0	0.1

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,5436)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	4	0.1	0.0	0.1
(1,5812)	1:141:A:GLN:HE21	1:141:A:GLN:HE22	4	0.1	0.0	0.1
(1,6683)	1:196:A:ASN:HB2	1:196:A:ASN:HD21	4	0.1	0.0	0.1
(1,322)	1:221:B:PHE:HZ	1:296:B:SER:H	3	1.39	0.54	1.11
(1,321)	1:221:B:PHE:HZ	1:233:B:CYS:H	3	0.75	0.67	0.44
(1,522)	1:236:B:VAL:HG11	1:289:B:TYR:HA	3	0.66	0.12	0.68
(1,522)	1:236:B:VAL:HG12	1:289:B:TYR:HA	3	0.66	0.12	0.68
(1,522)	1:236:B:VAL:HG13	1:289:B:TYR:HA	3	0.66	0.12	0.68
(1,473)	1:234:B:TYR:H	1:364:B:PHE:HE1	3	0.24	0.05	0.21
(1,4247)	1:52:A:ARG:HB3	1:52:A:ARG:H	3	0.23	0.02	0.23
(1,6965)	1:209:B:ARG:HA	1:53:A:GLY:HA2	3	0.23	0.03	0.24
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD11	3	0.21	0.0	0.21
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD12	3	0.21	0.0	0.21
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD13	3	0.21	0.0	0.21
(1,884)	1:253:B:PHE:HD1	1:253:B:PHE:H	3	0.21	0.04	0.21
(1,884)	1:253:B:PHE:HD2	1:253:B:PHE:H	3	0.21	0.04	0.21
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD21	3	0.2	0.0	0.2
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD22	3	0.2	0.0	0.2
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD23	3	0.2	0.0	0.2
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB1	3	0.19	0.07	0.2
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB2	3	0.19	0.07	0.2
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB3	3	0.19	0.07	0.2
(1,361)	1:227:B:ARG:HE	1:227:B:ARG:H	3	0.19	0.03	0.21
(1,2321)	1:333:B:PRO:HB2	1:334:B:LEU:H	3	0.18	0.05	0.21
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG21	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG22	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG23	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG21	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG22	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG23	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG21	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG22	3	0.17	0.06	0.18
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG23	3	0.17	0.06	0.18
(1,6032)	1:155:A:TYR:HB2	1:155:A:TYR:H	3	0.16	0.01	0.17
(1,6120)	1:161:A:CYS:HG	1:161:A:CYS:H	3	0.16	0.03	0.15
(1,3541)	1:12:A:LEU:HD21	1:169:A:GLN:HE21	3	0.16	0.02	0.15
(1,3541)	1:12:A:LEU:HD22	1:169:A:GLN:HE21	3	0.16	0.02	0.15
(1,3541)	1:12:A:LEU:HD23	1:169:A:GLN:HE21	3	0.16	0.02	0.15
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB2	3	0.15	0.03	0.15
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB3	3	0.15	0.03	0.15
(1,5506)	1:119:A:HIS:HE1	1:119:A:HIS:H	3	0.15	0.04	0.13
(1,6694)	1:197:A:GLN:HA	1:197:A:GLN:HG2	3	0.15	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6321)	1:174:A:GLN:HB3	1:174:A:GLN:H	3	0.14	0.02	0.13
(1,1750)	1:300:B:CYS:H	1:301:B:PHE:H	3	0.13	0.02	0.14
(1,2600)	1:351:B:ILE:HD11	1:389:B:LEU:H	3	0.13	0.01	0.13
(1,2600)	1:351:B:ILE:HD12	1:389:B:LEU:H	3	0.13	0.01	0.13
(1,2600)	1:351:B:ILE:HD13	1:389:B:LEU:H	3	0.13	0.01	0.13
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE1	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE2	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE3	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE1	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE2	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE3	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE1	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE2	3	0.13	0.02	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE3	3	0.13	0.02	0.11
(1,2919)	1:373:B:GLN:HB3	1:373:B:GLN:H	3	0.13	0.0	0.13
(1,286)	1:218:B:THR:HG21	1:361:B:TRP:HZ2	3	0.12	0.01	0.13
(1,286)	1:218:B:THR:HG22	1:361:B:TRP:HZ2	3	0.12	0.01	0.13
(1,286)	1:218:B:THR:HG23	1:361:B:TRP:HZ2	3	0.12	0.01	0.13
(1,472)	1:234:B:TYR:H	1:364:B:PHE:HD1	3	0.12	0.01	0.12
(1,660)	1:239:B:LEU:HD21	1:244:B:SER:HB2	3	0.12	0.02	0.11
(1,660)	1:239:B:LEU:HD22	1:244:B:SER:HB2	3	0.12	0.02	0.11
(1,660)	1:239:B:LEU:HD23	1:244:B:SER:HB2	3	0.12	0.02	0.11
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB2	3	0.12	0.01	0.12
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB3	3	0.12	0.01	0.12
(1,471)	1:234:B:TYR:H	1:254:B:LEU:H	3	0.12	0.0	0.12
(1,2044)	1:315:B:GLU:HA	1:315:B:GLU:HB3	3	0.12	0.0	0.12
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD11	3	0.12	0.01	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD12	3	0.12	0.01	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD13	3	0.12	0.01	0.11
(1,6251)	1:169:A:GLN:HB3	1:169:A:GLN:HE22	3	0.12	0.02	0.12
(1,4353)	1:58:A:GLN:HA	1:58:A:GLN:HB2	3	0.12	0.0	0.12
(1,5330)	1:112:A:ALA:HB1	1:115:A:GLN:HE21	3	0.11	0.0	0.11
(1,5330)	1:112:A:ALA:HB2	1:115:A:GLN:HE21	3	0.11	0.0	0.11
(1,5330)	1:112:A:ALA:HB3	1:115:A:GLN:HE21	3	0.11	0.0	0.11
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD11	3	0.11	0.01	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD12	3	0.11	0.01	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD13	3	0.11	0.01	0.1
(1,1719)	1:296:B:SER:HB3	1:296:B:SER:H	3	0.11	0.0	0.11
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD11	3	0.11	0.01	0.11
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD12	3	0.11	0.01	0.11
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD13	3	0.11	0.01	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG21	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG22	3	0.11	0.0	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG23	3	0.11	0.0	0.11
(1,3295)	1:396:B:GLN:HB3	1:396:B:GLN:H	3	0.1	0.0	0.1
(1,6118)	1:161:A:CYS:HB3	1:161:A:CYS:H	3	0.1	0.0	0.1
(1,2383)	1:339:B:LEU:HD11	1:392:B:ILE:HG12	2	0.8	0.1	0.8
(1,2383)	1:339:B:LEU:HD11	1:392:B:ILE:HG13	2	0.8	0.1	0.8
(1,2383)	1:339:B:LEU:HD12	1:392:B:ILE:HG12	2	0.8	0.1	0.8
(1,2383)	1:339:B:LEU:HD12	1:392:B:ILE:HG13	2	0.8	0.1	0.8
(1,2383)	1:339:B:LEU:HD13	1:392:B:ILE:HG12	2	0.8	0.1	0.8
(1,2383)	1:339:B:LEU:HD13	1:392:B:ILE:HG13	2	0.8	0.1	0.8
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD21	2	0.78	0.23	0.78
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD22	2	0.78	0.23	0.78
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD23	2	0.78	0.23	0.78
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE1	2	0.78	0.48	0.78
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE2	2	0.78	0.48	0.78
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE3	2	0.78	0.48	0.78
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE1	2	0.78	0.48	0.78
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE2	2	0.78	0.48	0.78
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE3	2	0.78	0.48	0.78
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD11	2	0.4	0.21	0.4
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD12	2	0.4	0.21	0.4
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD13	2	0.4	0.21	0.4
(1,6572)	1:191:A:ARG:HB3	1:191:A:ARG:H	2	0.37	0.01	0.37
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD21	2	0.24	0.09	0.24
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD22	2	0.24	0.09	0.24
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD23	2	0.24	0.09	0.24
(1,886)	1:253:B:PHE:HZ	1:253:B:PHE:H	2	0.22	0.0	0.22
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD21	2	0.22	0.01	0.22
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD22	2	0.22	0.01	0.22
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD23	2	0.22	0.01	0.22
(1,554)	1:237:B:GLU:HA	1:290:B:ARG:H	2	0.19	0.0	0.19
(1,5683)	1:129:A:ILE:HG21	1:193:A:ILE:HG21	2	0.19	0.02	0.19
(1,5683)	1:129:A:ILE:HG22	1:193:A:ILE:HG21	2	0.19	0.02	0.19
(1,5683)	1:129:A:ILE:HG23	1:193:A:ILE:HG21	2	0.19	0.02	0.19
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD11	2	0.18	0.06	0.18
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD12	2	0.18	0.06	0.18
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD13	2	0.18	0.06	0.18
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD11	2	0.18	0.06	0.18
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD12	2	0.18	0.06	0.18
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD13	2	0.18	0.06	0.18
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD11	2	0.18	0.06	0.18
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD12	2	0.18	0.06	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD13	2	0.18	0.06	0.18
(1,3767)	1:28:A:ARG:HE	1:28:A:ARG:H	2	0.18	0.08	0.18
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD11	2	0.18	0.0	0.18
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD12	2	0.18	0.0	0.18
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD13	2	0.18	0.0	0.18
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG21	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG22	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG23	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG21	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG22	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG23	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG21	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG22	2	0.17	0.0	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG23	2	0.17	0.0	0.17
(1,5693)	1:129:A:ILE:HD11	1:189:A:ARG:H	2	0.17	0.03	0.17
(1,5693)	1:129:A:ILE:HD12	1:189:A:ARG:H	2	0.17	0.03	0.17
(1,5693)	1:129:A:ILE:HD13	1:189:A:ARG:H	2	0.17	0.03	0.17
(1,6998)	1:11:A:HIS:HB3	1:253:B:PHE:HD1	2	0.16	0.06	0.16
(1,6998)	1:11:A:HIS:HB3	1:253:B:PHE:HD2	2	0.16	0.06	0.16
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG21	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG22	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG23	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG21	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG22	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG23	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG21	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG22	2	0.16	0.02	0.16
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG23	2	0.16	0.02	0.16
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG11	2	0.16	0.02	0.16
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG12	2	0.16	0.02	0.16
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG13	2	0.16	0.02	0.16
(1,6157)	1:162:A:TRP:HZ2	1:171:A:GLN:H	2	0.16	0.02	0.16
(1,2275)	1:328:B:ILE:HG21	1:330:B:ASP:H	2	0.15	0.02	0.15
(1,2275)	1:328:B:ILE:HG22	1:330:B:ASP:H	2	0.15	0.02	0.15
(1,2275)	1:328:B:ILE:HG23	1:330:B:ASP:H	2	0.15	0.02	0.15
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG11	2	0.15	0.03	0.15
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG12	2	0.15	0.03	0.15
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG13	2	0.15	0.03	0.15
(1,655)	1:239:B:LEU:HD11	1:289:B:TYR:HD1	2	0.15	0.03	0.15
(1,655)	1:239:B:LEU:HD11	1:289:B:TYR:HD2	2	0.15	0.03	0.15
(1,655)	1:239:B:LEU:HD12	1:289:B:TYR:HD1	2	0.15	0.03	0.15
(1,655)	1:239:B:LEU:HD12	1:289:B:TYR:HD2	2	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,655)	1:239:B:LEU:HD13	1:289:B:TYR:HD1	2	0.15	0.03	0.15
(1,655)	1:239:B:LEU:HD13	1:289:B:TYR:HD2	2	0.15	0.03	0.15
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD11	2	0.14	0.03	0.14
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD12	2	0.14	0.03	0.14
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD13	2	0.14	0.03	0.14
(1,6224)	1:168:A:HIS:HA	1:168:A:HIS:HD2	2	0.14	0.0	0.14
(1,529)	1:236:B:VAL:HG21	1:290:B:ARG:H	2	0.14	0.01	0.14
(1,529)	1:236:B:VAL:HG22	1:290:B:ARG:H	2	0.14	0.01	0.14
(1,529)	1:236:B:VAL:HG23	1:290:B:ARG:H	2	0.14	0.01	0.14
(1,2590)	1:351:B:ILE:HG21	1:385:B:LEU:H	2	0.14	0.01	0.14
(1,2590)	1:351:B:ILE:HG22	1:385:B:LEU:H	2	0.14	0.01	0.14
(1,2590)	1:351:B:ILE:HG23	1:385:B:LEU:H	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE1	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE2	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE3	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE1	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE2	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE3	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE1	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE2	2	0.14	0.01	0.14
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE3	2	0.14	0.01	0.14
(1,6050)	1:155:A:TYR:HE1	1:173:A:PHE:HZ	2	0.14	0.01	0.14
(1,6050)	1:155:A:TYR:HE2	1:173:A:PHE:HZ	2	0.14	0.01	0.14
(1,6491)	1:184:A:GLN:HA	1:187:A:SER:H	2	0.14	0.02	0.14
(1,2962)	1:375:B:TRP:HZ3	1:375:B:TRP:H	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB1	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB2	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB3	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB1	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB2	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB3	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB1	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB2	2	0.13	0.03	0.13
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB3	2	0.13	0.03	0.13
(1,292)	1:218:B:THR:HG21	1:375:B:TRP:HZ2	2	0.12	0.02	0.12
(1,292)	1:218:B:THR:HG22	1:375:B:TRP:HZ2	2	0.12	0.02	0.12
(1,292)	1:218:B:THR:HG23	1:375:B:TRP:HZ2	2	0.12	0.02	0.12
(1,5308)	1:111:A:ARG:HD3	1:115:A:GLN:HG2	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD21	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD22	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD23	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD21	2	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD22	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD23	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD21	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD22	2	0.12	0.02	0.12
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD23	2	0.12	0.02	0.12
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD11	2	0.12	0.02	0.12
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD12	2	0.12	0.02	0.12
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD13	2	0.12	0.02	0.12
(1,87)	1:209:B:ARG:HB2	1:209:B:ARG:HG3	2	0.12	0.0	0.12
(1,91)	1:209:B:ARG:HG3	1:209:B:ARG:HD2	2	0.12	0.0	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD21	2	0.12	0.0	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD22	2	0.12	0.0	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD23	2	0.12	0.0	0.12
(1,2051)	1:315:B:GLU:HB3	1:315:B:GLU:HG2	2	0.12	0.0	0.12
(1,2834)	1:367:B:HIS:HD2	1:370:B:GLN:H	2	0.12	0.0	0.12
(1,3501)	1:10:A:ARG:HG3	1:10:A:ARG:HD2	2	0.12	0.0	0.12
(1,5453)	1:116:A:GLU:HB3	1:116:A:GLU:HG2	2	0.12	0.0	0.12
(1,3009)	1:378:B:LEU:HD11	1:381:B:HIS:HB3	2	0.12	0.02	0.12
(1,3009)	1:378:B:LEU:HD12	1:381:B:HIS:HB3	2	0.12	0.02	0.12
(1,3009)	1:378:B:LEU:HD13	1:381:B:HIS:HB3	2	0.12	0.02	0.12
(1,3009)	1:378:B:LEU:HD21	1:381:B:HIS:HB3	2	0.12	0.02	0.12
(1,3009)	1:378:B:LEU:HD22	1:381:B:HIS:HB3	2	0.12	0.02	0.12
(1,3009)	1:378:B:LEU:HD23	1:381:B:HIS:HB3	2	0.12	0.02	0.12
(1,4045)	1:40:A:LEU:HD11	1:42:A:ASN:H	2	0.12	0.02	0.12
(1,4045)	1:40:A:LEU:HD12	1:42:A:ASN:H	2	0.12	0.02	0.12
(1,4045)	1:40:A:LEU:HD13	1:42:A:ASN:H	2	0.12	0.02	0.12
(1,4346)	1:57:A:ASN:HB2	1:57:A:ASN:H	2	0.12	0.02	0.12
(1,1639)	1:293:B:TRP:HZ3	1:293:B:TRP:H	2	0.12	0.0	0.12
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD21	2	0.12	0.0	0.12
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD22	2	0.12	0.0	0.12
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD23	2	0.12	0.0	0.12
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD21	2	0.12	0.0	0.12
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD22	2	0.12	0.0	0.12
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD23	2	0.12	0.0	0.12
(1,6412)	1:179:A:LEU:HD11	1:182:A:HIS:HB2	2	0.12	0.0	0.12
(1,6412)	1:179:A:LEU:HD12	1:182:A:HIS:HB2	2	0.12	0.0	0.12
(1,6412)	1:179:A:LEU:HD13	1:182:A:HIS:HB2	2	0.12	0.0	0.12
(1,6412)	1:179:A:LEU:HD21	1:182:A:HIS:HB2	2	0.12	0.0	0.12
(1,6412)	1:179:A:LEU:HD22	1:182:A:HIS:HB2	2	0.12	0.0	0.12
(1,6412)	1:179:A:LEU:HD23	1:182:A:HIS:HB2	2	0.12	0.0	0.12
(1,46)	1:206:B:SER:HA	1:206:B:SER:HB2	2	0.11	0.0	0.11
(1,83)	1:209:B:ARG:HB3	1:209:B:ARG:HG2	2	0.11	0.01	0.11

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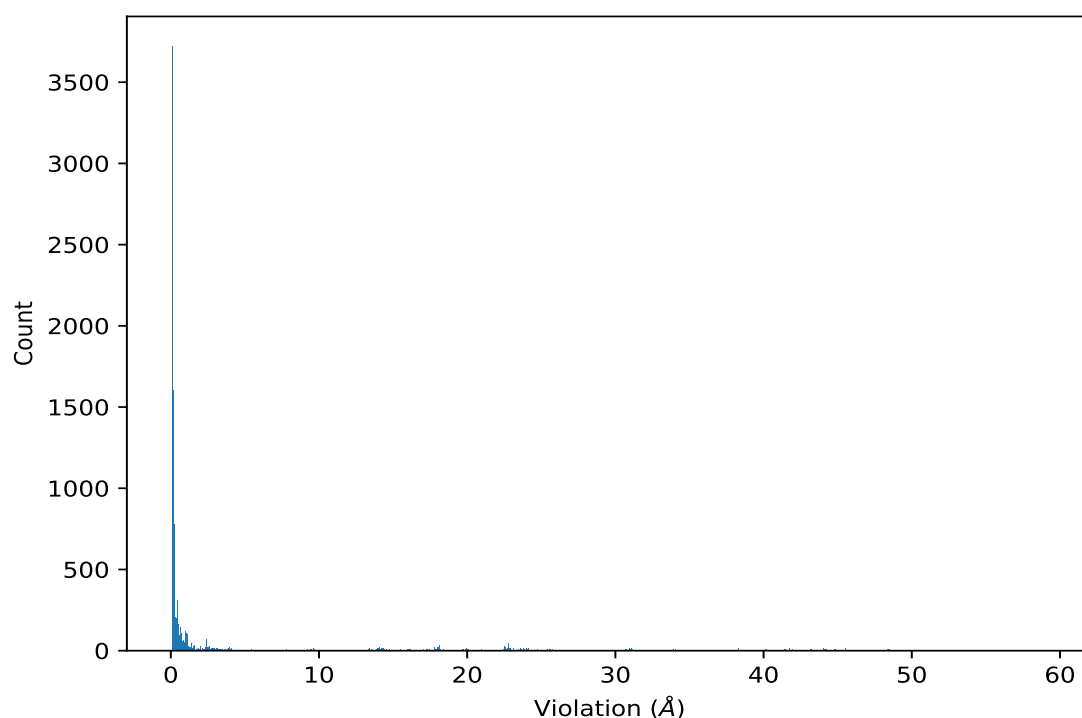
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1120)	1:272:B:LEU:HD11	1:308:B:GLU:H	2	0.11	0.0	0.11
(1,1120)	1:272:B:LEU:HD12	1:308:B:GLU:H	2	0.11	0.0	0.11
(1,1120)	1:272:B:LEU:HD13	1:308:B:GLU:H	2	0.11	0.0	0.11
(1,2103)	1:318:B:HIS:HB2	1:318:B:HIS:H	2	0.11	0.0	0.11
(1,5606)	1:124:A:ILE:HD11	1:125:A:PHE:H	2	0.11	0.0	0.11
(1,5606)	1:124:A:ILE:HD12	1:125:A:PHE:H	2	0.11	0.0	0.11
(1,5606)	1:124:A:ILE:HD13	1:125:A:PHE:H	2	0.11	0.0	0.11
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD11	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD12	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD13	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD11	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD12	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD13	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD11	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD12	2	0.1	0.0	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD13	2	0.1	0.0	0.1
(1,3281)	1:395:B:ASN:HB2	1:395:B:ASN:HD21	2	0.1	0.0	0.1
(1,4486)	1:72:A:GLN:HB3	1:72:A:GLN:H	2	0.1	0.0	0.1
(1,5631)	1:125:A:PHE:HA	1:151:A:SER:H	2	0.1	0.0	0.1
(1,5887)	1:145:A:ASP:HB3	1:145:A:ASP:H	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)
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	8	59.27
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	19	59.23
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	6	58.96
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	4	58.95
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	3	58.94
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	13	58.93
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	2	58.88
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	16	58.88
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	17	58.88
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	7	58.8
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	9	58.77
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	10	58.65
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	14	58.61
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	11	58.47
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	12	58.32
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	1	58.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	1	57.84
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	20	57.67
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	15	57.58
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	5	57.57
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	15	57.55
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	18	57.55
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	8	57.5
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	5	57.44
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	20	57.44
(1,6717)	2:399:C:DA:H1'	1:184:A:GLN:HG2	18	57.4
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	3	57.15
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	2	56.98
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	19	56.86
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	4	56.62
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	6	56.58
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	13	56.47
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	17	56.47
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	7	56.46
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	16	56.44
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	8	56.41
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	9	56.34
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	13	56.33
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	19	56.29
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	10	56.26
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	17	56.2
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	14	56.19
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	14	56.11
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	18	56.09
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	11	56.06
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	3	56.04
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	15	56.03
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	9	56.03
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	6	56.02
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	5	56.0
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	1	56.0
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	16	55.99
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	10	55.99
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	7	55.98
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	19	55.98
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	16	55.94
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	17	55.91
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	18	55.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	20	55.91
(1,6716)	2:399:C:DA:H1'	1:184:A:GLN:HG3	12	55.9
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	4	55.89
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	8	55.86
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	10	55.86
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	9	55.85
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	3	55.82
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	11	55.82
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	20	55.78
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	1	55.77
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	14	55.77
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	2	55.73
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	11	55.72
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	2	55.72
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	6	55.66
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	13	55.65
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	15	55.52
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	4	55.51
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	5	55.47
(1,6722)	2:399:C:DA:H8	1:181:A:GLU:HA	12	55.4
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	7	55.31
(1,6721)	2:399:C:DA:H4'	1:185:A:ALA:HA	12	55.05
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	8	54.59
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	13	54.47
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	17	54.38
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	14	54.3
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	18	54.28
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	3	54.22
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	10	54.21
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	9	54.19
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	19	54.17
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	1	54.15
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	16	54.13
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	11	53.95
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	2	53.87
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	20	53.87
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	6	53.8
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	15	53.69
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	4	53.65
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	5	53.64
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	7	53.43
(1,6718)	2:399:C:DA:H5''	1:185:A:ALA:HA	12	53.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	8	52.36
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	13	52.31
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	17	52.17
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	14	52.1
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	18	52.04
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	3	52.01
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	9	52.01
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	1	51.95
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	10	51.95
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	19	51.95
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	16	51.93
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	8	51.92
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	8	51.92
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	20	51.78
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	11	51.77
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	2	51.68
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	6	51.66
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	3	51.66
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	3	51.66
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	1	51.61
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	1	51.61
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	19	51.58
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	19	51.58
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	2	51.55
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	2	51.55
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	4	51.5
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	15	51.5
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	5	51.44
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	4	51.36
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	4	51.36
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	6	51.34
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	6	51.34
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	7	51.3
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	16	51.28
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	16	51.28
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	15	51.26
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	15	51.26
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	13	51.24
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	13	51.24
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	7	51.23
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	7	51.23
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	17	51.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	17	51.22
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	5	51.19
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	5	51.19
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	20	51.19
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	20	51.19
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	18	51.15
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	18	51.15
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	9	51.13
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	9	51.13
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	10	51.05
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	10	51.05
(1,6726)	2:400:C:DT:H5'	1:185:A:ALA:HA	12	51.02
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	14	50.98
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	14	50.98
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	8	50.85
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	11	50.83
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	11	50.83
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG2	12	50.81
(1,6724)	2:399:C:DA:H8	1:184:A:GLN:HG3	12	50.81
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	13	50.8
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	17	50.65
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	14	50.58
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	18	50.52
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	3	50.5
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	9	50.48
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	19	50.45
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	1	50.43
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	10	50.43
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	16	50.43
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	20	50.26
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	11	50.22
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	2	50.15
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	6	50.14
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	4	49.98
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	15	49.97
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	5	49.92
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	7	49.77
(1,6728)	2:400:C:DT:H5''	1:185:A:ALA:HA	12	49.49
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	19	48.74
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	19	48.74
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	7	48.5
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	7	48.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	18	48.48
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	18	48.48
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	6	48.47
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	6	48.47
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	16	48.47
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	16	48.47
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	5	48.46
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	5	48.46
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	10	48.45
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	10	48.45
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	15	48.45
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	15	48.45
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	2	48.41
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	2	48.41
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	11	48.41
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	11	48.41
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	17	48.41
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	17	48.41
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	9	48.4
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	9	48.4
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	1	48.39
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	1	48.39
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	14	48.39
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	14	48.39
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	3	48.38
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	3	48.38
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	8	48.38
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	8	48.38
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	20	48.35
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	20	48.35
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	4	48.32
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	4	48.32
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	13	48.03
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	13	48.03
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB2	12	47.85
(1,6723)	2:399:C:DA:H8	1:181:A:GLU:HB3	12	47.85
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	19	45.83
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	19	45.83
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	7	45.63
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	7	45.63
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	15	45.57
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	15	45.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	10	45.55
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	10	45.55
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	14	45.54
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	14	45.54
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	18	45.52
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	18	45.52
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	9	45.51
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	9	45.51
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	16	45.51
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	16	45.51
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	17	45.51
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	17	45.51
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	3	45.5
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	3	45.5
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	6	45.5
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	6	45.5
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	8	45.5
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	8	45.5
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	11	45.5
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	11	45.5
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	5	45.45
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	5	45.45
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	20	45.45
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	20	45.45
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	4	45.43
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	4	45.43
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	2	45.42
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	2	45.42
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	1	45.41
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	1	45.41
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	19	45.2
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	19	45.2
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	13	45.05
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	13	45.05
(1,6731)	2:400:C:DT:H5'	1:181:A:GLU:HB3	12	44.91
(1,6731)	2:400:C:DT:H5''	1:181:A:GLU:HB3	12	44.91
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	16	44.88
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	16	44.88
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	6	44.87
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	6	44.87
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	18	44.87
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	18	44.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	17	44.86
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	17	44.86
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	5	44.85
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	5	44.85
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	10	44.84
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	10	44.84
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	2	44.83
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	2	44.83
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	11	44.82
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	11	44.82
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	14	44.82
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	14	44.82
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	8	44.81
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	8	44.81
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	7	44.8
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	7	44.8
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	9	44.79
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	9	44.79
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	1	44.78
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	1	44.78
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	15	44.77
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	15	44.77
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	3	44.75
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	3	44.75
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	20	44.7
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	20	44.7
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	4	44.66
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	4	44.66
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	13	44.58
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	13	44.58
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	19	44.55
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	19	44.55
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	8	44.36
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	8	44.36
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	8	44.36
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	6	44.25
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	6	44.25
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	15	44.25
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	15	44.25
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	13	44.24
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	13	44.24
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	13	44.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	16	44.23
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	16	44.23
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	17	44.22
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	17	44.22
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	5	44.21
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	5	44.21
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	7	44.21
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	7	44.21
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	8	44.17
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	8	44.17
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	18	44.16
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	18	44.16
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	20	44.16
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	20	44.16
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	4	44.15
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	4	44.15
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	10	44.15
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	10	44.15
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	9	44.14
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	9	44.14
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	17	44.14
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	17	44.14
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	17	44.14
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	3	44.12
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	3	44.12
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	14	44.11
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	14	44.11
(1,6732)	2:400:C:DT:H5'	1:181:A:GLU:HB2	12	44.06
(1,6732)	2:400:C:DT:H5''	1:181:A:GLU:HB2	12	44.06
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	14	44.06
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	14	44.06
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	14	44.06
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	18	44.06
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	18	44.06
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	18	44.06
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	3	44.04
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	3	44.04
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	3	44.04
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	1	44.03
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	1	44.03
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	11	44.03
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	11	44.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	2	44.01
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	2	44.01
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	1	44.01
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	1	44.01
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	1	44.01
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	19	44.01
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	19	44.01
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	19	44.01
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	10	44.0
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	10	44.0
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	10	44.0
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	13	43.98
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	13	43.98
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	9	43.98
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	9	43.98
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	9	43.98
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	16	43.91
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	16	43.91
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	16	43.91
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	11	43.88
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	11	43.88
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	11	43.88
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	20	43.82
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	20	43.82
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	20	43.82
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	2	43.79
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	2	43.79
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	2	43.79
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	6	43.73
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	6	43.73
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	6	43.73
(1,6733)	2:400:C:DT:H5'	1:181:A:GLU:HA	12	43.6
(1,6733)	2:400:C:DT:H5''	1:181:A:GLU:HA	12	43.6
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	4	43.59
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	4	43.59
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	4	43.59
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	15	43.58
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	15	43.58
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	15	43.58
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	5	43.52
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	5	43.52
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	5	43.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	8	43.52
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	8	43.52
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	8	43.52
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	13	43.44
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	13	43.44
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	13	43.44
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	7	43.42
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	7	43.42
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	7	43.42
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	17	43.31
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	17	43.31
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	17	43.31
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	14	43.24
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	14	43.24
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	14	43.24
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	18	43.22
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	18	43.22
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	18	43.22
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	3	43.21
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	3	43.21
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	3	43.21
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	1	43.19
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	1	43.19
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	1	43.19
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	9	43.18
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	9	43.18
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	9	43.18
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	10	43.18
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	10	43.18
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	10	43.18
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	19	43.16
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	19	43.16
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	19	43.16
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB1	12	43.13
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB2	12	43.13
(1,6720)	2:399:C:DA:H4'	1:185:A:ALA:HB3	12	43.13
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	16	43.09
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	16	43.09
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	16	43.09
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	11	43.07
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	11	43.07
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	11	43.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	20	43.03
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	20	43.03
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	20	43.03
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	2	42.99
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	2	42.99
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	2	42.99
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	6	42.94
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	6	42.94
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	6	42.94
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	4	42.81
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	4	42.81
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	4	42.81
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	15	42.78
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	15	42.78
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	15	42.78
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	5	42.71
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	5	42.71
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	5	42.71
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	7	42.64
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	7	42.64
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	7	42.64
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB1	12	42.37
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB2	12	42.37
(1,6719)	2:399:C:DA:H1'	1:185:A:ALA:HB3	12	42.37
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	8	42.24
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	8	42.24
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	8	42.24
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	13	42.15
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	13	42.15
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	13	42.15
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	17	42.03
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	17	42.03
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	17	42.03
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	19	42.01
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	19	42.01
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	18	41.97
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	18	41.97
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	18	41.97
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	14	41.96
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	14	41.96
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	14	41.96
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	3	41.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	3	41.93
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	3	41.93
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	1	41.92
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	1	41.92
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	1	41.92
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	10	41.92
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	10	41.92
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	10	41.92
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	19	41.89
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	19	41.89
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	19	41.89
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	9	41.88
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	9	41.88
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	9	41.88
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	16	41.81
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	16	41.81
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	16	41.81
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	11	41.74
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	11	41.74
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	11	41.74
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	6	41.73
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	6	41.73
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	16	41.73
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	16	41.73
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	20	41.73
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	20	41.73
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	20	41.71
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	20	41.71
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	20	41.71
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	2	41.7
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	2	41.7
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	2	41.7
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	5	41.67
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	5	41.67
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	17	41.66
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	17	41.66
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	6	41.62
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	6	41.62
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	6	41.62
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	8	41.58
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	8	41.58
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	4	41.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	4	41.57
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	13	41.56
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	13	41.56
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	15	41.52
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	15	41.52
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	9	41.5
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	9	41.5
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	18	41.5
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	18	41.5
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	4	41.49
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	4	41.49
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	4	41.49
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	15	41.49
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	15	41.49
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	15	41.49
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	10	41.45
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	10	41.45
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	3	41.43
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	3	41.43
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	5	41.43
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	5	41.43
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	5	41.43
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	7	41.42
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	7	41.42
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	1	41.4
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	1	41.4
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	14	41.4
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	14	41.4
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	2	41.38
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	2	41.38
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	11	41.35
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	11	41.35
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	7	41.31
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	7	41.31
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	7	41.31
(1,6734)	2:400:C:DT:H5'	1:182:A:HIS:HA	12	41.12
(1,6734)	2:400:C:DT:H5''	1:182:A:HIS:HA	12	41.12
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB1	12	41.02
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB2	12	41.02
(1,6725)	2:399:C:DA:H3'	1:185:A:ALA:HB3	12	41.02
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB1	8	40.46
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB2	8	40.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	8	40.46
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	13	40.36
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	13	40.36
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	13	40.36
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	17	40.25
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	17	40.25
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	17	40.25
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	14	40.19
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	14	40.19
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	14	40.19
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	3	40.15
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	3	40.15
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	3	40.15
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	18	40.15
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	18	40.15
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	18	40.15
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	19	40.13
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	19	40.13
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	19	40.13
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	9	40.1
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	9	40.1
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	9	40.1
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	10	40.1
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	10	40.1
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	10	40.1
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	1	40.09
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	1	40.09
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	1	40.09
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	16	40.06
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	16	40.06
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	16	40.06
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	20	39.95
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	20	39.95
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	20	39.95
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	11	39.94
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	11	39.94
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	11	39.94
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	2	39.89
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	2	39.89
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB3	2	39.89
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB1	6	39.86
(1,6727)	2:400:C:DT:H5"	1:185:A:ALA:HB2	6	39.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB3	6	39.86
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB1	4	39.72
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB2	4	39.72
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB3	4	39.72
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB1	15	39.7
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB2	15	39.7
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB3	15	39.7
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB1	5	39.64
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB2	5	39.64
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB3	5	39.64
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB1	7	39.54
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB2	7	39.54
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB3	7	39.54
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB1	12	39.25
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB2	12	39.25
(1,6727)	2:400:C:DT:H5''	1:185:A:ALA:HB3	12	39.25
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	8	38.58
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	8	38.58
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	8	38.58
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	13	38.5
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	13	38.5
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	13	38.5
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	17	38.43
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	17	38.43
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	17	38.43
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	14	38.36
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	14	38.36
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	14	38.36
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	18	38.32
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	18	38.32
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	18	38.32
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	3	38.28
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	3	38.28
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	3	38.28
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	9	38.27
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	9	38.27
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	9	38.27
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	19	38.27
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	19	38.27
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	19	38.27
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	1	38.25
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	1	38.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	1	38.25
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	10	38.25
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	10	38.25
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	10	38.25
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	16	38.22
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	16	38.22
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	16	38.22
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	11	38.14
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	11	38.14
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	11	38.14
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	20	38.12
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	20	38.12
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	20	38.12
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	2	38.03
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	2	38.03
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	2	38.03
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	6	38.01
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	6	38.01
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	6	38.01
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	4	37.89
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	4	37.89
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	4	37.89
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	15	37.87
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	15	37.87
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	15	37.87
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	5	37.8
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	5	37.8
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	5	37.8
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	7	37.69
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	7	37.69
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	7	37.69
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB1	12	37.41
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB2	12	37.41
(1,6729)	2:400:C:DT:H4'	1:185:A:ALA:HB3	12	37.41
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	8	36.06
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	17	35.88
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	4	35.71
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	20	35.61
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	5	35.28
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	10	35.05
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	16	34.99
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	12	34.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	3	34.71
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	1	34.39
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	14	34.35
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	19	34.35
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	19	34.35
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	19	34.35
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	16	34.31
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	16	34.31
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	16	34.31
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	13	34.26
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	19	34.25
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	2	34.23
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	11	34.2
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	20	34.19
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	20	34.19
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	20	34.19
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	6	34.15
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	6	34.15
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	6	34.15
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	15	34.12
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	15	34.09
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	15	34.09
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	15	34.09
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	5	34.07
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	5	34.07
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	5	34.07
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	13	34.06
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	13	34.06
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	13	34.06
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	4	34.01
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	4	34.01
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	4	34.01
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	17	33.96
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	17	33.96
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	17	33.96
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	8	33.95
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	8	33.95
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	8	33.95
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	9	33.92
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	9	33.92
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	9	33.92
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	6	33.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	7	33.91
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	7	33.91
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	7	33.91
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	14	33.9
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	14	33.9
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	14	33.9
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	12	33.72
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	12	33.72
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	12	33.72
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	10	33.63
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	10	33.63
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	10	33.63
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	7	33.51
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	9	33.49
(1,6765)	2:408:C:DT:H5'	1:63:A:ASN:HA	18	33.47
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	11	33.46
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	11	33.46
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	11	33.46
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	2	33.4
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	2	33.4
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	2	33.4
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	18	32.97
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	18	32.97
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	18	32.97
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	3	32.93
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	3	32.93
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	3	32.93
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD21	1	32.87
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD22	1	32.87
(1,6730)	2:400:C:DT:H6	1:186:A:LEU:HD23	1	32.87
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	8	31.48
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	8	31.48
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	8	31.48
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	8	31.48
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	8	31.48
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	8	31.48
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	13	31.36
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	13	31.36
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	13	31.36
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	13	31.36
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	13	31.36
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	13	31.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	14	31.21
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	14	31.21
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	14	31.21
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	14	31.21
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	14	31.21
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	14	31.21
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	17	31.18
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	17	31.18
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	17	31.18
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	17	31.18
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	17	31.18
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	17	31.18
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	19	31.15
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	19	31.15
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	19	31.15
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	19	31.15
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	19	31.15
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	19	31.15
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	3	31.12
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	3	31.12
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	3	31.12
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	3	31.12
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	3	31.12
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	3	31.12
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	10	31.1
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	10	31.1
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	10	31.1
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	10	31.1
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	10	31.1
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	10	31.1
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	9	31.09
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	9	31.09
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	9	31.09
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	9	31.09
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	9	31.09
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	9	31.09
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	18	31.06
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	18	31.06
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	18	31.06
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	18	31.06
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	18	31.06
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	18	31.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	1	31.05
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	1	31.05
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	1	31.05
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	1	31.05
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	1	31.05
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	1	31.05
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	16	31.03
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	16	31.03
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	16	31.03
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	16	31.03
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	16	31.03
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	16	31.03
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	20	31.02
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	20	31.02
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	20	31.02
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	20	31.02
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	20	31.02
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	20	31.02
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	6	30.92
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	6	30.92
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	6	30.92
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	6	30.92
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	6	30.92
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	6	30.92
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	2	30.91
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	2	30.91
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	2	30.91
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	2	30.91
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	2	30.91
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	2	30.91
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	11	30.91
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	11	30.91
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	11	30.91
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	11	30.91
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	11	30.91
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	11	30.91
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	4	30.73
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	4	30.73
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	4	30.73
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	4	30.73
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	4	30.73
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	4	30.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	15	30.73
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	15	30.73
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	15	30.73
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	15	30.73
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	15	30.73
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	15	30.73
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	5	30.67
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	5	30.67
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	5	30.67
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	5	30.67
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	5	30.67
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	5	30.67
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	7	30.66
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	7	30.66
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	7	30.66
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	7	30.66
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	7	30.66
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	7	30.66
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB1	12	30.36
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB2	12	30.36
(1,6737)	2:401:C:DT:H5'	1:185:A:ALA:HB3	12	30.36
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB1	12	30.36
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB2	12	30.36
(1,6737)	2:401:C:DT:H5''	1:185:A:ALA:HB3	12	30.36
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	19	27.81
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	19	27.81
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	19	26.65
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	19	26.65
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	10	26.56
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	10	26.56
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	4	26.52
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	4	26.52
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	10	26.06
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	7	26.04
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	7	26.04
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	20	26.0
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	20	26.0
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	20	26.0
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	8	25.96
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	8	25.96
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	11	25.76
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	11	25.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	11	25.76
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	17	25.73
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	17	25.73
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	17	25.73
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	10	25.7
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	10	25.7
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	10	25.7
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	19	25.7
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	19	25.7
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	19	25.7
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	15	25.69
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	15	25.69
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	15	25.69
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	16	25.67
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	16	25.67
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	16	25.67
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	2	25.64
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	2	25.64
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	2	25.64
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	4	25.63
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	3	25.62
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	3	25.62
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	3	25.62
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	7	25.59
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	7	25.59
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	7	25.59
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	1	25.56
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	1	25.56
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	1	25.56
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	13	25.55
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	13	25.55
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	13	25.55
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	8	25.54
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	8	25.54
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	8	25.54
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	5	25.52
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	5	25.52
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	5	25.52
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	8	25.51
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	8	25.51
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	9	25.46
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	9	25.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	9	25.46
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	17	25.44
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	17	25.44
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	18	25.44
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	18	25.44
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	18	25.44
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	14	25.43
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	14	25.43
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	14	25.43
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	12	25.41
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	12	25.41
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	12	25.41
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	6	25.38
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	6	25.38
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	6	25.38
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	13	25.33
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	13	25.33
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	4	25.31
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	4	25.31
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	14	25.27
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	14	25.27
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	12	25.25
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	12	25.25
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD11	4	25.22
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD12	4	25.22
(1,6739)	2:401:C:DT:H6	1:26:A:ILE:HD13	4	25.22
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	10	25.17
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	10	25.17
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	8	25.13
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	8	25.13
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	11	25.11
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	11	25.11
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	17	25.08
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	19	25.0
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	12	24.92
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	12	24.92
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	13	24.91
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	2	24.91
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	2	24.91
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	1	24.83
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	17	24.78
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	17	24.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	1	24.77
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	1	24.77
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	7	24.75
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	6	24.75
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	6	24.75
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	11	24.69
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	12	24.58
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	3	24.56
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	3	24.56
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	4	24.46
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	4	24.46
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	6	24.38
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	6	24.38
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	12	24.37
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	12	24.37
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	10	24.36
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	10	24.36
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	20	24.33
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	20	24.33
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	20	24.33
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	10	24.28
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	10	24.14
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	10	24.14
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	10	24.14
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	11	24.14
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	11	24.14
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	11	24.14
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	17	24.13
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	17	24.13
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	17	24.13
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	19	24.11
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	19	24.11
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	19	24.11
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	15	24.1
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	15	24.1
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	15	24.1
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	3	24.08
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	3	24.08
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	3	24.08
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	13	24.07
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	13	24.07
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	7	24.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	7	24.06
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	1	24.03
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	1	24.03
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	1	24.03
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	2	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	2	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	2	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	5	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	5	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	5	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	8	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	8	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	8	24.02
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	7	24.0
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	7	24.0
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	7	24.0
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	16	24.0
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	16	24.0
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	16	24.0
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	14	23.96
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	14	23.96
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	14	23.96
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	18	23.96
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	18	23.96
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	18	23.96
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	12	23.94
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	12	23.94
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	12	23.94
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	11	23.94
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	11	23.94
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	20	23.89
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	20	23.89
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	20	23.89
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	20	23.89
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	19	23.87
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	19	23.87
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	19	23.87
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	19	23.87
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	13	23.86
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	13	23.86
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	13	23.86
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	1	23.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	1	23.83
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	4	23.82
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	4	23.82
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	4	23.82
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	13	23.81
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	13	23.81
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	10	23.81
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	10	23.81
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	10	23.81
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	10	23.81
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	2	23.81
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	2	23.81
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	9	23.76
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	9	23.76
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	9	23.76
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	14	23.73
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	14	23.73
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	14	23.73
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	14	23.73
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	1	23.71
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	1	23.71
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	8	23.68
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	19	23.68
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	1	23.68
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	20	23.66
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	20	23.66
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG21	6	23.65
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG22	6	23.65
(1,6738)	2:401:C:DT:H6	1:26:A:ILE:HG23	6	23.65
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	7	23.62
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	7	23.62
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	7	23.62
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	7	23.62
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	8	23.62
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	8	23.62
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	8	23.62
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	8	23.62
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	11	23.62
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	11	23.62
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	11	23.62
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	11	23.62
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	17	23.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	17	23.61
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	17	23.61
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	17	23.61
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	20	23.6
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	20	23.6
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	5	23.59
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	5	23.59
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	5	23.59
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	5	23.59
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	2	23.55
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	2	23.55
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	2	23.55
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	2	23.55
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	14	23.53
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	19	23.51
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	16	23.5
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	16	23.5
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	5	23.47
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	5	23.47
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	18	23.46
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	18	23.46
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	4	23.45
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	4	23.45
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	4	23.45
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	4	23.45
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	15	23.41
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	15	23.41
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	15	23.41
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	15	23.41
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	12	23.32
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	20	23.32
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	20	23.32
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	14	23.28
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	14	23.28
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	4	23.25
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	3	23.22
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	3	23.22
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	13	23.18
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	16	23.15
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	16	23.15
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	16	23.15
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	13	23.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	13	23.13
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	13	23.13
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	13	23.13
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	20	23.12
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	20	23.12
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	20	23.12
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	20	23.12
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	20	23.12
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	20	23.12
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	6	23.11
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	6	23.11
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	1	23.1
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	1	23.1
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	1	23.1
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	1	23.1
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	5	23.09
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	11	23.09
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	11	23.04
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	11	23.04
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	5	23.03
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	6	23.02
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	6	23.02
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	6	23.02
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	9	22.97
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	9	22.97
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	9	22.97
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	9	22.97
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	15	22.94
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	15	22.94
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	12	22.94
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	12	22.94
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	12	22.94
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	12	22.94
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	16	22.94
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	16	22.94
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	16	22.94
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	16	22.94
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	17	22.94
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	17	22.94
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	17	22.94
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	3	22.91
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	3	22.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	3	22.91
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	3	22.91
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	5	22.87
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	5	22.87
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	5	22.87
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	14	22.87
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	14	22.87
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	18	22.87
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	18	22.87
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	18	22.87
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	18	22.87
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	19	22.86
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	19	22.86
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	19	22.86
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	19	22.86
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	19	22.86
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	19	22.86
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	20	22.85
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	20	22.85
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	20	22.85
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	10	22.83
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	10	22.83
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	10	22.83
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	10	22.83
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	10	22.83
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	10	22.83
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	2	22.8
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	2	22.8
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA2	6	22.8
(1,6735)	2:401:C:DT:H5'	1:25:A:GLY:HA3	6	22.8
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA2	6	22.8
(1,6735)	2:401:C:DT:H5''	1:25:A:GLY:HA3	6	22.8
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	15	22.78
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	15	22.78
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	15	22.78
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	15	22.78
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	15	22.78
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	15	22.78
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	5	22.78
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	5	22.78
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	19	22.77
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	19	22.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	11	22.77
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	11	22.77
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	11	22.77
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	11	22.77
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	11	22.77
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	11	22.77
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	2	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	2	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	2	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	2	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	2	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	2	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	7	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	7	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	7	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	7	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	7	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	7	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	17	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	17	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	17	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	17	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	17	22.76
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	17	22.76
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	3	22.75
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	3	22.75
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	3	22.75
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	3	22.75
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	3	22.75
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	3	22.75
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	8	22.75
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	8	22.75
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	8	22.75
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	8	22.75
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	8	22.75
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	8	22.75
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	9	22.73
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	9	22.73
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	16	22.73
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	16	22.73
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	16	22.73
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	16	22.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	16	22.73
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	16	22.73
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	13	22.7
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	13	22.7
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	13	22.7
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	13	22.7
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	13	22.7
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	13	22.7
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	8	22.69
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	1	22.68
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	1	22.68
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	1	22.68
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	1	22.68
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	1	22.68
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	1	22.68
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	15	22.65
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	15	22.65
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	16	22.62
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	5	22.61
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	5	22.61
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	5	22.61
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	5	22.61
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	5	22.61
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	5	22.61
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	10	22.6
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	10	22.6
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	10	22.6
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	14	22.57
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	14	22.57
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	14	22.57
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	14	22.57
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	14	22.57
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	14	22.57
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	14	22.57
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	14	22.57
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	14	22.57
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	11	22.56
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	11	22.56
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	11	22.56
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	12	22.56
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	12	22.56
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	12	22.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	12	22.56
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	12	22.56
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	12	22.56
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	6	22.55
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	6	22.55
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	6	22.55
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	6	22.55
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	6	22.55
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	6	22.55
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	9	22.54
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	9	22.54
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	9	22.54
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	9	22.54
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	9	22.54
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	9	22.54
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	6	22.53
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	2	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	2	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	2	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	18	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	18	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	18	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	19	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	19	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	19	22.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	7	22.51
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	7	22.51
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	7	22.51
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	18	22.51
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	18	22.51
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	18	22.51
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	18	22.51
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	18	22.51
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	18	22.51
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	9	22.49
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	9	22.49
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	9	22.49
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	18	22.48
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	18	22.48
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB2	7	22.45
(1,6763)	2:407:C:DT:H6	1:62:A:LEU:HB3	7	22.45
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	2	22.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	15	22.42
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	15	22.42
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	15	22.42
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	18	22.42
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	7	22.38
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	15	22.36
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	15	22.36
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	5	22.35
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	5	22.35
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD11	4	22.33
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD12	4	22.33
(1,6736)	2:401:C:DT:H5'	1:26:A:ILE:HD13	4	22.33
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD11	4	22.33
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD12	4	22.33
(1,6736)	2:401:C:DT:H5''	1:26:A:ILE:HD13	4	22.33
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	8	22.14
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	8	22.14
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	8	22.14
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	17	22.13
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	17	22.13
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	17	22.13
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	8	22.05
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	8	22.05
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	10	22.04
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	6	22.0
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	18	21.96
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	18	21.96
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	4	21.91
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	4	21.91
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	17	21.89
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	17	21.89
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	3	21.86
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	20	21.83
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	20	21.79
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	12	21.72
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	12	21.72
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	12	21.72
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	20	21.62
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	20	21.62
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	3	21.61
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	3	21.61
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	5	21.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	5	21.55
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	12	21.52
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	12	21.52
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	3	21.46
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	3	21.46
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	3	21.46
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	9	21.46
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	9	21.46
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	14	21.34
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	16	21.26
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	20	21.24
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	3	21.15
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	17	21.1
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	2	21.1
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	11	21.06
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	16	21.03
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	15	21.02
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	1	21.0
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	10	20.99
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	1	20.99
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	4	20.98
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	4	20.98
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	4	20.98
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	13	20.97
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	13	20.97
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	18	20.95
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	16	20.91
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	16	20.91
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	5	20.91
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	19	20.91
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	12	20.9
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	12	20.87
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	2	20.86
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	15	20.86
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	4	20.85
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	7	20.81
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	15	20.8
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	17	20.8
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	8	20.79
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	18	20.76
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	13	20.73
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	14	20.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	9	20.71
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	4	20.68
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	8	20.66
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	13	20.61
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	13	20.61
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	13	20.61
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	6	20.6
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	11	20.6
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	5	20.59
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	11	20.58
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	11	20.58
(1,6746)	2:403:C:DT:H6	1:26:A:ILE:HB	6	20.57
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	13	20.49
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD11	1	20.45
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD12	1	20.45
(1,6764)	2:407:C:DT:H6	1:62:A:LEU:HD13	1	20.45
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	20	20.36
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	20	20.36
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	20	20.36
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	15	20.27
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	15	20.27
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	9	20.15
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	9	20.15
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	10	20.07
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	10	20.07
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	10	20.07
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	19	20.07
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	19	20.07
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	19	20.07
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	3	20.07
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	16	20.04
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	15	20.03
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	15	20.03
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	15	20.03
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	11	20.02
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	11	20.02
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	11	20.02
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	17	19.99
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	17	19.99
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	17	19.99
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	6	19.98
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	6	19.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:2:A:GLU:HB2	1:202:B:ALA:H	9	19.98
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	2	19.97
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	2	19.97
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	2	19.97
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	7	19.96
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	7	19.96
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	7	19.96
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	16	19.96
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	16	19.96
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	16	19.96
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	3	19.95
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	3	19.95
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	3	19.95
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	10	19.94
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	10	19.94
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	8	19.91
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	8	19.91
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	8	19.91
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	9	19.9
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	9	19.9
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	1	19.87
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	1	19.87
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	1	19.87
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	1	19.87
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	1	19.87
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	13	19.87
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	13	19.87
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	13	19.87
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	14	19.86
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	19	19.83
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	19	19.83
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	5	19.8
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	5	19.8
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	5	19.8
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	14	19.76
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	14	19.76
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	14	19.76
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	12	19.75
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	12	19.75
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD13	12	19.75
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD11	9	19.71
(1,6741)	2:402:C:DT:H5"	1:26:A:ILE:HD12	9	19.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	9	19.71
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	6	19.7
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	6	19.7
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	6	19.7
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	18	19.7
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	18	19.7
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	18	19.7
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG2	16	19.68
(1,3)	1:2:A:GLU:HA	1:201:B:GLU:HG3	16	19.68
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	2	19.66
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	2	19.66
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	19	19.65
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	19	19.65
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	19	19.65
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	7	19.64
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	7	19.61
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	7	19.61
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	14	19.56
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	14	19.56
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	20	19.51
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD11	4	19.49
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD12	4	19.49
(1,6741)	2:402:C:DT:H5''	1:26:A:ILE:HD13	4	19.49
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	18	19.19
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	18	19.19
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB2	3	19.12
(1,6760)	2:406:C:DA:H1'	1:66:A:PHE:HB3	3	19.12
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	20	19.09
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	2	19.09
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	15	19.02
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	11	18.98
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	17	18.98
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	10	18.92
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	19	18.88
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	5	18.87
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	15	18.86
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	14	18.81
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	3	18.77
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	7	18.75
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	4	18.74
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	16	18.74
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	2	18.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	8	18.72
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG2	16	18.72
(1,4)	1:2:A:GLU:HB2	1:201:B:GLU:HG3	16	18.72
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	1	18.65
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	18	18.65
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	12	18.62
(1,7)	1:2:A:GLU:HA	1:202:B:ALA:H	9	18.55
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	13	18.5
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	9	18.46
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	20	18.46
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	20	18.46
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	20	18.46
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	10	18.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	10	18.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	10	18.41
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	20	18.4
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	20	18.4
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	20	18.4
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	20	18.4
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	20	18.4
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	20	18.4
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	17	18.33
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	17	18.33
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	17	18.33
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	11	18.31
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	11	18.31
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	11	18.31
(1,6747)	2:403:C:DT:H6	1:26:A:ILE:HA	6	18.28
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	10	18.25
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	10	18.25
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	10	18.25
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	19	18.23
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	19	18.23
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	19	18.23
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	15	18.22
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	15	18.22
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	15	18.22
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	3	18.21
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	3	18.21
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	3	18.21
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	18	18.2
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	5	18.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	5	18.18
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	5	18.18
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	1	18.15
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	1	18.15
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	1	18.15
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	19	18.15
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	19	18.15
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	19	18.15
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	19	18.15
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	19	18.15
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	19	18.15
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	16	18.14
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	16	18.14
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	16	18.14
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	10	18.14
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	10	18.14
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	10	18.14
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	10	18.14
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	10	18.14
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	10	18.14
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	2	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	2	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	2	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	7	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	7	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	7	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	18	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	18	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	18	18.11
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	15	18.11
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	15	18.11
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	15	18.11
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	15	18.11
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	15	18.11
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	15	18.11
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	8	18.1
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	8	18.1
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	8	18.1
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	14	18.1
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	14	18.1
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	14	18.1
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	11	18.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	11	18.1
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	11	18.1
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	11	18.1
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	11	18.1
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	11	18.1
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	17	18.08
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	17	18.08
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	17	18.08
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	17	18.08
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	17	18.08
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	17	18.08
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	12	18.07
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	12	18.07
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	12	18.07
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	2	18.05
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	2	18.05
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	2	18.05
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	2	18.05
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	2	18.05
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	2	18.05
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	16	18.05
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	16	18.05
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	16	18.05
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	16	18.05
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	16	18.05
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	16	18.05
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	7	18.04
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	7	18.04
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	7	18.04
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	7	18.04
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	7	18.04
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	7	18.04
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	3	18.03
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	3	18.03
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	3	18.03
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	3	18.03
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	3	18.03
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	3	18.03
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	4	18.02
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	4	18.02
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	4	18.02
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	8	17.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	8	17.99
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	8	17.99
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	8	17.99
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	8	17.99
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	8	17.99
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	13	17.96
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	13	17.96
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	13	17.96
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	1	17.96
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	1	17.96
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	1	17.96
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	1	17.96
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	1	17.96
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	1	17.96
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	13	17.96
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	13	17.96
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	13	17.96
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	13	17.96
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	13	17.96
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	13	17.96
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	9	17.92
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	9	17.92
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	9	17.92
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	5	17.9
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	5	17.9
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	5	17.9
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	5	17.9
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	5	17.9
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	5	17.9
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	12	17.86
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	12	17.86
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	12	17.86
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	12	17.86
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	12	17.86
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	12	17.86
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	14	17.86
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	14	17.86
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	14	17.86
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	14	17.86
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	14	17.86
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	14	17.86
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	9	17.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	9	17.82
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	9	17.82
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	9	17.82
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	9	17.82
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	9	17.82
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	6	17.81
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	6	17.81
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	6	17.81
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	6	17.81
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	6	17.81
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	6	17.81
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	18	17.81
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	18	17.81
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	18	17.81
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	18	17.81
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	18	17.81
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	18	17.81
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG21	6	17.8
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG22	6	17.8
(1,6744)	2:403:C:DT:H6	1:26:A:ILE:HG23	6	17.8
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD11	4	17.62
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD12	4	17.62
(1,6742)	2:402:C:DT:H5'	1:26:A:ILE:HD13	4	17.62
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD11	4	17.62
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD12	4	17.62
(1,6742)	2:402:C:DT:H5''	1:26:A:ILE:HD13	4	17.62
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	3	17.58
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	12	17.52
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	12	17.52
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	12	17.52
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	1	17.47
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	1	17.47
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	1	17.47
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	10	17.46
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	10	17.46
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	13	17.46
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	13	17.46
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	13	17.46
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	5	17.44
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	5	17.44
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	7	17.42
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	7	17.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	4	17.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	4	17.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	4	17.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	11	17.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	11	17.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	11	17.41
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	5	17.35
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	5	17.35
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	5	17.35
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	12	17.33
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	12	17.33
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	6	17.33
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	6	17.33
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	6	17.33
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	17	17.31
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	17	17.31
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	17	17.31
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	3	17.28
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	3	17.28
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	8	17.26
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	8	17.26
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	8	17.26
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	20	17.25
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	20	17.25
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	1	17.19
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	1	17.19
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	14	17.17
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	14	17.17
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	8	17.12
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	8	17.12
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	11	17.11
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	11	17.11
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	6	17.07
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	6	17.07
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	13	17.06
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	13	17.06
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	19	17.06
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	19	17.06
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	18	17.05
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	18	17.05
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	17	17.04
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	17	17.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	2	17.02
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	2	17.02
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	4	17.02
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	4	17.02
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	9	17.02
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	9	17.02
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	15	17.01
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	15	17.01
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	14	16.6
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	14	16.6
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	14	16.6
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	7	16.59
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	7	16.59
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	7	16.59
(1,6762)	2:407:C:DT:H5'	1:59:A:ALA:HA	16	16.58
(1,6762)	2:407:C:DT:H5''	1:59:A:ALA:HA	16	16.58
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	16	16.49
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	16	16.49
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	16	16.49
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	15	16.43
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	15	16.43
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	15	16.43
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	20	16.32
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	20	16.32
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	20	16.31
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	20	16.31
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	19	16.25
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	19	16.25
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	17	16.24
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	17	16.24
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	14	16.22
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	14	16.22
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	11	16.2
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	11	16.2
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	10	16.17
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	10	16.17
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	10	16.15
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	10	16.15
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	19	16.15
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	19	16.15
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	5	16.15
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	5	16.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	20	16.12
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	20	16.12
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	20	16.12
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	8	16.09
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	8	16.09
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	4	16.09
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	4	16.09
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	11	16.08
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	11	16.08
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	15	16.06
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	15	16.06
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	17	16.06
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	17	16.06
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	14	16.05
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	14	16.05
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	5	16.04
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	5	16.04
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	7	16.04
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	7	16.04
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	2	16.03
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	2	16.03
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	2	16.03
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	2	16.01
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	2	16.01
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	3	15.99
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	3	15.99
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	7	15.99
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	7	15.99
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	8	15.97
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	8	15.97
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	2	15.95
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	2	15.95
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	16	15.91
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	16	15.91
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	1	15.9
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	1	15.9
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	4	15.9
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	4	15.9
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	12	15.88
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	12	15.88
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	13	15.82
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	13	15.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	18	15.82
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	18	15.82
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	15	15.77
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	15	15.77
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	18	15.7
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	18	15.7
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	9	15.65
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	9	15.65
(1,6748)	2:403:C:DT:H5'	1:26:A:ILE:HA	6	15.58
(1,6748)	2:403:C:DT:H5''	1:26:A:ILE:HA	6	15.58
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	7	15.57
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	7	15.57
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	9	15.57
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	9	15.57
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	1	15.54
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	1	15.54
(1,5)	1:2:A:GLU:HA	1:202:B:ALA:HA	9	15.54
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	12	15.51
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	12	15.51
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	9	15.5
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	9	15.5
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	13	15.49
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	13	15.49
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	19	15.45
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	19	15.45
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	18	15.42
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	18	15.42
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	18	15.42
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	10	15.38
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	10	15.38
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	18	15.37
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	18	15.37
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	16	15.35
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	16	15.35
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	15	15.33
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	15	15.33
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	12	15.29
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	12	15.29
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	3	15.27
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	3	15.27
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	13	15.25
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	13	15.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA2	6	15.22
(1,6745)	2:403:C:DT:H6	1:25:A:GLY:HA3	6	15.22
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	2	15.21
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	2	15.21
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	5	15.21
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	5	15.21
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	17	15.15
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	17	15.15
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	8	15.1
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	8	15.1
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	11	14.77
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	11	14.77
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	6	14.76
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	6	14.76
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	3	14.75
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	3	14.75
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	3	14.75
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	14	14.74
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	14	14.74
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	20	14.61
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	20	14.61
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	20	14.61
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	3	14.57
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	3	14.57
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	4	14.56
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	4	14.56
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	1	14.55
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	1	14.55
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	16	14.55
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	16	14.55
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	11	14.44
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	11	14.44
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	11	14.44
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	10	14.43
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	10	14.43
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	10	14.43
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	17	14.43
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	17	14.43
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	17	14.43
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	15	14.39
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	15	14.39
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	15	14.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	19	14.39
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	19	14.39
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	19	14.39
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	7	14.36
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	7	14.36
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	7	14.36
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	3	14.35
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	3	14.35
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	3	14.35
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	5	14.32
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	5	14.32
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	5	14.32
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	8	14.32
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	8	14.32
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	8	14.32
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	1	14.3
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	1	14.3
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	1	14.3
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	7	14.3
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	7	14.3
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	7	14.3
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	20	14.3
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	20	14.3
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	20	14.3
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	20	14.3
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	2	14.29
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	2	14.29
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	2	14.29
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	16	14.29
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	16	14.29
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	16	14.29
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	14	14.28
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	14	14.28
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	14	14.28
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	19	14.27
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	19	14.27
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	19	14.27
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	19	14.27
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	10	14.24
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	10	14.24
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	10	14.24
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	18	14.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	18	14.24
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	18	14.24
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	12	14.22
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	12	14.22
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	12	14.22
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	5	14.21
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	5	14.21
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	5	14.21
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	10	14.2
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	10	14.2
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	10	14.2
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	10	14.2
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	12	14.18
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	12	14.18
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	12	14.18
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	14	14.18
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	14	14.18
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	14	14.18
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	14	14.18
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	13	14.16
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	13	14.16
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	13	14.16
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	4	14.13
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	4	14.13
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	4	14.13
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	18	14.1
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	18	14.1
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	18	14.1
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	11	14.08
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	11	14.08
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	11	14.08
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	11	14.08
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	9	14.07
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	9	14.07
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	9	14.07
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	17	14.07
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	17	14.07
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	17	14.07
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	17	14.07
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	9	14.05
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	9	14.05
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	9	14.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	5	14.05
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	5	14.05
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	5	14.05
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	5	14.05
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	8	14.05
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	8	14.05
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	8	14.05
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	8	14.05
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	7	14.03
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	7	14.03
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	7	14.03
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	7	14.03
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	6	14.02
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	6	14.02
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	6	14.02
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	19	14.02
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	19	14.02
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	19	14.02
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	11	14.01
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	11	14.01
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	11	14.01
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	8	13.98
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	8	13.98
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	8	13.98
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	2	13.98
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	2	13.98
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	2	13.98
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	2	13.98
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	14	13.96
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	14	13.96
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	14	13.96
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	1	13.95
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	1	13.95
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	1	13.95
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	4	13.95
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	4	13.95
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	4	13.95
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	4	13.95
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG21	6	13.94
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG22	6	13.94
(1,6749)	2:404:C:DC:H5	1:26:A:ILE:HG23	6	13.94
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	2	13.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	2	13.93
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	2	13.93
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	13	13.92
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	13	13.92
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	13	13.92
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	3	13.91
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	3	13.91
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	3	13.91
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB1	9	13.91
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB2	9	13.91
(1,6)	1:2:A:GLU:HA	1:202:B:ALA:HB3	9	13.91
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	17	13.88
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	17	13.88
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	17	13.88
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	20	13.87
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	20	13.87
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	20	13.87
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	15	13.86
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	15	13.86
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	15	13.86
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	15	13.81
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	15	13.81
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	15	13.81
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	15	13.81
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	4	13.74
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	4	13.74
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	4	13.74
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	20	13.72
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	20	13.72
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	3	13.63
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	3	13.63
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	15	13.59
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	15	13.59
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	16	13.59
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	16	13.59
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	13	13.57
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	13	13.57
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	13	13.57
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	13	13.57
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	1	13.56
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	1	13.56
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	1	13.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	1	13.56
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	10	13.54
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	10	13.54
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	11	13.54
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	11	13.54
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	17	13.52
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	17	13.52
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	19	13.51
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	19	13.51
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	1	13.46
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	1	13.46
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	5	13.45
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	5	13.45
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	12	13.45
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	12	13.45
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	9	13.44
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	9	13.44
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	9	13.44
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	9	13.44
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB1	16	13.43
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB2	16	13.43
(1,6761)	2:406:C:DA:H8	1:59:A:ALA:HB3	16	13.43
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	8	13.43
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	8	13.43
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	18	13.43
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	18	13.43
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	14	13.42
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	14	13.42
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	7	13.41
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	7	13.41
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	2	13.39
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	2	13.39
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	12	13.37
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	12	13.37
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	12	13.37
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	12	13.37
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	16	13.37
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	16	13.37
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	16	13.37
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	16	13.37
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	18	13.34
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	18	13.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	18	13.34
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	18	13.34
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	3	13.33
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	3	13.33
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	3	13.33
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	3	13.33
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	4	13.31
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	4	13.31
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	13	13.27
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	13	13.27
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA2	6	13.26
(1,6743)	2:403:C:DT:H5'	1:25:A:GLY:HA3	6	13.26
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA2	6	13.26
(1,6743)	2:403:C:DT:H5''	1:25:A:GLY:HA3	6	13.26
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB2	20	13.22
(1,6758)	2:406:C:DA:H1'	1:57:A:ASN:HB3	20	13.22
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	9	13.17
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	9	13.17
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA2	6	13.08
(1,6740)	2:402:C:DT:H4'	1:27:A:GLY:HA3	6	13.08
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	20	12.68
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	10	12.51
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	17	12.5
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	19	12.5
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	11	12.49
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	5	12.38
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	14	12.38
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	2	12.33
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	8	12.33
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	7	12.28
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	7	12.23
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	4	12.2
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	15	12.2
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	8	12.07
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	18	12.06
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	17	12.01
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	10	12.0
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	11	11.98
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	19	11.98
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	5	11.96
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	13	11.95
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	12	11.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	2	11.91
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	1	11.86
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	13	11.84
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	9	11.83
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	16	11.82
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	3	11.78
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	15	11.77
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	18	11.74
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	9	11.73
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	6	11.7
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	12	11.65
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	1	11.55
(1,6751)	2:404:C:DC:H6	1:26:A:ILE:H	6	11.55
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	14	11.54
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	3	11.48
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	4	11.45
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	16	11.34
(1,6757)	2:405:C:DA:H1'	1:58:A:GLN:HA	20	11.21
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	7	10.85
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	8	10.76
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	17	10.7
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	10	10.68
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	19	10.65
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	5	10.64
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	18	10.64
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	11	10.63
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	12	10.58
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	2	10.56
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	13	10.5
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	9	10.45
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	15	10.41
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	6	10.37
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	1	10.27
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	14	10.23
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	3	10.17
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	4	10.17
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	16	10.06
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	5	10.04
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	5	10.04
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	7	10.02
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	7	10.02
(1,6755)	2:405:C:DA:H4'	1:58:A:GLN:HA	20	9.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	8	9.92
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	8	9.92
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	10	9.92
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	10	9.92
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	18	9.78
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	18	9.78
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	12	9.74
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	12	9.74
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	17	9.73
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	17	9.73
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	3	9.73
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	3	9.73
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	16	9.72
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	16	9.72
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	2	9.7
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	2	9.7
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	18	9.7
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	13	9.69
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	13	9.69
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	2	9.68
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	9	9.68
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	6	9.67
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	20	9.67
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	11	9.65
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	11	9.65
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	17	9.65
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	15	9.64
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	15	9.63
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	15	9.63
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	5	9.63
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	11	9.63
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	15	9.61
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	15	9.61
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	20	9.61
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	20	9.61
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	14	9.61
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	9	9.6
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	9	9.6
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	7	9.6
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	13	9.6
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	20	9.59
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	20	9.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	3	9.58
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	6	9.56
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	6	9.56
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	4	9.55
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	19	9.54
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	19	9.54
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	10	9.53
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	1	9.51
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	1	9.51
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	1	9.51
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	12	9.51
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	3	9.48
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	3	9.48
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	11	9.46
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	11	9.46
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	12	9.46
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	12	9.46
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	10	9.44
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	10	9.44
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	19	9.44
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	4	9.43
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	4	9.43
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	17	9.42
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	17	9.42
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	16	9.42
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	18	9.41
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	18	9.41
(1,6750)	2:404:C:DC:H5	1:30:A:LYS:HA	8	9.41
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	1	9.39
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	1	9.39
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	14	9.31
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	14	9.31
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	19	9.3
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	19	9.3
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	5	9.28
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	5	9.28
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	7	9.26
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	7	9.26
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	2	9.24
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	2	9.24
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	18	9.22
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	18	9.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	8	9.22
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	8	9.22
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	13	9.22
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	13	9.22
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB2	16	9.21
(1,6759)	2:406:C:DA:H1'	1:58:A:GLN:HB3	16	9.21
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	9	9.17
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	9	9.17
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	14	9.17
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	14	9.17
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	7	9.08
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	7	9.08
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	6	9.04
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	6	9.04
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA2	4	9.01
(1,6752)	2:404:C:DC:H6	1:27:A:GLY:HA3	4	9.01
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	9	8.99
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	9	8.99
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	12	8.91
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	12	8.91
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	19	8.81
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	19	8.81
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	15	8.75
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	15	8.75
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	10	8.73
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	10	8.73
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	2	8.6
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	2	8.6
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	13	8.6
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	13	8.6
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	5	8.56
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	5	8.56
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	17	8.52
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	17	8.52
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	8	8.42
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	8	8.42
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	11	8.07
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	11	8.07
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	6	8.04
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	6	8.04
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	14	7.98
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	14	7.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	3	7.82
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	3	7.82
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	1	7.8
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	1	7.8
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	4	7.8
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	4	7.8
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	16	7.8
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	16	7.8
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	8	6.8
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	4	6.67
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	20	6.57
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB2	20	6.44
(1,6754)	2:405:C:DA:H8	1:57:A:ASN:HB3	20	6.44
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	9	6.42
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	18	6.4
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	14	6.38
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	14	6.38
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	17	6.27
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	5	6.19
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	8	6.19
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	6	6.16
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	1	6.13
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	19	6.07
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	19	6.07
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	7	6.0
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	2	5.98
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	3	5.97
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	12	5.96
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	12	5.96
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	16	5.95
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	8	5.9
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	8	5.9
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	20	5.88
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	14	5.85
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	10	5.76
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	11	5.76
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	11	5.76
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	11	5.71
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	17	5.68
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	17	5.68
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	10	5.63
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	10	5.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	7	5.58
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	7	5.58
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	19	5.56
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	13	5.54
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	3	5.52
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	3	5.52
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	2	5.5
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	2	5.5
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	12	5.48
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	15	5.44
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	5	5.43
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	5	5.43
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	13	5.43
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	13	5.43
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	18	5.42
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	18	5.42
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	15	5.41
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	15	5.41
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	9	5.3
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	9	5.3
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	8	5.26
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	5	5.24
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	1	5.21
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	1	5.21
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	19	5.17
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	6	5.17
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	6	5.17
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	5	5.12
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	20	5.08
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	4	5.08
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	4	5.08
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	20	5.05
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	20	5.05
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	20	5.03
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	20	5.03
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	20	4.96
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	20	4.96
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	7	4.9
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	18	4.88
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	17	4.88
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	19	4.87
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	4	4.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	8	4.78
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG2	16	4.75
(1,6756)	2:405:C:DA:H4'	1:58:A:GLN:HG3	16	4.75
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	5	4.69
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	5	4.69
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	20	4.69
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	20	4.69
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	19	4.67
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	8	4.63
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	4	4.63
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	2	4.61
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	8	4.58
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	8	4.58
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	17	4.58
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	17	4.58
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	16	4.57
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	17	4.55
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	9	4.53
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	1	4.53
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	1	4.51
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	14	4.43
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	20	4.39
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	11	4.37
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	4	4.36
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	15	4.35
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	15	4.35
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	15	4.35
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	4	4.29
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	16	4.26
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	18	4.25
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	18	4.25
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	19	4.24
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	8	4.2
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	8	4.2
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	14	4.17
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	5	4.16
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	18	4.15
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	4	4.11
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	3	4.11
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	20	4.1
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	4	4.1
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	4	4.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	2	4.09
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	6	4.09
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	6	4.09
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	19	4.08
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	18	4.08
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	18	4.08
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	6	4.07
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	9	4.07
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	9	4.07
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	17	4.06
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	15	4.06
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	15	4.06
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	14	4.05
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	7	4.03
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	5	4.02
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	3	4.02
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	2	4.02
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	2	4.02
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	9	4.01
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	1	4.0
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	15	4.0
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	15	4.0
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	7	4.0
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	7	4.0
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	9	3.99
(1,6976)	1:213:B:ASP:HA	1:58:A:GLN:HB3	14	3.97
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	11	3.97
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	11	3.97
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	12	3.97
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	12	3.97
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	14	3.97
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	14	3.97
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	13	3.96
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	13	3.96
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	17	3.96
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	17	3.96
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	20	3.96
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	20	3.96
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	2	3.95
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	5	3.95
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	5	3.95
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	10	3.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	10	3.95
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	17	3.94
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	18	3.94
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	6	3.94
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	6	3.94
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	8	3.93
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	8	3.93
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	3	3.93
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	3	3.93
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	5	3.91
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	5	3.91
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	6	3.91
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	17	3.91
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	1	3.9
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	8	3.88
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	1	3.88
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	1	3.88
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	4	3.88
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	4	3.88
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	10	3.85
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	19	3.84
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	19	3.84
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	2	3.82
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	10	3.82
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	14	3.81
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	15	3.81
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	12	3.8
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	5	3.8
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	16	3.79
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	16	3.79
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	8	3.78
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	17	3.78
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	9	3.78
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	10	3.74
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	18	3.74
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB2	8	3.74
(1,6753)	2:405:C:DA:H3'	1:30:A:LYS:HB3	8	3.74
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	9	3.73
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	9	3.73
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	16	3.71
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	16	3.71
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	7	3.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	19	3.67
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	19	3.67
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	4	3.66
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	7	3.63
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	2	3.61
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	9	3.61
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	9	3.61
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	9	3.61
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	9	3.61
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	17	3.6
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	18	3.59
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	3	3.57
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	10	3.56
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	19	3.55
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	1	3.55
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	16	3.55
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	6	3.53
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	2	3.52
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	19	3.51
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	7	3.51
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	1	3.5
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	3	3.48
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	10	3.48
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	14	3.47
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	19	3.45
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	13	3.45
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	18	3.45
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	18	3.45
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	19	3.44
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	19	3.44
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	19	3.44
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	2	3.44
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	9	3.44
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	16	3.43
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	3	3.42
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	17	3.41
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	16	3.41
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	13	3.39
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	13	3.39
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	4	3.36
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	15	3.36
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	17	3.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	15	3.36
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	15	3.36
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	15	3.36
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	15	3.36
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	11	3.35
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	11	3.33
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	4	3.33
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	11	3.32
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	7	3.31
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	13	3.3
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	18	3.29
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	4	3.29
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	1	3.27
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	19	3.27
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	6	3.26
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	1	3.26
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	3	3.25
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	12	3.25
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	19	3.25
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	20	3.23
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	20	3.23
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	7	3.22
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	5	3.21
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	11	3.21
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	16	3.21
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	13	3.2
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	13	3.2
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	13	3.2
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	13	3.2
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	2	3.19
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	9	3.18
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	9	3.18
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	14	3.18
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	14	3.18
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	14	3.17
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	15	3.17
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	15	3.16
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	7	3.16
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	7	3.16
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	8	3.15
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	13	3.15
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	10	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	6	3.14
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	3	3.13
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	4	3.12
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	2	3.12
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	11	3.12
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	13	3.12
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	7	3.12
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	15	3.11
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	9	3.11
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	9	3.11
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	1	3.1
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	14	3.1
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	13	3.09
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	13	3.09
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	16	3.08
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	16	3.08
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	9	3.08
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	3	3.08
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	14	3.07
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	3	3.07
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	3	3.07
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	17	3.06
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	5	3.05
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	5	3.05
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	4	3.05
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	4	3.05
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	14	3.05
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	9	3.05
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	9	3.05
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	18	3.05
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	16	3.04
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	16	3.03
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	6	3.02
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	6	3.02
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	12	3.01
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	14	3.0
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	17	3.0
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	7	3.0
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	18	3.0
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	18	3.0
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	18	3.0
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	18	3.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	3	2.99
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	10	2.99
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	10	2.99
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	10	2.99
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	2	2.99
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	8	2.99
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	8	2.99
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	4	2.98
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	12	2.98
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	1	2.94
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	11	2.94
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	11	2.94
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	15	2.94
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	15	2.94
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	16	2.93
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	16	2.93
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	16	2.93
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	7	2.92
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	7	2.92
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	18	2.91
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	18	2.91
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	18	2.91
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	15	2.91
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	20	2.9
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	15	2.89
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	13	2.88
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	13	2.88
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	1	2.88
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	1	2.88
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	15	2.87
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	15	2.87
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	10	2.87
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	19	2.86
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	19	2.86
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	3	2.86
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	11	2.86
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	1	2.85
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	2	2.85
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	2	2.85
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	17	2.85
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	17	2.85
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	15	2.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	4	2.83
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	4	2.83
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	9	2.83
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	10	2.82
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	10	2.82
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	11	2.81
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	11	2.81
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	11	2.81
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	7	2.81
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	10	2.81
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	4	2.8
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	4	2.8
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	20	2.8
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	20	2.8
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	5	2.79
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	8	2.79
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	13	2.79
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	9	2.77
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	9	2.77
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	9	2.77
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	12	2.77
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	1	2.76
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	1	2.76
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	19	2.76
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	19	2.76
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	5	2.74
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	2	2.73
(1,6979)	1:213:B:ASP:HA	1:58:A:GLN:HG2	12	2.73
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	18	2.72
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	12	2.71
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	15	2.71
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	15	2.71
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	18	2.71
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	18	2.71
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	17	2.71
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	17	2.71
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	14	2.7
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	5	2.7
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	5	2.7
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	12	2.69
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	8	2.69
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	7	2.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	18	2.66
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	18	2.66
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	12	2.66
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	18	2.66
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	5	2.65
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	10	2.64
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	10	2.64
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	18	2.64
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	7	2.63
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	7	2.63
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	3	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	3	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	3	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	8	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	8	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	8	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	13	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	13	2.62
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	13	2.62
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	17	2.61
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	2	2.61
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	2	2.61
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	2	2.61
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	2	2.61
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	9	2.61
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	2	2.61
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	2	2.61
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	2	2.61
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	2	2.61
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	15	2.6
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	15	2.6
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	4	2.59
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	4	2.59
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	4	2.59
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	4	2.59
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	8	2.59
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	6	2.58
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	20	2.57
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	20	2.57
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	20	2.57
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	7	2.57
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	7	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	6	2.57
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	17	2.56
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	17	2.56
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	17	2.56
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	17	2.56
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	3	2.56
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	4	2.55
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	20	2.55
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	19	2.55
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	19	2.55
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	8	2.54
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	13	2.54
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	17	2.53
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	17	2.53
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	9	2.53
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	10	2.53
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	9	2.52
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	20	2.52
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	20	2.52
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE1	3	2.52
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE2	3	2.52
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE3	3	2.52
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE1	3	2.52
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE2	3	2.52
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE3	3	2.52
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	16	2.51
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	19	2.51
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	19	2.51
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	19	2.51
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	19	2.51
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	19	2.51
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	19	2.51
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	2	2.49
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	2	2.49
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	3	2.49
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	3	2.49
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	1	2.48
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	7	2.48
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	17	2.48
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	17	2.48
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	17	2.46
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	17	2.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	17	2.46
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	8	2.46
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	8	2.46
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	8	2.46
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	8	2.46
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	1	2.46
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	1	2.46
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	18	2.46
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	20	2.45
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	7	2.44
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	7	2.44
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	7	2.44
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	12	2.44
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	12	2.44
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	1	2.43
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	1	2.43
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	13	2.43
(1,6978)	1:213:B:ASP:HA	1:58:A:GLN:HG3	15	2.43
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	1	2.43
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	1	2.43
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	1	2.43
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	1	2.43
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	4	2.43
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	4	2.43
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	1	2.43
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	1	2.43
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	10	2.43
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	10	2.43
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	11	2.43
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	11	2.43
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	18	2.43
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	18	2.43
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	3	2.42
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	3	2.42
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	14	2.42
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	5	2.42
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	5	2.42
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	5	2.42
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	5	2.42
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	8	2.42
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	8	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	2	2.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	2	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	3	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	3	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	4	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	4	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	5	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	5	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	6	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	6	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	7	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	7	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	8	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	8	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	9	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	9	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	12	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	12	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	13	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	13	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	14	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	14	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	15	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	15	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	16	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	16	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	17	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	17	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	19	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	19	2.42
(1,3356)	2:412:D:DT:H5'	2:412:D:DT:H6	20	2.42
(1,3356)	2:412:D:DT:H5''	2:412:D:DT:H6	20	2.42
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	20	2.41
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	20	2.41
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	20	2.41
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	20	2.41
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	19	2.38
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	19	2.38
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	9	2.38
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	4	2.38
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	4	2.38
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	2	2.37
(1,6977)	1:213:B:ASP:HA	1:58:A:GLN:HB2	5	2.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	10	2.37
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	10	2.37
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	3	2.36
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	3	2.36
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	3	2.36
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	3	2.36
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	3	2.36
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	3	2.36
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	6	2.35
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	6	2.35
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	20	2.35
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	20	2.35
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	13	2.34
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	13	2.34
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	7	2.34
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	6	2.32
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	6	2.32
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	6	2.32
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	6	2.32
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	6	2.32
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	7	2.31
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	14	2.29
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	14	2.29
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	5	2.28
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	12	2.27
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	10	2.27
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	10	2.27
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	10	2.27
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	16	2.26
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	20	2.26
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	4	2.25
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	9	2.25
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	19	2.24
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	19	2.24
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	5	2.24
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	5	2.24
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	7	2.22
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	7	2.22
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	7	2.22
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	7	2.22
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	11	2.21
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	11	2.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	9	2.19
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	9	2.19
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	13	2.19
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	13	2.19
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	10	2.17
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	8	2.14
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	10	2.14
(1,322)	1:221:B:PHE:HZ	1:296:B:SER:H	2	2.14
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	6	2.13
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	16	2.13
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	16	2.13
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	17	2.13
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	17	2.13
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	15	2.13
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	17	2.13
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	17	2.13
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	6	2.12
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	6	2.12
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	19	2.11
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	16	2.11
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	1	2.11
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	1	2.11
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	5	2.11
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	2	2.09
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	10	2.07
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	6	2.06
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	6	2.06
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	7	2.06
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	13	2.06
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	13	2.04
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	14	2.04
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	14	2.04
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	13	2.04
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	13	2.04
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	10	2.02
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	10	2.02
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	10	2.02
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	10	2.02
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	11	2.02
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	11	2.02
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	11	2.02
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	11	2.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	12	2.02
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	12	2.02
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	12	2.02
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	12	2.02
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	14	2.02
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	14	2.02
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	12	2.02
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	12	2.02
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	2	2.01
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	2	2.01
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	18	2.0
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	16	2.0
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	6	2.0
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	6	2.0
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	9	1.99
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	15	1.98
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	11	1.98
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	10	1.97
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	10	1.97
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	16	1.95
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	16	1.95
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE1	1	1.95
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE2	1	1.95
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE3	1	1.95
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE1	1	1.95
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE2	1	1.95
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE3	1	1.95
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	19	1.94
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	19	1.94
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	8	1.94
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	8	1.94
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	12	1.92
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	12	1.92
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	6	1.92
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	5	1.91
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	8	1.89
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	8	1.89
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	3	1.89
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	3	1.89
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	2	1.88
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	2	1.88
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	7	1.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	19	1.88
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	5	1.86
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	1	1.86
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	6	1.86
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	11	1.85
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	11	1.85
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	2	1.85
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	2	1.85
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	3	1.84
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	3	1.84
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	1	1.84
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	14	1.83
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	14	1.83
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	14	1.83
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	14	1.83
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	16	1.8
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	16	1.8
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	20	1.79
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	8	1.79
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	19	1.79
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	18	1.79
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	16	1.79
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	16	1.79
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	2	1.77
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	2	1.77
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	8	1.76
(1,6981)	1:213:B:ASP:HB2	1:58:A:GLN:HB3	14	1.75
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	19	1.75
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	16	1.73
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	16	1.73
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	17	1.72
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	18	1.72
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	10	1.7
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB2	10	1.7
(1,6958)	1:208:B:PRO:HB3	1:165:A:PHE:HB3	10	1.7
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	3	1.7
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	3	1.7
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	3	1.7
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	10	1.69
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	15	1.69
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	8	1.68
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	14	1.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	14	1.67
(1,321)	1:221:B:PHE:HZ	1:233:B:CYS:H	2	1.67
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	7	1.64
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	7	1.64
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	13	1.64
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	19	1.63
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	13	1.63
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	18	1.62
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	12	1.62
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	12	1.62
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	17	1.62
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	7	1.62
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	12	1.62
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	10	1.61
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	13	1.61
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	8	1.61
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	14	1.6
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	14	1.6
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	4	1.6
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	4	1.6
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	18	1.59
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	2	1.59
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	4	1.59
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	9	1.59
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	15	1.59
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	3	1.58
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	5	1.58
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	1	1.58
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	5	1.58
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	6	1.58
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	10	1.58
(1,1404)	1:282:B:GLN:HB2	1:282:B:GLN:HE22	20	1.58
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	1	1.57
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	1	1.57
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	1	1.57
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	1	1.57
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	1	1.56
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	15	1.56
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	15	1.56
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	8	1.56
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	2	1.56
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	2	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	5	1.56
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	5	1.56
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	7	1.56
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	7	1.56
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	15	1.56
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	9	1.56
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	15	1.55
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	15	1.55
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	4	1.55
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	3	1.55
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	6	1.54
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	8	1.54
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	3	1.54
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	3	1.54
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	17	1.54
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	17	1.54
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	6	1.53
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	6	1.53
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	11	1.53
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	11	1.53
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	19	1.53
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	19	1.53
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	6	1.53
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	4	1.52
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	4	1.52
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	17	1.52
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	16	1.51
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	16	1.51
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	19	1.51
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	4	1.5
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	4	1.5
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	14	1.5
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	14	1.5
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	20	1.5
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	20	1.5
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	4	1.5
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	2	1.49
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	1	1.49
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	1	1.49
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	13	1.49
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	13	1.49
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	10	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	10	1.48
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	2	1.48
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	2	1.48
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	2	1.48
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	14	1.48
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	20	1.47
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	17	1.47
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	17	1.47
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	10	1.47
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	14	1.45
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	7	1.45
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	7	1.45
(1,6983)	1:213:B:ASP:HB2	1:58:A:GLN:HB2	20	1.44
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	15	1.44
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	8	1.42
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	8	1.42
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	18	1.42
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	2	1.41
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	2	1.41
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	13	1.41
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	13	1.41
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	16	1.41
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	2	1.4
(1,6957)	1:208:B:PRO:HA	1:165:A:PHE:HD1	15	1.4
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	1	1.4
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	1	1.4
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	7	1.4
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	4	1.39
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	4	1.39
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	8	1.39
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	8	1.39
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	19	1.39
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	19	1.39
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	6	1.39
(1,6989)	1:214:B:PRO:HG2	1:58:A:GLN:HG2	11	1.38
(1,6989)	1:214:B:PRO:HG3	1:58:A:GLN:HG2	11	1.38
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	5	1.38
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	5	1.38
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	15	1.38
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	15	1.38
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	16	1.38
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	16	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	20	1.38
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	16	1.37
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	19	1.37
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	19	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	3	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	3	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	6	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	6	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	7	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	7	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	14	1.37
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	14	1.37
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	14	1.37
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	5	1.37
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	5	1.37
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	5	1.37
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	2	1.37
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	5	1.37
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	1	1.36
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	1	1.36
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	10	1.36
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	10	1.36
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	20	1.36
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	20	1.36
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	15	1.36
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	15	1.36
(1,6980)	1:213:B:ASP:HB3	1:58:A:GLN:HB3	14	1.35
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	12	1.35
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	12	1.35
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	16	1.35
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	9	1.34
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	9	1.34
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	12	1.34
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	12	1.34
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	18	1.34
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	18	1.34
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	3	1.34
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	13	1.34
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	13	1.34
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	11	1.34
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	20	1.33
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	17	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	17	1.32
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	12	1.32
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5'	11	1.31
(1,6784)	2:399:C:DA:H8	2:400:C:DT:H5''	11	1.31
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	13	1.31
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	3	1.3
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	1	1.3
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	1	1.3
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	9	1.3
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	9	1.3
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	10	1.29
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	10	1.29
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	13	1.29
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	20	1.29
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	20	1.29
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	1	1.29
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	1	1.29
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	20	1.28
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	18	1.27
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	6	1.26
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	6	1.26
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	3	1.25
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	17	1.25
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	17	1.25
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE1	3	1.25
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE2	3	1.25
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE3	3	1.25
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE1	3	1.25
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE2	3	1.25
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE3	3	1.25
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	7	1.24
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	7	1.24
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	7	1.24
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	3	1.23
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	3	1.23
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	19	1.22
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	19	1.22
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE1	2	1.22
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE2	2	1.22
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE3	2	1.22
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE1	2	1.22
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE2	2	1.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE3	2	1.22
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	3	1.21
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	3	1.21
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	13	1.21
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	17	1.2
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB2	16	1.2
(1,6963)	1:208:B:PRO:HG2	1:165:A:PHE:HB3	16	1.2
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB2	16	1.2
(1,6963)	1:208:B:PRO:HG3	1:165:A:PHE:HB3	16	1.2
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	7	1.2
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	7	1.2
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB2	16	1.19
(1,6959)	1:208:B:PRO:HB2	1:165:A:PHE:HB3	16	1.19
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	20	1.19
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	4	1.19
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	4	1.19
(1,319)	1:221:B:PHE:HE1	1:296:B:SER:H	2	1.19
(1,319)	1:221:B:PHE:HE2	1:296:B:SER:H	2	1.19
(1,319)	1:221:B:PHE:HE1	1:296:B:SER:H	1	1.18
(1,319)	1:221:B:PHE:HE2	1:296:B:SER:H	1	1.18
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	18	1.17
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	20	1.17
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	20	1.17
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	20	1.17
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	12	1.16
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD21	10	1.16
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD22	10	1.16
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD23	10	1.16
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	1	1.16
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	1	1.16
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	1	1.16
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	14	1.16
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	14	1.16
(1,319)	1:221:B:PHE:HE1	1:296:B:SER:H	7	1.16
(1,319)	1:221:B:PHE:HE2	1:296:B:SER:H	7	1.16
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	4	1.15
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	4	1.15
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	4	1.15
(1,573)	1:237:B:GLU:HG2	1:290:B:ARG:HB3	17	1.15
(1,573)	1:237:B:GLU:HG2	1:290:B:ARG:HB3	20	1.15
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	4	1.14
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	5	1.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	12	1.14
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	12	1.14
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	12	1.14
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	12	1.14
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	12	1.14
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	12	1.14
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	12	1.14
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	12	1.14
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	12	1.14
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	10	1.14
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	10	1.14
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG21	18	1.14
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG22	18	1.14
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG23	18	1.14
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	7	1.14
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	7	1.14
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	7	1.14
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	4	1.13
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	10	1.13
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	10	1.13
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	15	1.13
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	15	1.13
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	15	1.13
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	15	1.13
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	15	1.13
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	15	1.13
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	15	1.13
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	15	1.13
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	15	1.13
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	13	1.13
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	13	1.13
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	13	1.13
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	15	1.12
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	15	1.12
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	5	1.12
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	19	1.12
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	17	1.12
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	17	1.12
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	17	1.12
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	18	1.12
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	18	1.12
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	18	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	18	1.12
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	18	1.12
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	18	1.12
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	18	1.12
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	18	1.12
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	18	1.12
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	20	1.12
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	20	1.12
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	20	1.12
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	18	1.12
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	18	1.12
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	12	1.12
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	12	1.12
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	12	1.12
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	5	1.11
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	12	1.11
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	10	1.11
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	10	1.11
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	10	1.11
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	10	1.11
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	10	1.11
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	10	1.11
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	10	1.11
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	10	1.11
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	10	1.11
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	2	1.11
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	2	1.11
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	2	1.11
(1,322)	1:221:B:PHE:HZ	1:296:B:SER:H	7	1.11
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	17	1.1
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	6	1.1
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	16	1.1
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	3	1.1
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	3	1.1
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	3	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	3	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	3	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	3	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	3	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	3	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	3	1.1
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	9	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	9	1.1
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	9	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	9	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	9	1.1
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	9	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	9	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	9	1.1
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	9	1.1
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	7	1.1
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	7	1.1
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	7	1.1
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	12	1.1
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	12	1.1
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	12	1.1
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	15	1.09
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	11	1.09
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	19	1.09
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	19	1.09
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	19	1.09
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	19	1.09
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	19	1.09
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	19	1.09
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	19	1.09
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	19	1.09
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	19	1.09
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	11	1.09
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	11	1.09
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	11	1.09
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	13	1.09
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	13	1.09
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	13	1.09
(1,573)	1:237:B:GLU:HG2	1:290:B:ARG:HB3	1	1.09
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG21	13	1.09
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG22	13	1.09
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG23	13	1.09
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	9	1.09
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	9	1.09
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	9	1.09
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	20	1.09
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	20	1.09
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	20	1.09
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	9	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	9	1.08
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	18	1.08
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	18	1.08
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	18	1.08
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	17	1.08
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	17	1.08
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	17	1.08
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	2	1.08
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	2	1.08
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	2	1.08
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	3	1.08
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	3	1.08
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	3	1.08
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	15	1.07
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	15	1.07
(1,6982)	1:213:B:ASP:HB3	1:58:A:GLN:HB2	20	1.07
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	18	1.07
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	18	1.07
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	20	1.07
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	20	1.07
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	16	1.07
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	16	1.07
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	16	1.07
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	14	1.06
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	14	1.06
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	14	1.06
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	14	1.06
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	14	1.06
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	14	1.06
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	14	1.06
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	14	1.06
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	14	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	9	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	9	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	9	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	15	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	15	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	15	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	18	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	18	1.06
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	18	1.06
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	6	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	6	1.06
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	6	1.06
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	9	1.06
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	10	1.06
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	10	1.06
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	10	1.06
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	9	1.05
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	11	1.05
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	11	1.05
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	1	1.05
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	14	1.05
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	14	1.05
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	14	1.05
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	13	1.05
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	13	1.05
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	13	1.05
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	7	1.05
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	7	1.05
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	7	1.05
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	10	1.05
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	11	1.05
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	11	1.05
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	11	1.05
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	11	1.05
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	11	1.05
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	11	1.05
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	5	1.05
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	5	1.05
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	5	1.05
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	11	1.05
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	11	1.05
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	11	1.05
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	15	1.05
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	15	1.05
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	15	1.05
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	12	1.04
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	12	1.04
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	17	1.04
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	17	1.04
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	17	1.04
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	17	1.04
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	17	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	17	1.04
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	17	1.04
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	17	1.04
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	17	1.04
(1,2686)	1:357:B:PHE:HD1	1:378:B:LEU:HG	3	1.04
(1,2686)	1:357:B:PHE:HD2	1:378:B:LEU:HG	3	1.04
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	6	1.04
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	6	1.04
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	6	1.04
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	19	1.04
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	19	1.04
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	19	1.04
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	7	1.04
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	7	1.04
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	6	1.04
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	6	1.04
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	6	1.04
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	9	1.03
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	9	1.03
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	18	1.03
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	13	1.03
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	13	1.03
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	13	1.03
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD11	11	1.03
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD12	11	1.03
(1,4525)	1:73:A:LEU:HD21	1:76:A:LEU:HD13	11	1.03
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD11	11	1.03
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD12	11	1.03
(1,4525)	1:73:A:LEU:HD22	1:76:A:LEU:HD13	11	1.03
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD11	11	1.03
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD12	11	1.03
(1,4525)	1:73:A:LEU:HD23	1:76:A:LEU:HD13	11	1.03
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	14	1.03
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	14	1.03
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	14	1.03
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	8	1.03
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	8	1.03
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	8	1.03
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	7	1.02
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	7	1.02
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	17	1.02
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	1	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	1	1.02
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	1	1.02
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	16	1.02
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	16	1.02
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	16	1.02
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	13	1.02
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	16	1.02
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	16	1.02
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	16	1.02
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	16	1.02
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	16	1.02
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	16	1.02
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	13	1.02
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	13	1.02
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	13	1.02
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	10	1.01
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	10	1.01
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	10	1.01
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	12	1.01
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	12	1.01
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	12	1.01
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD21	10	1.01
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD22	10	1.01
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD23	10	1.01
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	5	1.01
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	5	1.01
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	16	1.01
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	16	1.01
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	12	1.01
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	12	1.01
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	12	1.01
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	12	1.01
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	12	1.01
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	12	1.01
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	9	1.01
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	9	1.01
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	9	1.01
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	12	1.0
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	7	1.0
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	7	1.0
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD21	15	1.0
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD22	15	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD23	15	1.0
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	16	1.0
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	8	1.0
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	8	1.0
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	8	1.0
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	15	1.0
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	15	1.0
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	15	1.0
(1,1674)	1:294:B:PHE:HA	1:360:B:CYS:HG	11	1.0
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD21	14	1.0
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD22	14	1.0
(1,1596)	1:291:B:VAL:HB	1:321:B:LEU:HD23	14	1.0
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	16	1.0
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	16	1.0
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	16	1.0
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	9	1.0
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	9	1.0
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	9	1.0
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	2	1.0
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	2	1.0
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	15	1.0
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	15	1.0
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	15	1.0
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	15	1.0
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	15	1.0
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	15	1.0
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	18	0.99
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	18	0.99
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	18	0.99
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	5	0.99
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	5	0.99
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	5	0.99
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	4	0.99
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	4	0.99
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	4	0.99
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	4	0.99
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	4	0.99
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	4	0.99
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	13	0.98
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	13	0.98
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	13	0.98
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	8	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	8	0.98
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	8	0.98
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	15	0.98
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	15	0.98
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	15	0.98
(1,778)	1:246:B:LYS:HE2	1:246:B:LYS:H	11	0.98
(1,778)	1:246:B:LYS:HE3	1:246:B:LYS:H	11	0.98
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	7	0.98
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	7	0.98
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	7	0.98
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	7	0.98
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	7	0.98
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	7	0.98
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	20	0.98
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	20	0.98
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	20	0.98
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	20	0.98
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	20	0.98
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	20	0.98
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	1	0.98
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	1	0.98
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	1	0.98
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	8	0.98
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	8	0.98
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	8	0.98
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	4	0.97
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	4	0.97
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	6	0.97
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	3	0.97
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	3	0.97
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	3	0.97
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	9	0.96
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	9	0.96
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	9	0.96
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	10	0.96
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	10	0.96
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	10	0.96
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	20	0.96
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	20	0.96
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	20	0.96
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	4	0.96
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	4	0.96

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	4	0.96
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	6	0.96
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	6	0.96
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	6	0.96
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	6	0.96
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	6	0.96
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	6	0.96
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	14	0.95
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	14	0.95
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	14	0.95
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	16	0.95
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	16	0.95
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	16	0.95
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	5	0.95
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	5	0.95
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	5	0.95
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD21	14	0.94
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD22	14	0.94
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD23	14	0.94
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	5	0.93
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	5	0.93
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	5	0.93
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	4	0.93
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	19	0.93
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	19	0.93
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	19	0.93
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	6	0.93
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	6	0.93
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	6	0.93
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	12	0.92
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	12	0.92
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	12	0.92
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	13	0.92
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	13	0.92
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	13	0.92
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE1	12	0.92
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE2	12	0.92
(1,317)	1:221:B:PHE:HD1	1:352:B:MET:HE3	12	0.92
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE1	12	0.92
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE2	12	0.92
(1,317)	1:221:B:PHE:HD2	1:352:B:MET:HE3	12	0.92
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	16	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	14	0.91
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	14	0.91
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	20	0.91
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	20	0.91
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	20	0.91
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	8	0.91
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	8	0.91
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	8	0.91
(1,322)	1:221:B:PHE:HZ	1:296:B:SER:H	1	0.91
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	1	0.9
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	1	0.9
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	14	0.9
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	14	0.9
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	6	0.9
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	17	0.9
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	20	0.9
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	20	0.9
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	20	0.9
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	14	0.9
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	14	0.9
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	14	0.9
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	16	0.9
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	16	0.9
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	16	0.9
(1,2383)	1:339:B:LEU:HD11	1:392:B:ILE:HG12	3	0.89
(1,2383)	1:339:B:LEU:HD11	1:392:B:ILE:HG13	3	0.89
(1,2383)	1:339:B:LEU:HD12	1:392:B:ILE:HG12	3	0.89
(1,2383)	1:339:B:LEU:HD12	1:392:B:ILE:HG13	3	0.89
(1,2383)	1:339:B:LEU:HD13	1:392:B:ILE:HG12	3	0.89
(1,2383)	1:339:B:LEU:HD13	1:392:B:ILE:HG13	3	0.89
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	17	0.89
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	17	0.89
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	17	0.89
(1,6986)	1:213:B:ASP:HB3	1:58:A:GLN:HG2	11	0.88
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	9	0.88
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	13	0.88
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	13	0.87
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	16	0.87
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	16	0.87
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	16	0.87
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	11	0.87
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	4	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	4	0.87
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	4	0.87
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	2	0.87
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	2	0.87
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	2	0.87
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	10	0.87
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	10	0.87
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	10	0.87
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	2	0.86
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	16	0.86
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	18	0.86
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	18	0.86
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	18	0.86
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	18	0.86
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	17	0.86
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	17	0.86
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	17	0.86
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	18	0.85
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	18	0.85
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	7	0.85
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD21	18	0.85
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD22	18	0.85
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD23	18	0.85
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	13	0.85
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	13	0.85
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	13	0.85
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	6	0.85
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	11	0.85
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	9	0.85
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	9	0.85
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	9	0.85
(1,6960)	1:208:B:PRO:HB3	1:165:A:PHE:HD1	20	0.84
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	11	0.84
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	1	0.84
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	1	0.84
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	1	0.84
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	4	0.84
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	6	0.84
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	6	0.84
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	6	0.84
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	11	0.84
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	11	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	11	0.84
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	9	0.83
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	9	0.83
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	9	0.83
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	2	0.83
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	2	0.83
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	2	0.83
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	15	0.83
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	15	0.83
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	15	0.83
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	9	0.82
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	16	0.82
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	1	0.82
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	19	0.82
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	19	0.82
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	19	0.82
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	5	0.82
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	5	0.82
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	5	0.82
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	10	0.82
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	10	0.82
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	10	0.82
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	10	0.82
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	10	0.82
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	10	0.82
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	3	0.81
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	8	0.81
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	8	0.81
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	8	0.81
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	13	0.8
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	13	0.8
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	10	0.8
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	3	0.8
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	6	0.8
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	5	0.8
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	5	0.8
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	5	0.8
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	14	0.8
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	14	0.8
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	14	0.8
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	14	0.8
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	14	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	14	0.8
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	14	0.8
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	14	0.8
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	14	0.8
(1,316)	1:221:B:PHE:HD1	1:296:B:SER:H	1	0.8
(1,316)	1:221:B:PHE:HD2	1:296:B:SER:H	1	0.8
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	4	0.8
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	4	0.8
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	4	0.8
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	10	0.79
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	17	0.79
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	17	0.79
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	17	0.79
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	17	0.79
(1,522)	1:236:B:VAL:HG11	1:289:B:TYR:HA	1	0.79
(1,522)	1:236:B:VAL:HG12	1:289:B:TYR:HA	1	0.79
(1,522)	1:236:B:VAL:HG13	1:289:B:TYR:HA	1	0.79
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	2	0.78
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	14	0.78
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	12	0.78
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	12	0.78
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	12	0.78
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	15	0.78
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	15	0.78
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	15	0.78
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	1	0.78
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	1	0.78
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	1	0.78
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	9	0.77
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	9	0.77
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	9	0.77
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	8	0.77
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	8	0.77
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	8	0.77
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	8	0.77
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	8	0.77
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	8	0.77
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	11	0.76
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	11	0.76
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	11	0.76
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	16	0.76
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	8	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	7	0.76
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	7	0.76
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	7	0.76
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	7	0.76
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	13	0.76
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	13	0.76
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	13	0.76
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	3	0.76
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	3	0.76
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	3	0.76
(1,316)	1:221:B:PHE:HD1	1:296:B:SER:H	7	0.76
(1,316)	1:221:B:PHE:HD2	1:296:B:SER:H	7	0.76
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	11	0.75
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	17	0.75
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	6	0.75
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	6	0.75
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	6	0.75
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	4	0.75
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	4	0.75
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	4	0.75
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	9	0.75
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	9	0.75
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	9	0.75
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	1	0.74
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	15	0.74
(1,6987)	1:213:B:ASP:HB2	1:58:A:GLN:HG2	12	0.73
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	9	0.73
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	18	0.73
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	18	0.73
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	18	0.73
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	5	0.73
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	5	0.73
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	5	0.73
(1,1320)	1:278:B:VAL:HG11	1:319:B:VAL:HG21	19	0.73
(1,1320)	1:278:B:VAL:HG11	1:319:B:VAL:HG22	19	0.73
(1,1320)	1:278:B:VAL:HG11	1:319:B:VAL:HG23	19	0.73
(1,1320)	1:278:B:VAL:HG12	1:319:B:VAL:HG21	19	0.73
(1,1320)	1:278:B:VAL:HG12	1:319:B:VAL:HG22	19	0.73
(1,1320)	1:278:B:VAL:HG12	1:319:B:VAL:HG23	19	0.73
(1,1320)	1:278:B:VAL:HG13	1:319:B:VAL:HG21	19	0.73
(1,1320)	1:278:B:VAL:HG13	1:319:B:VAL:HG22	19	0.73
(1,1320)	1:278:B:VAL:HG13	1:319:B:VAL:HG23	19	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	13	0.73
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	13	0.73
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	13	0.73
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	9	0.72
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	9	0.72
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	10	0.72
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	20	0.72
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	16	0.72
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	16	0.72
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	16	0.72
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	15	0.72
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	15	0.72
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	15	0.72
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	3	0.72
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	20	0.72
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	9	0.72
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	9	0.72
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	9	0.72
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	14	0.72
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	14	0.72
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	14	0.72
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	3	0.72
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	3	0.72
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	3	0.72
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	14	0.72
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	14	0.72
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	14	0.72
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	9	0.72
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	9	0.72
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	9	0.72
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	17	0.72
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	17	0.72
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	17	0.72
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	7	0.71
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	5	0.71
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	5	0.71
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	5	0.71
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	5	0.71
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	5	0.71
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	5	0.71
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	5	0.71
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	5	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	5	0.71
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	1	0.71
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	12	0.71
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	12	0.71
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	12	0.71
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	7	0.71
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	7	0.71
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	7	0.71
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	1	0.71
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	1	0.71
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	1	0.71
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	19	0.71
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	19	0.71
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	19	0.71
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	17	0.7
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	17	0.7
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	17	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	3	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	4	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	5	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	6	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	8	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	9	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	11	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	17	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	18	0.7
(1,5760)	1:138:A:GLU:HB3	1:138:A:GLU:H	19	0.7
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	7	0.7
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	7	0.7
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	7	0.7
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	20	0.7
(1,3063)	1:382:B:SER:HB2	1:382:B:SER:H	7	0.7
(1,3063)	1:382:B:SER:HB2	1:382:B:SER:H	8	0.7
(1,3063)	1:382:B:SER:HB2	1:382:B:SER:H	14	0.7
(1,2383)	1:339:B:LEU:HD11	1:392:B:ILE:HG12	20	0.7
(1,2383)	1:339:B:LEU:HD11	1:392:B:ILE:HG13	20	0.7
(1,2383)	1:339:B:LEU:HD12	1:392:B:ILE:HG12	20	0.7
(1,2383)	1:339:B:LEU:HD12	1:392:B:ILE:HG13	20	0.7
(1,2383)	1:339:B:LEU:HD13	1:392:B:ILE:HG12	20	0.7
(1,2383)	1:339:B:LEU:HD13	1:392:B:ILE:HG13	20	0.7
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	14	0.7
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	14	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	14	0.7
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	16	0.7
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	16	0.7
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	16	0.7
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	7	0.69
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	8	0.69
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	2	0.69
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	6	0.69
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	5	0.69
(1,3063)	1:382:B:SER:HB2	1:382:B:SER:H	5	0.69
(1,3063)	1:382:B:SER:HB2	1:382:B:SER:H	9	0.69
(1,3063)	1:382:B:SER:HB2	1:382:B:SER:H	20	0.69
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	8	0.68
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	7	0.68
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	7	0.68
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	7	0.68
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	7	0.68
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	7	0.68
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	7	0.68
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	7	0.68
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	7	0.68
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	7	0.68
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	8	0.68
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	14	0.68
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	16	0.68
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	16	0.68
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	16	0.68
(1,522)	1:236:B:VAL:HG11	1:289:B:TYR:HA	11	0.68
(1,522)	1:236:B:VAL:HG12	1:289:B:TYR:HA	11	0.68
(1,522)	1:236:B:VAL:HG13	1:289:B:TYR:HA	11	0.68
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	12	0.67
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	12	0.67
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	12	0.67
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	12	0.67
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	12	0.67
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	12	0.67
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	12	0.67
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	12	0.67
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	12	0.67
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	13	0.67
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	13	0.67
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	13	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	13	0.67
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	13	0.67
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	13	0.67
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	13	0.67
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	13	0.67
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	13	0.67
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	9	0.67
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	6	0.67
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	6	0.67
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	7	0.67
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	7	0.67
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	8	0.67
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	8	0.67
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	13	0.67
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	13	0.67
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	14	0.67
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	14	0.67
(1,3066)	1:382:B:SER:HB2	1:383:B:GLN:H	7	0.67
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	7	0.67
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	7	0.67
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	7	0.67
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	5	0.67
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	5	0.67
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	5	0.67
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	5	0.67
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	5	0.67
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	5	0.67
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	10	0.67
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	10	0.67
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	10	0.67
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	3	0.66
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	9	0.66
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	4	0.66
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	2	0.66
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	2	0.66
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	3	0.66
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	3	0.66
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	5	0.66
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	5	0.66
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	12	0.66
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	12	0.66
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	19	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	19	0.66
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	4	0.66
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	4	0.66
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	4	0.66
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	16	0.65
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	16	0.65
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	5	0.65
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	5	0.65
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	4	0.65
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	4	0.65
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	4	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	16	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	16	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	16	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	16	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	16	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	16	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	16	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	16	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	16	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	17	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	17	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	17	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	17	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	17	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	17	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	17	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	17	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	17	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	19	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	19	0.65
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	19	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	19	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	19	0.65
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	19	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	19	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	19	0.65
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	19	0.65
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	11	0.65
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	20	0.65
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	1	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	1	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	4	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	4	0.65
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	9	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	9	0.65
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	10	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	10	0.65
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	15	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	15	0.65
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	16	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	16	0.65
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	17	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	17	0.65
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	20	0.65
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	20	0.65
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	19	0.65
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	19	0.65
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	19	0.65
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	14	0.65
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	14	0.65
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	14	0.65
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	14	0.65
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	14	0.65
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	14	0.65
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	17	0.64
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	5	0.64
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	5	0.64
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	15	0.64
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	15	0.64
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	15	0.64
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	15	0.64
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	15	0.64
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	15	0.64
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	15	0.64
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	15	0.64
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	15	0.64
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	1	0.64
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	2	0.64
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	8	0.64
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	14	0.64
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	1	0.64
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	1	0.64
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	1	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	1	0.64
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	3	0.64
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	3	0.64
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	3	0.64
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	19	0.64
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	19	0.64
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	19	0.64
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	11	0.64
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	11	0.64
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	11	0.64
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	17	0.64
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	17	0.64
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	17	0.64
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	1	0.63
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	19	0.63
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	19	0.63
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	19	0.63
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	20	0.63
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	20	0.63
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	20	0.63
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	20	0.63
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	20	0.63
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	20	0.63
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	20	0.63
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	20	0.63
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	20	0.63
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	20	0.63
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	20	0.63
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	20	0.63
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	8	0.63
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	15	0.63
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	18	0.63
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	18	0.63
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	16	0.63
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	3	0.63
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	3	0.63
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	3	0.63
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD21	7	0.62
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD22	7	0.62
(1,6375)	1:176:A:TRP:H	1:179:A:LEU:HD23	7	0.62
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	6	0.62
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	6	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	6	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	6	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	6	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	6	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	6	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	6	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	6	0.62
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	10	0.62
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	10	0.62
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	10	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	10	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	10	0.62
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	10	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	10	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	10	0.62
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	10	0.62
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	10	0.62
(1,3357)	2:413:D:DT:H5'	2:413:D:DT:H6	11	0.62
(1,3357)	2:413:D:DT:H5''	2:413:D:DT:H6	11	0.62
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	15	0.62
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	15	0.62
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	15	0.62
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	20	0.62
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	20	0.62
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	20	0.62
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	5	0.61
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	17	0.61
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	10	0.61
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	10	0.61
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	10	0.61
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	2	0.61
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD11	15	0.61
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD12	15	0.61
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD13	15	0.61
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	6	0.6
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	6	0.6
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	9	0.6
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	9	0.6
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	9	0.6
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	9	0.6
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	9	0.6
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	9	0.6
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	9	0.6
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	9	0.6
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	11	0.6
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	16	0.6
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	14	0.6
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	12	0.6
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	12	0.6
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	12	0.6
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	12	0.6
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	2	0.6
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	2	0.6
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	2	0.6
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	4	0.6
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	15	0.6
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	20	0.6
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	8	0.59
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	8	0.59
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	8	0.59
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	11	0.59
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	11	0.59
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	11	0.59
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	18	0.59
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	5	0.59
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	7	0.59
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	10	0.59
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	6	0.58
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	6	0.58
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	6	0.58
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	7	0.58
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	5	0.58
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	7	0.58
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	1	0.58
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	9	0.58
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	9	0.58
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	9	0.58
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	9	0.58
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	9	0.58
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	9	0.58
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	1	0.57
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	7	0.57
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	19	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	12	0.57
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	12	0.57
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	12	0.57
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	4	0.57
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	4	0.57
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	4	0.57
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	4	0.57
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	4	0.57
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	4	0.57
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	4	0.57
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	4	0.57
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	4	0.57
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	11	0.57
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	11	0.57
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	20	0.57
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	18	0.57
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	18	0.57
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	8	0.57
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	8	0.57
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	8	0.57
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	8	0.57
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	6	0.57
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	9	0.57
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	3	0.57
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	13	0.57
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	16	0.56
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	16	0.56
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	16	0.56
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	17	0.56
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	19	0.56
(1,2687)	1:357:B:PHE:HE1	1:378:B:LEU:HG	3	0.56
(1,2687)	1:357:B:PHE:HE2	1:378:B:LEU:HG	3	0.56
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	12	0.56
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	12	0.56
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	12	0.56
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	12	0.56
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	12	0.56
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	12	0.56
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	1	0.56
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	1	0.56
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	1	0.56
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	7	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	7	0.56
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	7	0.56
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	17	0.56
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	17	0.56
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	17	0.56
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	5	0.56
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	5	0.56
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	5	0.56
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	14	0.55
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	14	0.55
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	14	0.55
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	6	0.55
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	6	0.55
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	8	0.55
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	8	0.55
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	8	0.55
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	8	0.55
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	8	0.55
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	8	0.55
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	8	0.55
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	8	0.55
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	8	0.55
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD21	1	0.55
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD22	1	0.55
(1,830)	1:250:B:HIS:HD2	1:283:B:LEU:HD23	1	0.55
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	18	0.55
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	18	0.55
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	18	0.55
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	10	0.54
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	10	0.54
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	10	0.54
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	10	0.54
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	10	0.54
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	10	0.54
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	10	0.54
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	10	0.54
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	10	0.54
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	14	0.54
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	12	0.54
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	18	0.54
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	18	0.54
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	17	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	17	0.54
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	17	0.54
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	20	0.54
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	20	0.54
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	20	0.54
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	16	0.53
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	18	0.53
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	18	0.53
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	18	0.53
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	18	0.53
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	18	0.53
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	18	0.53
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	18	0.53
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	18	0.53
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	18	0.53
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	7	0.53
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	7	0.53
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	7	0.53
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	7	0.53
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	7	0.53
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	7	0.53
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	7	0.53
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	7	0.53
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	7	0.53
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	15	0.53
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	15	0.53
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	15	0.53
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	15	0.53
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	15	0.53
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	15	0.53
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	15	0.53
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	15	0.53
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	15	0.53
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	7	0.53
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	7	0.53
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	7	0.53
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	10	0.53
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	19	0.53
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	19	0.53
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	19	0.53
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	19	0.53
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	6	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	6	0.52
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	3	0.52
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	12	0.52
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	12	0.52
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	12	0.52
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	12	0.52
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	12	0.52
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	12	0.52
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	12	0.52
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	12	0.52
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	12	0.52
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	6	0.52
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	6	0.52
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	6	0.52
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	18	0.52
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	18	0.52
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	18	0.52
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	18	0.52
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	18	0.52
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	19	0.52
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	8	0.52
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	8	0.52
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	14	0.52
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	3	0.52
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	3	0.52
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	3	0.52
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	3	0.52
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	3	0.52
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	3	0.52
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	17	0.52
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	2	0.52
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	2	0.52
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	2	0.52
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	2	0.52
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	2	0.52
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	2	0.52
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	3	0.52
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	3	0.52
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	3	0.52
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	3	0.52
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	3	0.52
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	3	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	20	0.51
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	5	0.51
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	5	0.51
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	5	0.51
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	14	0.51
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	14	0.51
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	14	0.51
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	14	0.51
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	14	0.51
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	14	0.51
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	14	0.51
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	14	0.51
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	14	0.51
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	8	0.51
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	8	0.51
(1,573)	1:237:B:GLU:HG2	1:290:B:ARG:HB3	15	0.51
(1,522)	1:236:B:VAL:HG11	1:289:B:TYR:HA	18	0.51
(1,522)	1:236:B:VAL:HG12	1:289:B:TYR:HA	18	0.51
(1,522)	1:236:B:VAL:HG13	1:289:B:TYR:HA	18	0.51
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	14	0.51
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	14	0.51
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	14	0.51
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	14	0.51
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	14	0.51
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	14	0.51
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	1	0.5
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	15	0.5
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	19	0.5
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	19	0.5
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	19	0.5
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	19	0.5
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	19	0.5
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	19	0.5
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	19	0.5
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	19	0.5
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	19	0.5
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	6	0.5
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	6	0.5
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	7	0.5
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	7	0.5
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	13	0.5
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	13	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	12	0.5
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	12	0.5
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	4	0.5
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	4	0.5
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	4	0.5
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	4	0.5
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	4	0.5
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	4	0.5
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	6	0.5
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	6	0.5
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	6	0.5
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	6	0.5
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	6	0.5
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	6	0.5
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	12	0.5
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	12	0.5
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	12	0.5
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	4	0.5
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	4	0.5
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	4	0.5
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	4	0.5
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	4	0.5
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	4	0.5
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	11	0.49
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	11	0.49
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	17	0.49
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	17	0.49
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	1	0.49
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	1	0.49
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	1	0.49
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	1	0.49
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	1	0.49
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	1	0.49
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	1	0.49
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	1	0.49
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	1	0.49
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	5	0.49
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	5	0.49
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	5	0.49
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	5	0.49
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	5	0.49
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	5	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	5	0.49
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	5	0.49
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	5	0.49
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	1	0.49
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	2	0.49
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	2	0.49
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	3	0.49
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	3	0.49
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	9	0.49
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	9	0.49
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	10	0.49
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	10	0.49
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	19	0.49
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	19	0.49
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	20	0.49
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	20	0.49
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	5	0.49
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	5	0.49
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	17	0.49
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	17	0.49
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	17	0.49
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	17	0.49
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	17	0.49
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	6	0.49
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	6	0.49
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	6	0.49
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	6	0.49
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	20	0.49
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	20	0.49
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	20	0.49
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	20	0.49
(1,776)	1:246:B:LYS:HD3	1:246:B:LYS:H	15	0.49
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	19	0.49
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	19	0.49
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	19	0.49
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	6	0.48
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	6	0.48
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	3	0.48
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	3	0.48
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	3	0.48
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	13	0.48
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	13	0.48
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	13	0.48
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	13	0.48
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	13	0.48
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	13	0.48
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	13	0.48
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	13	0.48
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	12	0.48
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	5	0.48
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	5	0.48
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	12	0.48
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	12	0.48
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	15	0.48
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	15	0.48
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	18	0.48
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	18	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	1	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	1	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	2	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	2	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	4	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	4	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	7	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	7	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	9	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	9	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	10	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	10	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	13	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	13	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	15	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	15	0.48
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	16	0.48
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	16	0.48
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	12	0.48
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	20	0.47
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	4	0.47
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	4	0.47
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	5	0.47
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	5	0.47
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	17	0.47
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	17	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	4	0.47
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	4	0.47
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	18	0.47
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	18	0.47
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	6	0.47
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	6	0.47
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	6	0.47
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	6	0.47
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	6	0.47
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	6	0.47
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	6	0.47
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	6	0.47
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	6	0.47
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	5	0.47
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	8	0.47
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	8	0.47
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	8	0.47
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	1	0.47
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	1	0.47
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	14	0.47
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	14	0.47
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	16	0.47
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	16	0.47
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	6	0.47
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	6	0.47
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	14	0.47
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	14	0.47
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	18	0.47
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	18	0.47
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	20	0.47
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	20	0.47
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	15	0.47
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	15	0.47
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	15	0.47
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	15	0.47
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	15	0.47
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	15	0.47
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	18	0.47
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	18	0.47
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	18	0.47
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	18	0.47
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	18	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	18	0.47
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	2	0.47
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	4	0.47
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	4	0.47
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	4	0.47
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	18	0.47
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	18	0.47
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	18	0.47
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	8	0.46
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	8	0.46
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	1	0.46
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	1	0.46
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	10	0.46
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	10	0.46
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	11	0.46
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	11	0.46
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	14	0.46
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	14	0.46
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	9	0.46
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	9	0.46
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	16	0.46
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	16	0.46
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	10	0.46
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	10	0.46
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	10	0.46
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	11	0.46
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	11	0.46
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	11	0.46
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	11	0.46
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	11	0.46
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	11	0.46
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	11	0.46
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	11	0.46
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	11	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	8	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	8	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	8	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	8	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	8	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	8	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	8	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	8	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	8	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	20	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	20	0.46
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	20	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	20	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	20	0.46
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	20	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	20	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	20	0.46
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	20	0.46
(1,4619)	1:76:A:LEU:HD11	1:94:A:TRP:HZ3	13	0.46
(1,4619)	1:76:A:LEU:HD12	1:94:A:TRP:HZ3	13	0.46
(1,4619)	1:76:A:LEU:HD13	1:94:A:TRP:HZ3	13	0.46
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	18	0.46
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	18	0.46
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	18	0.46
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	19	0.46
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	19	0.46
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	19	0.46
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	4	0.46
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	4	0.46
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	11	0.46
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	11	0.46
(1,3400)	2:417:D:DT:H5'	2:417:D:DT:H6	17	0.46
(1,3400)	2:417:D:DT:H5''	2:417:D:DT:H6	17	0.46
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	3	0.46
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	3	0.46
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	19	0.46
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	19	0.46
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	1	0.46
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	1	0.46
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	1	0.46
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	8	0.46
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	8	0.46
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	8	0.46
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	10	0.46
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	10	0.46
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	10	0.46
(1,665)	1:239:B:LEU:H	1:288:B:ILE:HG12	9	0.46
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	1	0.46
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	1	0.46
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	1	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	1	0.45
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	1	0.45
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	16	0.45
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	16	0.45
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	13	0.45
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	19	0.45
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	19	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	2	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	2	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	3	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	3	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	6	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	6	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	9	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	9	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	12	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	12	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	13	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	13	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	15	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	15	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	16	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	16	0.45
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	18	0.45
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	18	0.45
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	5	0.45
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	5	0.45
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	15	0.45
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	15	0.45
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	13	0.45
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	13	0.45
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	13	0.45
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	17	0.45
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	17	0.45
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	17	0.45
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	7	0.45
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	7	0.45
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	7	0.45
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	1	0.45
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	1	0.45
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	1	0.45
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	1	0.45
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	1	0.45
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	1	0.45
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	1	0.45
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	1	0.45
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	17	0.45
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	17	0.45
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	17	0.45
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	17	0.45
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	17	0.45
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	17	0.45
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	17	0.45
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	17	0.45
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	17	0.45
(1,3340)	2:410:D:DT:H5'	2:410:D:DT:H6	8	0.45
(1,3340)	2:410:D:DT:H5''	2:410:D:DT:H6	8	0.45
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	4	0.45
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	4	0.45
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	4	0.45
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	11	0.45
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	19	0.45
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	9	0.44
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	9	0.44
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	5	0.44
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	7	0.44
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	7	0.44
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	8	0.44
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	8	0.44
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	19	0.44
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	19	0.44
(1,6856)	2:403:C:DT:H5'	2:403:C:DT:H6	20	0.44
(1,6856)	2:403:C:DT:H5''	2:403:C:DT:H6	20	0.44
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	12	0.44
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	12	0.44
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	14	0.44
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	14	0.44
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	3	0.44
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	3	0.44
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	3	0.44
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	4	0.44
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	4	0.44
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	4	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	2	0.44
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	2	0.44
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	2	0.44
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	2	0.44
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	2	0.44
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	2	0.44
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	2	0.44
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	2	0.44
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	2	0.44
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD21	3	0.44
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD22	3	0.44
(1,5682)	1:129:A:ILE:HG21	1:190:A:LEU:HD23	3	0.44
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD21	3	0.44
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD22	3	0.44
(1,5682)	1:129:A:ILE:HG22	1:190:A:LEU:HD23	3	0.44
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD21	3	0.44
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD22	3	0.44
(1,5682)	1:129:A:ILE:HG23	1:190:A:LEU:HD23	3	0.44
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	4	0.44
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	4	0.44
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	4	0.44
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	4	0.44
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	4	0.44
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	4	0.44
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	4	0.44
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	4	0.44
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	4	0.44
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	4	0.44
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE1	8	0.44
(1,2698)	1:358:B:LYS:H	1:372:B:PHE:HE2	8	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	2	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	2	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	2	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	2	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	2	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	2	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	8	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	8	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	8	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	8	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	8	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	13	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	13	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	13	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	13	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	13	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	13	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	19	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	19	0.44
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	19	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	19	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	19	0.44
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	19	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	5	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	5	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	5	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	12	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	12	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	12	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	18	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	18	0.44
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	18	0.44
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	16	0.44
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	16	0.44
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	16	0.44
(1,321)	1:221:B:PHE:HZ	1:233:B:CYS:H	1	0.44
(1,6988)	1:214:B:PRO:HG2	1:58:A:GLN:HG3	2	0.43
(1,6988)	1:214:B:PRO:HG3	1:58:A:GLN:HG3	2	0.43
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	2	0.43
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	1	0.43
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	1	0.43
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	1	0.43
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	1	0.43
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	1	0.43
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	2	0.43
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	2	0.43
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	2	0.43
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	2	0.43
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	2	0.43
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	2	0.43
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	2	0.43
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	2	0.43
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	2	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	2	0.43
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	2	0.43
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	2	0.43
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	18	0.43
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	18	0.43
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	18	0.43
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	18	0.43
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	18	0.43
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	18	0.43
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	18	0.43
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	18	0.43
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	18	0.43
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	9	0.43
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	9	0.43
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	9	0.43
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	5	0.43
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	15	0.43
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	2	0.43
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	2	0.43
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	2	0.43
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	17	0.43
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	17	0.43
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	17	0.43
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	3	0.43
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	1	0.43
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	15	0.43
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	15	0.43
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	15	0.43
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	15	0.43
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	10	0.43
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	10	0.43
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	10	0.43
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	10	0.43
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	10	0.43
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	10	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	3	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	3	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	3	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	6	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	6	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	6	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	7	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	7	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	7	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	13	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	13	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	13	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	19	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	19	0.43
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	19	0.43
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	11	0.43
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	11	0.43
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	11	0.43
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	1	0.43
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	8	0.43
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	8	0.43
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	8	0.43
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	4	0.42
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	4	0.42
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB2	18	0.42
(1,6991)	1:215:B:HIS:HD1	1:61:A:ASN:HB3	18	0.42
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	12	0.42
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	12	0.42
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	7	0.42
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	11	0.42
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	3	0.42
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	3	0.42
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	3	0.42
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	3	0.42
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	3	0.42
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	3	0.42
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	3	0.42
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	3	0.42
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	3	0.42
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	9	0.42
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	9	0.42
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	9	0.42
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	20	0.42
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	20	0.42
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	20	0.42
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	20	0.42
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	20	0.42
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	20	0.42
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	18	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	1	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	1	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	1	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	8	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	8	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	8	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	17	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	17	0.42
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	17	0.42
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	15	0.42
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	15	0.42
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	15	0.42
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	15	0.42
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	15	0.42
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	15	0.42
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	17	0.42
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	17	0.42
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	17	0.42
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	17	0.42
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	17	0.42
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	17	0.42
(1,159)	1:212:B:MET:HE1	1:253:B:PHE:HA	14	0.42
(1,159)	1:212:B:MET:HE2	1:253:B:PHE:HA	14	0.42
(1,159)	1:212:B:MET:HE3	1:253:B:PHE:HA	14	0.42
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	11	0.41
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	11	0.41
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	2	0.41
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	2	0.41
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	3	0.41
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	3	0.41
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	10	0.41
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	10	0.41
(1,6592)	1:191:A:ARG:HD2	1:192:A:ALA:H	15	0.41
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	16	0.41
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	16	0.41
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	16	0.41
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	16	0.41
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	16	0.41
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	16	0.41
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	16	0.41
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	16	0.41
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	2	0.41
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	2	0.41
(1,3560)	1:13:A:MET:HE1	1:14:A:ASP:H	5	0.41
(1,3560)	1:13:A:MET:HE2	1:14:A:ASP:H	5	0.41
(1,3560)	1:13:A:MET:HE3	1:14:A:ASP:H	5	0.41
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	2	0.41
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	14	0.41
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	14	0.41
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	7	0.41
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	7	0.41
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	7	0.41
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	7	0.41
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	7	0.41
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	7	0.41
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	11	0.41
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	11	0.41
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	11	0.41
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	11	0.41
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	11	0.41
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	11	0.41
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	9	0.41
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	12	0.41
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	9	0.41
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	9	0.41
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	9	0.41
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	3	0.41
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	3	0.41
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	3	0.41
(1,319)	1:221:B:PHE:HE1	1:296:B:SER:H	6	0.41
(1,319)	1:221:B:PHE:HE2	1:296:B:SER:H	6	0.41
(1,316)	1:221:B:PHE:HD1	1:296:B:SER:H	2	0.41
(1,316)	1:221:B:PHE:HD2	1:296:B:SER:H	2	0.41
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	13	0.4
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	13	0.4
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	15	0.4
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	15	0.4
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	6	0.4
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	6	0.4
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	16	0.4
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	16	0.4
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	16	0.4
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	20	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	20	0.4
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	20	0.4
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	6	0.4
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	6	0.4
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	7	0.4
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	7	0.4
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	13	0.4
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	4	0.4
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	4	0.4
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	4	0.4
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	5	0.4
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	5	0.4
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	5	0.4
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	7	0.4
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	7	0.4
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	7	0.4
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	1	0.4
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	1	0.4
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	1	0.4
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	6	0.4
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	14	0.4
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	14	0.4
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	14	0.4
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	14	0.4
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	14	0.4
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	14	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	4	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	4	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	4	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	14	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	14	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	14	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	16	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	16	0.4
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	16	0.4
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	9	0.4
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	13	0.4
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	17	0.39
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	17	0.39
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	7	0.39
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	7	0.39
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	13	0.39
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	19	0.39
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	19	0.39
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	20	0.39
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	20	0.39
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	5	0.39
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	5	0.39
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	5	0.39
(1,6445)	1:181:A:GLU:HG2	1:182:A:HIS:H	13	0.39
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	8	0.39
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	11	0.39
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	11	0.39
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	11	0.39
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	11	0.39
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	11	0.39
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	11	0.39
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	4	0.39
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	9	0.39
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	9	0.39
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	9	0.39
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	8	0.39
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	18	0.39
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	18	0.39
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	18	0.39
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	10	0.39
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	14	0.39
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	6	0.39
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	12	0.39
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	12	0.39
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	12	0.39
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	12	0.39
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	12	0.39
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	12	0.39
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	12	0.38
(1,6572)	1:191:A:ARG:HB3	1:191:A:ARG:H	8	0.38
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	2	0.38
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	19	0.38
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	19	0.38
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	19	0.38
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	5	0.38
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	5	0.38
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	3	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	3	0.38
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	3	0.38
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	14	0.38
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	14	0.38
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	14	0.38
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	11	0.38
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	11	0.38
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	17	0.38
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	17	0.38
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	17	0.38
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	17	0.38
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	17	0.38
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	17	0.38
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	1	0.38
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	5	0.38
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD11	9	0.38
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD12	9	0.38
(1,829)	1:250:B:HIS:HD2	1:283:B:LEU:HD13	9	0.38
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	17	0.38
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	6	0.38
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	2	0.37
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	2	0.37
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	3	0.37
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	3	0.37
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	4	0.37
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	4	0.37
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	1	0.37
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	1	0.37
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	1	0.37
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	2	0.37
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	12	0.37
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	6	0.37
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	6	0.37
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	6	0.37
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	11	0.37
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	11	0.37
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	11	0.37
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	11	0.37
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	11	0.37
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	11	0.37
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	11	0.37
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	11	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	11	0.37
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	2	0.37
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	9	0.37
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	16	0.37
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	8	0.37
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD21	10	0.37
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD22	10	0.37
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD23	10	0.37
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD21	10	0.37
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD22	10	0.37
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD23	10	0.37
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	11	0.37
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	11	0.37
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	11	0.37
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	11	0.37
(1,319)	1:221:B:PHE:HE1	1:296:B:SER:H	12	0.37
(1,319)	1:221:B:PHE:HE2	1:296:B:SER:H	12	0.37
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	20	0.36
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	20	0.36
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5'	8	0.36
(1,6813)	2:401:C:DT:H6	2:401:C:DT:H5''	8	0.36
(1,6572)	1:191:A:ARG:HB3	1:191:A:ARG:H	14	0.36
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	3	0.36
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	13	0.36
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	1	0.36
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	15	0.36
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG21	2	0.36
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG22	2	0.36
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG23	2	0.36
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG21	2	0.36
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG22	2	0.36
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG23	2	0.36
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	4	0.36
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	11	0.36
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	11	0.36
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	11	0.36
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD1	14	0.36
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD2	14	0.36
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD1	14	0.36
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD2	14	0.36
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD1	14	0.36
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD2	14	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	3	0.36
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	5	0.35
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	5	0.35
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	6	0.35
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	6	0.35
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB2	12	0.35
(1,6996)	1:11:A:HIS:HB3	1:253:B:PHE:HB3	12	0.35
(1,6961)	1:208:B:PRO:HB2	1:165:A:PHE:HD1	11	0.35
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	1	0.35
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	10	0.35
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	10	0.35
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	10	0.35
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	10	0.35
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	10	0.35
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	10	0.35
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	10	0.35
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	17	0.35
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	17	0.35
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	17	0.35
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	17	0.35
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	17	0.35
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	17	0.35
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	1	0.35
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	16	0.35
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD11	9	0.35
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD12	9	0.35
(1,5681)	1:129:A:ILE:HG21	1:190:A:LEU:HD13	9	0.35
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD11	9	0.35
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD12	9	0.35
(1,5681)	1:129:A:ILE:HG22	1:190:A:LEU:HD13	9	0.35
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD11	9	0.35
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD12	9	0.35
(1,5681)	1:129:A:ILE:HG23	1:190:A:LEU:HD13	9	0.35
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	8	0.35
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	13	0.35
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	13	0.35
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	14	0.35
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	14	0.35
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	2	0.35
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	5	0.35
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	2	0.35
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	2	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	2	0.35
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	2	0.35
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	7	0.35
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	7	0.35
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	7	0.35
(1,1309)	1:278:B:VAL:HG11	1:281:B:LEU:HD21	19	0.35
(1,1309)	1:278:B:VAL:HG11	1:281:B:LEU:HD22	19	0.35
(1,1309)	1:278:B:VAL:HG11	1:281:B:LEU:HD23	19	0.35
(1,1309)	1:278:B:VAL:HG12	1:281:B:LEU:HD21	19	0.35
(1,1309)	1:278:B:VAL:HG12	1:281:B:LEU:HD22	19	0.35
(1,1309)	1:278:B:VAL:HG12	1:281:B:LEU:HD23	19	0.35
(1,1309)	1:278:B:VAL:HG13	1:281:B:LEU:HD21	19	0.35
(1,1309)	1:278:B:VAL:HG13	1:281:B:LEU:HD22	19	0.35
(1,1309)	1:278:B:VAL:HG13	1:281:B:LEU:HD23	19	0.35
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD11	2	0.35
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD12	2	0.35
(1,979)	1:259:B:LYS:HA	1:261:B:LEU:HD13	2	0.35
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	13	0.35
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	13	0.35
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	13	0.35
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	13	0.35
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	13	0.35
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	13	0.35
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	7	0.35
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	7	0.35
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	7	0.35
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	17	0.34
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	17	0.34
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	9	0.34
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	9	0.34
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	9	0.34
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	1	0.34
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	1	0.34
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	1	0.34
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	1	0.34
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	1	0.34
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	1	0.34
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	10	0.34
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	1	0.34
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	1	0.34
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	1	0.34
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	12	0.34
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	12	0.34
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	15	0.34
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	20	0.34
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	19	0.34
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	2	0.34
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	2	0.34
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	2	0.34
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	4	0.33
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	4	0.33
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	4	0.33
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	13	0.33
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	6	0.33
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	2	0.33
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	2	0.33
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	2	0.33
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	11	0.33
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	11	0.33
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	11	0.33
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	5	0.33
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	5	0.33
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	5	0.33
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	16	0.33
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	5	0.33
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	7	0.33
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	10	0.33
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD21	3	0.33
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD22	3	0.33
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD23	3	0.33
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	19	0.33
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	16	0.33
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	16	0.33
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	16	0.33
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	16	0.33
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	16	0.33
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	16	0.33
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	4	0.33
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	3	0.33
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	3	0.33
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	3	0.33
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	3	0.33
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	3	0.33
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	11	0.33
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	11	0.33
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	11	0.33
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	11	0.32
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	10	0.32
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	1	0.32
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	1	0.32
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	20	0.32
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	20	0.32
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	20	0.32
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	14	0.32
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	20	0.32
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	20	0.32
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	20	0.32
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	20	0.32
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	20	0.32
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	20	0.32
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	3	0.32
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG21	6	0.32
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG22	6	0.32
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG23	6	0.32
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG21	6	0.32
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG22	6	0.32
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG23	6	0.32
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG21	6	0.32
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG22	6	0.32
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG23	6	0.32
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	9	0.32
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	9	0.32
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG21	7	0.32
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG22	7	0.32
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG23	7	0.32
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG21	7	0.32
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG22	7	0.32
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG23	7	0.32
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	17	0.32
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	6	0.32
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	6	0.32
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	6	0.32
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	13	0.32
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	13	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	13	0.32
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	7	0.32
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	7	0.32
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	7	0.32
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	18	0.32
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	18	0.32
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	18	0.32
(1,2621)	1:353:B:THR:H	1:357:B:PHE:HE1	1	0.32
(1,2621)	1:353:B:THR:H	1:357:B:PHE:HE2	1	0.32
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	18	0.32
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	8	0.32
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	8	0.32
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	5	0.32
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	5	0.32
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	5	0.32
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	13	0.32
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	13	0.32
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	13	0.32
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	16	0.32
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	3	0.32
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	3	0.32
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	3	0.32
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	7	0.32
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	7	0.32
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	7	0.32
(1,473)	1:234:B:TYR:H	1:364:B:PHE:HE1	10	0.32
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	12	0.32
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	12	0.32
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	12	0.32
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	15	0.31
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	18	0.31
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	18	0.31
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	18	0.31
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	19	0.31
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	19	0.31
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	19	0.31
(1,3886)	1:36:A:GLU:HA	1:93:A:THR:HB	4	0.31
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	11	0.31
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	11	0.31
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	14	0.31
(1,3560)	1:13:A:MET:HE1	1:14:A:ASP:H	6	0.31
(1,3560)	1:13:A:MET:HE2	1:14:A:ASP:H	6	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3560)	1:13:A:MET:HE3	1:14:A:ASP:H	6	0.31
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	2	0.31
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	4	0.31
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	4	0.31
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	4	0.31
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	19	0.31
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	19	0.31
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	19	0.31
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	3	0.31
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	3	0.31
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	3	0.31
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	14	0.31
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	17	0.31
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	17	0.31
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	17	0.31
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	17	0.31
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	2	0.31
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	19	0.31
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	19	0.31
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	19	0.31
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	15	0.31
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	15	0.31
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	15	0.31
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	18	0.31
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	18	0.31
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	18	0.31
(1,6985)	1:213:B:ASP:HB2	1:58:A:GLN:HG3	13	0.3
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	11	0.3
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	17	0.3
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	8	0.3
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	8	0.3
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	8	0.3
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	10	0.3
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	10	0.3
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	10	0.3
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	11	0.3
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	11	0.3
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	11	0.3
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	17	0.3
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	17	0.3
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	17	0.3
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	6	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	6	0.3
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	6	0.3
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	17	0.3
(1,3560)	1:13:A:MET:HE1	1:14:A:ASP:H	13	0.3
(1,3560)	1:13:A:MET:HE2	1:14:A:ASP:H	13	0.3
(1,3560)	1:13:A:MET:HE3	1:14:A:ASP:H	13	0.3
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	16	0.3
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	16	0.3
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	16	0.3
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	8	0.3
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	8	0.3
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	8	0.3
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	10	0.3
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	19	0.3
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	19	0.3
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	19	0.3
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE1	1	0.3
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE2	1	0.3
(1,320)	1:221:B:PHE:HE1	1:352:B:MET:HE3	1	0.3
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE1	1	0.3
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE2	1	0.3
(1,320)	1:221:B:PHE:HE2	1:352:B:MET:HE3	1	0.3
(1,6992)	1:251:B:ARG:HG3	1:8:A:GLY:HA3	13	0.29
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	12	0.29
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	4	0.29
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	9	0.29
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	18	0.29
(1,5696)	1:129:A:ILE:HD11	1:190:A:LEU:H	10	0.29
(1,5696)	1:129:A:ILE:HD12	1:190:A:LEU:H	10	0.29
(1,5696)	1:129:A:ILE:HD13	1:190:A:LEU:H	10	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	2	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	2	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	2	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	4	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	4	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	4	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	5	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	5	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	5	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	7	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	7	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	9	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	9	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	9	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	11	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	11	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	11	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	14	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	14	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	14	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	15	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	15	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	15	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	16	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	16	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	16	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	18	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	18	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	18	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	19	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	19	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	19	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD11	20	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD12	20	0.29
(1,4402)	1:62:A:LEU:HB3	1:62:A:LEU:HD13	20	0.29
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	12	0.29
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	20	0.29
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	20	0.29
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	20	0.29
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	1	0.29
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	1	0.29
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	1	0.29
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	3	0.29
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	3	0.29
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	3	0.29
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	15	0.29
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	15	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	4	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	4	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	4	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	11	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	11	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	16	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	16	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	16	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	17	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	17	0.29
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	17	0.29
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	6	0.29
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	7	0.29
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	9	0.29
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	12	0.29
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	12	0.29
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	12	0.29
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD21	15	0.29
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD22	15	0.29
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD23	15	0.29
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD21	15	0.29
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD22	15	0.29
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD23	15	0.29
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	8	0.29
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	8	0.29
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	8	0.29
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	8	0.29
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	8	0.29
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	8	0.29
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	8	0.29
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	8	0.29
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	8	0.29
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	14	0.28
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	8	0.28
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	8	0.28
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	17	0.28
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	15	0.28
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	15	0.28
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	15	0.28
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	15	0.28
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	15	0.28
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	15	0.28
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	15	0.28
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	15	0.28
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	15	0.28
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD21	14	0.28
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD22	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD23	14	0.28
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	9	0.28
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	9	0.28
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	9	0.28
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	9	0.28
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	9	0.28
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	9	0.28
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD21	15	0.28
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD22	15	0.28
(1,5969)	1:151:A:SER:H	1:190:A:LEU:HD23	15	0.28
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	14	0.28
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	14	0.28
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	14	0.28
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	15	0.28
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	15	0.28
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	15	0.28
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	12	0.28
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	12	0.28
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	12	0.28
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	17	0.28
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	4	0.28
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	4	0.28
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	4	0.28
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	4	0.28
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	9	0.28
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	9	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	2	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	2	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	2	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	9	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	9	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	9	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	18	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	18	0.28
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	18	0.28
(1,910)	1:254:B:LEU:HD21	1:274:B:PHE:HA	7	0.28
(1,910)	1:254:B:LEU:HD22	1:274:B:PHE:HA	7	0.28
(1,910)	1:254:B:LEU:HD23	1:274:B:PHE:HA	7	0.28
(1,910)	1:254:B:LEU:HD21	1:274:B:PHE:HA	19	0.28
(1,910)	1:254:B:LEU:HD22	1:274:B:PHE:HA	19	0.28
(1,910)	1:254:B:LEU:HD23	1:274:B:PHE:HA	19	0.28
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	18	0.28
(1,378)	1:230:B:THR:HG21	1:297:B:TRP:H	9	0.28
(1,378)	1:230:B:THR:HG22	1:297:B:TRP:H	9	0.28
(1,378)	1:230:B:THR:HG23	1:297:B:TRP:H	9	0.28
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	20	0.27
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	20	0.27
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	12	0.27
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	15	0.27
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	16	0.27
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	15	0.27
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	19	0.27
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	19	0.27
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB1	4	0.27
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB2	4	0.27
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB3	4	0.27
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	13	0.27
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	9	0.27
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	9	0.27
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	9	0.27
(1,2233)	1:324:B:PHE:HD1	1:353:B:THR:H	3	0.27
(1,2233)	1:324:B:PHE:HD2	1:353:B:THR:H	3	0.27
(1,1848)	1:309:B:VAL:HA	1:309:B:VAL:HG21	8	0.27
(1,1848)	1:309:B:VAL:HA	1:309:B:VAL:HG22	8	0.27
(1,1848)	1:309:B:VAL:HA	1:309:B:VAL:HG23	8	0.27
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	19	0.27
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	7	0.27
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	7	0.27
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	1	0.27
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	1	0.27
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	1	0.27
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	8	0.27
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	8	0.27
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	8	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	4	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	4	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	4	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	7	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	7	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	7	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	11	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	11	0.27
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	7	0.27
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	7	0.27
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	7	0.27
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	3	0.26
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	3	0.26
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	14	0.26
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	7	0.26
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	7	0.26
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	7	0.26
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	7	0.26
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	7	0.26
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	7	0.26
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	7	0.26
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	7	0.26
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	7	0.26
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	12	0.26
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	12	0.26
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	12	0.26
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	12	0.26
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	12	0.26
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	12	0.26
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	12	0.26
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	12	0.26
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	12	0.26
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	2	0.26
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	12	0.26
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	1	0.26
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	1	0.26
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	10	0.26
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	10	0.26
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	10	0.26
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	4	0.26
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	4	0.26
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	4	0.26
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	14	0.26
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	14	0.26
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	14	0.26
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	19	0.26
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	19	0.26
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	19	0.26
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	8	0.26
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3886)	1:36:A:GLU:HA	1:93:A:THR:HB	1	0.26
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	15	0.26
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	5	0.26
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	5	0.26
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	5	0.26
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD11	12	0.26
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD12	12	0.26
(1,2984)	1:376:B:ASP:HB2	1:378:B:LEU:HD13	12	0.26
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	14	0.26
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	12	0.26
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	12	0.26
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	6	0.26
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	6	0.26
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	6	0.26
(1,1321)	1:278:B:VAL:HG21	1:319:B:VAL:HG21	13	0.26
(1,1321)	1:278:B:VAL:HG21	1:319:B:VAL:HG22	13	0.26
(1,1321)	1:278:B:VAL:HG21	1:319:B:VAL:HG23	13	0.26
(1,1321)	1:278:B:VAL:HG22	1:319:B:VAL:HG21	13	0.26
(1,1321)	1:278:B:VAL:HG22	1:319:B:VAL:HG22	13	0.26
(1,1321)	1:278:B:VAL:HG22	1:319:B:VAL:HG23	13	0.26
(1,1321)	1:278:B:VAL:HG23	1:319:B:VAL:HG21	13	0.26
(1,1321)	1:278:B:VAL:HG23	1:319:B:VAL:HG22	13	0.26
(1,1321)	1:278:B:VAL:HG23	1:319:B:VAL:HG23	13	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	6	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	6	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	6	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	8	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	8	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	8	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	14	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	14	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	14	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	15	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	15	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	15	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	16	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	16	0.26
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	16	0.26
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD1	2	0.26
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD2	2	0.26
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD1	2	0.26
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD2	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD1	2	0.26
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD2	2	0.26
(1,884)	1:253:B:PHE:HD1	1:253:B:PHE:H	10	0.26
(1,884)	1:253:B:PHE:HD2	1:253:B:PHE:H	10	0.26
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	10	0.26
(1,318)	1:221:B:PHE:HE1	1:296:B:SER:HB2	7	0.26
(1,318)	1:221:B:PHE:HE1	1:296:B:SER:HB3	7	0.26
(1,318)	1:221:B:PHE:HE2	1:296:B:SER:HB2	7	0.26
(1,318)	1:221:B:PHE:HE2	1:296:B:SER:HB3	7	0.26
(1,6993)	1:251:B:ARG:HG3	1:8:A:GLY:HA2	11	0.25
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	15	0.25
(1,6965)	1:209:B:ARG:HA	1:53:A:GLY:HA2	3	0.25
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	5	0.25
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	6	0.25
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	18	0.25
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	18	0.25
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	18	0.25
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	18	0.25
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	18	0.25
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	18	0.25
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	18	0.25
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	18	0.25
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	18	0.25
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	9	0.25
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	13	0.25
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	13	0.25
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	13	0.25
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	6	0.25
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	6	0.25
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	6	0.25
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	6	0.25
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	6	0.25
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	6	0.25
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	14	0.25
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	14	0.25
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	14	0.25
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	2	0.25
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	2	0.25
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	2	0.25
(1,4247)	1:52:A:ARG:HB3	1:52:A:ARG:H	13	0.25
(1,3767)	1:28:A:ARG:HE	1:28:A:ARG:H	2	0.25
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	16	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	5	0.25
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	1	0.25
(1,3087)	1:383:B:GLN:H	1:383:B:GLN:HE22	18	0.25
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	8	0.25
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	8	0.25
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	8	0.25
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	2	0.25
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	2	0.25
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	13	0.25
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	13	0.25
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	13	0.25
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	13	0.25
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	8	0.25
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	8	0.25
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	8	0.25
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	20	0.25
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	20	0.25
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	20	0.25
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD11	1	0.25
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD12	1	0.25
(1,461)	1:234:B:TYR:HD1	1:277:B:LEU:HD13	1	0.25
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD11	1	0.25
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD12	1	0.25
(1,461)	1:234:B:TYR:HD2	1:277:B:LEU:HD13	1	0.25
(1,6965)	1:209:B:ARG:HA	1:53:A:GLY:HA2	13	0.24
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	13	0.24
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	13	0.24
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	3	0.24
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	12	0.24
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	7	0.24
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	1	0.24
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	13	0.24
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	13	0.24
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	13	0.24
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	13	0.24
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	13	0.24
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	13	0.24
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	16	0.24
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	16	0.24
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	16	0.24
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	16	0.24
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	16	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	16	0.24
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	9	0.24
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	18	0.24
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	18	0.24
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	18	0.24
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	18	0.24
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	18	0.24
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	18	0.24
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	18	0.24
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	18	0.24
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	18	0.24
(1,5856)	1:143:A:LEU:HD21	1:146:A:ALA:H	20	0.24
(1,5856)	1:143:A:LEU:HD22	1:146:A:ALA:H	20	0.24
(1,5856)	1:143:A:LEU:HD23	1:146:A:ALA:H	20	0.24
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	3	0.24
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	3	0.24
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	18	0.24
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	18	0.24
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	18	0.24
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	3	0.24
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	3	0.24
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	3	0.24
(1,3886)	1:36:A:GLU:HA	1:93:A:THR:HB	8	0.24
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	10	0.24
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	10	0.24
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	10	0.24
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	15	0.24
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	15	0.24
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	15	0.24
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	20	0.24
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	18	0.24
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	18	0.24
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	18	0.24
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	2	0.24
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG21	11	0.24
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG22	11	0.24
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG23	11	0.24
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG21	11	0.24
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG22	11	0.24
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG23	11	0.24
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG21	11	0.24
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG22	11	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG23	11	0.24
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	14	0.24
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	14	0.24
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	14	0.24
(1,1338)	1:279:B:PRO:HA	1:282:B:GLN:HB2	4	0.24
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	1	0.24
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	10	0.24
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	9	0.24
(1,6984)	1:213:B:ASP:HB3	1:58:A:GLN:HG3	13	0.23
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	16	0.23
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	16	0.23
(1,6868)	2:404:C:DC:H2''	2:404:C:DC:H5	1	0.23
(1,6868)	2:404:C:DC:H2''	2:404:C:DC:H5	2	0.23
(1,6868)	2:404:C:DC:H2''	2:404:C:DC:H5	6	0.23
(1,6868)	2:404:C:DC:H2''	2:404:C:DC:H5	7	0.23
(1,6868)	2:404:C:DC:H2''	2:404:C:DC:H5	10	0.23
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	12	0.23
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	19	0.23
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	19	0.23
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	19	0.23
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	19	0.23
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	19	0.23
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	19	0.23
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	19	0.23
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	19	0.23
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	19	0.23
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	11	0.23
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD11	4	0.23
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD12	4	0.23
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD13	4	0.23
(1,6367)	1:176:A:TRP:HB2	1:177:A:ASP:H	15	0.23
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	3	0.23
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	12	0.23
(1,5820)	1:141:A:GLN:HE21	1:194:A:LEU:HD21	6	0.23
(1,5820)	1:141:A:GLN:HE21	1:194:A:LEU:HD22	6	0.23
(1,5820)	1:141:A:GLN:HE21	1:194:A:LEU:HD23	6	0.23
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	13	0.23
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	13	0.23
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	9	0.23
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	9	0.23
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	9	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	3	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	3	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	17	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	17	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	17	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	19	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	19	0.23
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	19	0.23
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	1	0.23
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	3	0.23
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	9	0.23
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	10	0.23
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	13	0.23
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	13	0.23
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	13	0.23
(1,4619)	1:76:A:LEU:HD11	1:94:A:TRP:HZ3	18	0.23
(1,4619)	1:76:A:LEU:HD12	1:94:A:TRP:HZ3	18	0.23
(1,4619)	1:76:A:LEU:HD13	1:94:A:TRP:HZ3	18	0.23
(1,4619)	1:76:A:LEU:HD11	1:94:A:TRP:HZ3	19	0.23
(1,4619)	1:76:A:LEU:HD12	1:94:A:TRP:HZ3	19	0.23
(1,4619)	1:76:A:LEU:HD13	1:94:A:TRP:HZ3	19	0.23
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	15	0.23
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	15	0.23
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	15	0.23
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	20	0.23
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	20	0.23
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	20	0.23
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	3	0.23
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	16	0.23
(1,4247)	1:52:A:ARG:HB3	1:52:A:ARG:H	4	0.23
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	12	0.23
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	12	0.23
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	13	0.23
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	13	0.23
(1,4015)	1:39:A:ARG:H	1:47:A:LYS:HA	2	0.23
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	10	0.23
(1,3104)	1:385:B:LEU:HA	1:385:B:LEU:HD21	18	0.23
(1,3104)	1:385:B:LEU:HA	1:385:B:LEU:HD22	18	0.23
(1,3104)	1:385:B:LEU:HA	1:385:B:LEU:HD23	18	0.23
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	17	0.23
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	17	0.23
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2727)	1:361:B:TRP:HB2	1:361:B:TRP:H	12	0.23
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	6	0.23
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	11	0.23
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	1	0.23
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	1	0.23
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD11	18	0.23
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD12	18	0.23
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD13	18	0.23
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD11	18	0.23
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD12	18	0.23
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD13	18	0.23
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD11	18	0.23
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD12	18	0.23
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD13	18	0.23
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	16	0.23
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	16	0.23
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	16	0.23
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	16	0.23
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	7	0.23
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	20	0.23
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	20	0.23
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	20	0.23
(1,264)	1:217:B:PHE:HA	1:365:B:VAL:HG21	19	0.23
(1,264)	1:217:B:PHE:HA	1:365:B:VAL:HG22	19	0.23
(1,264)	1:217:B:PHE:HA	1:365:B:VAL:HG23	19	0.23
(1,6998)	1:11:A:HIS:HB3	1:253:B:PHE:HD1	10	0.22
(1,6998)	1:11:A:HIS:HB3	1:253:B:PHE:HD2	10	0.22
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	2	0.22
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	2	0.22
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	8	0.22
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	13	0.22
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	19	0.22
(1,6868)	2:404:C:DC:H2"	2:404:C:DC:H5	20	0.22
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	6	0.22
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	9	0.22
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	16	0.22
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD21	14	0.22
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD22	14	0.22
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD23	14	0.22
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	2	0.22
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	2	0.22
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	2	0.22
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	2	0.22
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	2	0.22
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	2	0.22
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	2	0.22
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	2	0.22
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	12	0.22
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD11	6	0.22
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD12	6	0.22
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD13	6	0.22
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	8	0.22
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	16	0.22
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	5	0.22
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	5	0.22
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	17	0.22
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	17	0.22
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	17	0.22
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	17	0.22
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	17	0.22
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	17	0.22
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	17	0.22
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	17	0.22
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	17	0.22
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	17	0.22
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	17	0.22
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	17	0.22
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	13	0.22
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	13	0.22
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	13	0.22
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	9	0.22
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	9	0.22
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	9	0.22
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	7	0.22
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	16	0.22
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	1	0.22
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	1	0.22
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	1	0.22
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	9	0.22
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	9	0.22
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	9	0.22
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	11	0.22
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	17	0.22
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	17	0.22
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	19	0.22
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	19	0.22
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	1	0.22
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD11	6	0.22
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD12	6	0.22
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD13	6	0.22
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD11	10	0.22
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD12	10	0.22
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD13	10	0.22
(1,3886)	1:36:A:GLU:HA	1:93:A:THR:HB	20	0.22
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	2	0.22
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	2	0.22
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	8	0.22
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	8	0.22
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	1	0.22
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	1	0.22
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	1	0.22
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	1	0.22
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	1	0.22
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	1	0.22
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	1	0.22
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	1	0.22
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	1	0.22
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	7	0.22
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	8	0.22
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	9	0.22
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	13	0.22
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	20	0.22
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	8	0.22
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	10	0.22
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	10	0.22
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	10	0.22
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	15	0.22
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	15	0.22
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	5	0.22
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	5	0.22
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	5	0.22
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	5	0.22
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	5	0.22
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	5	0.22
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	5	0.22
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	5	0.22
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD1	10	0.22
(1,1678)	1:294:B:PHE:HD1	1:324:B:PHE:HD2	10	0.22
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD1	10	0.22
(1,1678)	1:294:B:PHE:HD2	1:324:B:PHE:HD2	10	0.22
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	1	0.22
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	1	0.22
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	6	0.22
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	6	0.22
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	6	0.22
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	11	0.22
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	15	0.22
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	15	0.22
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	15	0.22
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	5	0.22
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	8	0.22
(1,886)	1:253:B:PHE:HZ	1:253:B:PHE:H	10	0.22
(1,886)	1:253:B:PHE:HZ	1:253:B:PHE:H	14	0.22
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD11	6	0.22
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD12	6	0.22
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD13	6	0.22
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	1	0.22
(1,414)	1:232:B:LEU:HD21	1:293:B:TRP:HZ2	2	0.22
(1,414)	1:232:B:LEU:HD22	1:293:B:TRP:HZ2	2	0.22
(1,414)	1:232:B:LEU:HD23	1:293:B:TRP:HZ2	2	0.22
(1,361)	1:227:B:ARG:HE	1:227:B:ARG:H	13	0.22
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	17	0.22
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	17	0.22
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	17	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	6	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	6	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	7	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	7	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	8	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	8	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	9	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	9	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	10	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	10	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	11	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	12	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	12	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	13	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	13	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	14	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	14	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	16	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	16	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	18	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	18	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	19	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	19	0.22
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	20	0.22
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	20	0.22
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	2	0.21
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	8	0.21
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	14	0.21
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	19	0.21
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD21	6	0.21
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD22	6	0.21
(1,6636)	1:194:A:LEU:HA	1:194:A:LEU:HD23	6	0.21
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	10	0.21
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	10	0.21
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	10	0.21
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	10	0.21
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	10	0.21
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	10	0.21
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	10	0.21
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	10	0.21
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	10	0.21
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD21	3	0.21
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD22	3	0.21
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD23	3	0.21
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	4	0.21
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	20	0.21
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	9	0.21
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	5	0.21
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	1	0.21
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	9	0.21
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	2	0.21
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	4	0.21
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	4	0.21
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	10	0.21
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	10	0.21
(1,5683)	1:129:A:ILE:HG21	1:193:A:ILE:HG21	7	0.21
(1,5683)	1:129:A:ILE:HG22	1:193:A:ILE:HG21	7	0.21
(1,5683)	1:129:A:ILE:HG23	1:193:A:ILE:HG21	7	0.21
(1,5506)	1:119:A:HIS:HE1	1:119:A:HIS:H	3	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	2	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	2	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	5	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	5	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	6	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	6	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	8	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	8	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	9	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	9	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	10	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	10	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	12	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	12	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	18	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	18	0.21
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	20	0.21
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	20	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	1	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	1	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	1	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	14	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	14	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	14	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	16	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	16	0.21
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	16	0.21
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	6	0.21
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	8	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	1	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	1	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	2	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	2	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	4	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	8	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	8	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	9	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	9	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	12	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	12	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	14	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	14	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	16	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	16	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	18	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	18	0.21
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	20	0.21
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	20	0.21
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	11	0.21
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	11	0.21
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	3	0.21
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	3	0.21
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	3	0.21
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	4	0.21
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	4	0.21
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	4	0.21
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG21	20	0.21
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG22	20	0.21
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG23	20	0.21
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG21	20	0.21
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG22	20	0.21
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG23	20	0.21
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG21	20	0.21
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG22	20	0.21
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG23	20	0.21
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD11	15	0.21
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD12	15	0.21
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD13	15	0.21
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	14	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	3	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	3	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	5	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	5	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	8	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	11	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	11	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	12	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	12	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	13	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	13	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	14	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	14	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	15	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	15	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	19	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	19	0.21
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	20	0.21
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	20	0.21
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	12	0.21
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	13	0.21
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	15	0.21
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	15	0.21
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	15	0.21
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	15	0.21
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	15	0.21
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	15	0.21
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	15	0.21
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	15	0.21
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	15	0.21
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	13	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	1	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	2	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	3	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	4	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	5	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	10	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	12	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	15	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	16	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	17	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	18	0.21
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	19	0.21
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	13	0.21
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	16	0.21
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	13	0.21
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	12	0.21
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	13	0.21
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	13	0.21
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	20	0.21
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	20	0.21
(1,2321)	1:333:B:PRO:HB2	1:334:B:LEU:H	6	0.21
(1,2321)	1:333:B:PRO:HB2	1:334:B:LEU:H	8	0.21
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	6	0.21
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	6	0.21
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	8	0.21
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	8	0.21
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	10	0.21
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	10	0.21
(1,1708)	1:295:B:ILE:HD11	1:296:B:SER:H	3	0.21
(1,1708)	1:295:B:ILE:HD12	1:296:B:SER:H	3	0.21
(1,1708)	1:295:B:ILE:HD13	1:296:B:SER:H	3	0.21
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	12	0.21
(1,1688)	1:295:B:ILE:HB	1:295:B:ILE:H	7	0.21
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	19	0.21
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	19	0.21
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	13	0.21
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	16	0.21
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	19	0.21
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	3	0.21
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	3	0.21
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	3	0.21
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	9	0.21
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	9	0.21
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	13	0.21
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	13	0.21
(1,922)	1:254:B:LEU:HD21	1:277:B:LEU:H	5	0.21
(1,922)	1:254:B:LEU:HD22	1:277:B:LEU:H	5	0.21
(1,922)	1:254:B:LEU:HD23	1:277:B:LEU:H	5	0.21
(1,884)	1:253:B:PHE:HD1	1:253:B:PHE:H	14	0.21
(1,884)	1:253:B:PHE:HD2	1:253:B:PHE:H	14	0.21
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	20	0.21
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	4	0.21
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	4	0.21
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	4	0.21
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD11	1	0.21
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD12	1	0.21
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD13	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD11	19	0.21
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD12	19	0.21
(1,615)	1:239:B:LEU:HA	1:239:B:LEU:HD13	19	0.21
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	14	0.21
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	15	0.21
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	17	0.21
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	17	0.21
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	17	0.21
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG21	18	0.21
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG22	18	0.21
(1,487)	1:235:B:GLU:HG3	1:363:B:THR:HG23	18	0.21
(1,473)	1:234:B:TYR:H	1:364:B:PHE:HE1	14	0.21
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	11	0.21
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	11	0.21
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	11	0.21
(1,361)	1:227:B:ARG:HE	1:227:B:ARG:H	11	0.21
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	1	0.21
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	1	0.21
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	2	0.21
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	2	0.21
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	3	0.21
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	3	0.21
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	4	0.21
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	4	0.21
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	5	0.21
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	5	0.21
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	15	0.21
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	15	0.21
(1,259)	1:217:B:PHE:HE1	1:217:B:PHE:H	17	0.21
(1,259)	1:217:B:PHE:HE2	1:217:B:PHE:H	17	0.21
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	3	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	4	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	5	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	7	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	10	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	13	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	15	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	17	0.2
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	20	0.2
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	7	0.2
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	16	0.2
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD21	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD22	1	0.2
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD23	1	0.2
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD21	18	0.2
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD22	18	0.2
(1,6506)	1:186:A:LEU:HA	1:186:A:LEU:HD23	18	0.2
(1,6479)	1:184:A:GLN:HB2	1:184:A:GLN:HE21	15	0.2
(1,6479)	1:184:A:GLN:HB3	1:184:A:GLN:HE21	15	0.2
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	6	0.2
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	16	0.2
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD11	16	0.2
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD12	16	0.2
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD13	16	0.2
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	2	0.2
(1,6149)	1:162:A:TRP:HE1	1:172:A:PRO:HA	5	0.2
(1,6148)	1:162:A:TRP:HE1	1:171:A:GLN:H	4	0.2
(1,6120)	1:161:A:CYS:HG	1:161:A:CYS:H	20	0.2
(1,5856)	1:143:A:LEU:HD21	1:146:A:ALA:H	9	0.2
(1,5856)	1:143:A:LEU:HD22	1:146:A:ALA:H	9	0.2
(1,5856)	1:143:A:LEU:HD23	1:146:A:ALA:H	9	0.2
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	15	0.2
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	15	0.2
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	18	0.2
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	18	0.2
(1,5693)	1:129:A:ILE:HD11	1:189:A:ARG:H	17	0.2
(1,5693)	1:129:A:ILE:HD12	1:189:A:ARG:H	17	0.2
(1,5693)	1:129:A:ILE:HD13	1:189:A:ARG:H	17	0.2
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	13	0.2
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB1	8	0.2
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB2	8	0.2
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB3	8	0.2
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	1	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	1	0.2
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	3	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	3	0.2
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	11	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	11	0.2
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	15	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	15	0.2
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	16	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	16	0.2
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	17	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	19	0.2
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	19	0.2
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	20	0.2
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	20	0.2
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	20	0.2
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	20	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	3	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	3	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	3	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	5	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	5	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	5	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	17	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	17	0.2
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	17	0.2
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	3	0.2
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	3	0.2
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	5	0.2
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	5	0.2
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	6	0.2
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	6	0.2
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	7	0.2
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	7	0.2
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	13	0.2
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	13	0.2
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	4	0.2
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	8	0.2
(1,4247)	1:52:A:ARG:HB3	1:52:A:ARG:H	16	0.2
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	10	0.2
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	10	0.2
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	15	0.2
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	17	0.2
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	17	0.2
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	17	0.2
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	4	0.2
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	4	0.2
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	6	0.2
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	6	0.2
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	7	0.2
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	7	0.2
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	9	0.2
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	10	0.2
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	10	0.2
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	18	0.2
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	18	0.2
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	20	0.2
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	1	0.2
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	4	0.2
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	9	0.2
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	6	0.2
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	11	0.2
(1,3392)	2:417:D:DT:H1'	2:417:D:DT:H6	14	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	2	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	3	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	6	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	7	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	9	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	10	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	12	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	14	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	15	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	16	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	19	0.2
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	20	0.2
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	13	0.2
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	15	0.2
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	14	0.2
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	20	0.2
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	13	0.2
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	10	0.2
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	8	0.2
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	8	0.2
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	17	0.2
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	17	0.2
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	19	0.2
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	19	0.2
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	2	0.2
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	2	0.2
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	2	0.2
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	2	0.2
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	2	0.2
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	2	0.2
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	2	0.2
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	2	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	1	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	1	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	2	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	2	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	3	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	3	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	4	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	4	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	5	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	5	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	7	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	7	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	9	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	9	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	11	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	11	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	12	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	12	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	14	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	14	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	15	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	15	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	16	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	16	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	17	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	17	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	18	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	18	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	19	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	19	0.2
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	20	0.2
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	20	0.2
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	6	0.2
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	19	0.2
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	19	0.2
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	19	0.2
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	8	0.2
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	14	0.2
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	15	0.2
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	20	0.2
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD21	19	0.2
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD22	19	0.2
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD23	19	0.2
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD21	19	0.2
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD22	19	0.2
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD23	19	0.2
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	1	0.2
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	1	0.2
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	2	0.2
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	2	0.2
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	3	0.2
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	3	0.2
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	10	0.2
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	10	0.2
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	16	0.2
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	16	0.2
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	18	0.2
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	18	0.2
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	7	0.2
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	7	0.2
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	7	0.2
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	3	0.2
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	4	0.2
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	11	0.2
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	11	0.2
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	11	0.2
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	7	0.2
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	1	0.2
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	1	0.2
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	1	0.2
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	1	0.2
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	1	0.2
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	1	0.2
(1,473)	1:234:B:TYR:H	1:364:B:PHE:HE1	18	0.2
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG11	13	0.2
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG12	13	0.2
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG13	13	0.2
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG11	13	0.2
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG12	13	0.2
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG13	13	0.2
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG11	13	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG12	13	0.2
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG13	13	0.2
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB2	18	0.19
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB3	18	0.19
(1,6965)	1:209:B:ARG:HA	1:53:A:GLY:HA2	16	0.19
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	1	0.19
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	11	0.19
(1,6664)	1:195:A:GLN:HB3	1:195:A:GLN:H	18	0.19
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	5	0.19
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	12	0.19
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	12	0.19
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	12	0.19
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD11	9	0.19
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD12	9	0.19
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD13	9	0.19
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD21	18	0.19
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD22	18	0.19
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD23	18	0.19
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	14	0.19
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	14	0.19
(1,6056)	1:155:A:TYR:H	1:179:A:LEU:HG	14	0.19
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	12	0.19
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	12	0.19
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	12	0.19
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	12	0.19
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	12	0.19
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	12	0.19
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	12	0.19
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	12	0.19
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	12	0.19
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	3	0.19
(1,5874)	1:144:A:ARG:HB3	1:150:A:VAL:HG11	17	0.19
(1,5874)	1:144:A:ARG:HB3	1:150:A:VAL:HG12	17	0.19
(1,5874)	1:144:A:ARG:HB3	1:150:A:VAL:HG13	17	0.19
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	14	0.19
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	14	0.19
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	14	0.19
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	14	0.19
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	6	0.19
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	6	0.19
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	6	0.19
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	6	0.19
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	6	0.19
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	4	0.19
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	4	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	7	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	7	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	7	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	9	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	9	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	9	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	15	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	15	0.19
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	15	0.19
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	1	0.19
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	1	0.19
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	1	0.19
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	3	0.19
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	3	0.19
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	3	0.19
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	12	0.19
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	12	0.19
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	12	0.19
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	8	0.19
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	7	0.19
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	11	0.19
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	14	0.19
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	17	0.19
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	18	0.19
(1,4619)	1:76:A:LEU:HD11	1:94:A:TRP:HZ3	3	0.19
(1,4619)	1:76:A:LEU:HD12	1:94:A:TRP:HZ3	3	0.19
(1,4619)	1:76:A:LEU:HD13	1:94:A:TRP:HZ3	3	0.19
(1,4619)	1:76:A:LEU:HD11	1:94:A:TRP:HZ3	12	0.19
(1,4619)	1:76:A:LEU:HD12	1:94:A:TRP:HZ3	12	0.19
(1,4619)	1:76:A:LEU:HD13	1:94:A:TRP:HZ3	12	0.19
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	10	0.19
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	10	0.19
(1,4550)	1:75:A:PHE:HE1	1:75:A:PHE:H	15	0.19
(1,4550)	1:75:A:PHE:HE2	1:75:A:PHE:H	15	0.19
(1,4265)	1:52:A:ARG:HG3	1:53:A:GLY:H	17	0.19
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	14	0.19
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	14	0.19
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD11	20	0.19
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD12	20	0.19
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD13	20	0.19
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	11	0.19
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	11	0.19
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	11	0.19
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	1	0.19
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	1	0.19
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	16	0.19
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	16	0.19
(1,3669)	1:18:A:PHE:HE1	1:18:A:PHE:H	17	0.19
(1,3669)	1:18:A:PHE:HE2	1:18:A:PHE:H	17	0.19
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	5	0.19
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	19	0.19
(1,3453)	1:6:A:ALA:HB1	1:7:A:SER:H	12	0.19
(1,3453)	1:6:A:ALA:HB2	1:7:A:SER:H	12	0.19
(1,3453)	1:6:A:ALA:HB3	1:7:A:SER:H	12	0.19
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	1	0.19
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	4	0.19
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	5	0.19
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	11	0.19
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	17	0.19
(1,3262)	1:394:B:GLN:HB3	1:394:B:GLN:H	18	0.19
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	12	0.19
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	12	0.19
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	12	0.19
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	12	0.19
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	12	0.19
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	12	0.19
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	12	0.19
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	12	0.19
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	12	0.19
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	19	0.19
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	19	0.19
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	19	0.19
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	19	0.19
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	19	0.19
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	19	0.19
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	19	0.19
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	19	0.19
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	19	0.19
(1,3089)	1:383:B:GLN:HA	1:386:B:SER:H	18	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	6	0.19
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	14	0.19
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	16	0.19
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	12	0.19
(1,2727)	1:361:B:TRP:HB2	1:361:B:TRP:H	1	0.19
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	4	0.19
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	4	0.19
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	11	0.19
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	11	0.19
(1,2346)	1:335:B:TYR:HE1	1:335:B:TYR:H	16	0.19
(1,2346)	1:335:B:TYR:HE2	1:335:B:TYR:H	16	0.19
(1,2277)	1:328:B:ILE:HG21	1:385:B:LEU:HD21	20	0.19
(1,2277)	1:328:B:ILE:HG21	1:385:B:LEU:HD22	20	0.19
(1,2277)	1:328:B:ILE:HG21	1:385:B:LEU:HD23	20	0.19
(1,2277)	1:328:B:ILE:HG22	1:385:B:LEU:HD21	20	0.19
(1,2277)	1:328:B:ILE:HG22	1:385:B:LEU:HD22	20	0.19
(1,2277)	1:328:B:ILE:HG22	1:385:B:LEU:HD23	20	0.19
(1,2277)	1:328:B:ILE:HG23	1:385:B:LEU:HD21	20	0.19
(1,2277)	1:328:B:ILE:HG23	1:385:B:LEU:HD22	20	0.19
(1,2277)	1:328:B:ILE:HG23	1:385:B:LEU:HD23	20	0.19
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	1	0.19
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	1	0.19
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	1	0.19
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	1	0.19
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	1	0.19
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	1	0.19
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	1	0.19
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	1	0.19
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	1	0.19
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	1	0.19
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	1	0.19
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	1	0.19
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	1	0.19
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	1	0.19
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	1	0.19
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	1	0.19
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	1	0.19
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	1	0.19
(1,1943)	1:312:B:PHE:HE1	1:312:B:PHE:H	13	0.19
(1,1943)	1:312:B:PHE:HE2	1:312:B:PHE:H	13	0.19
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	20	0.19
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	20	0.19
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	9	0.19
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	9	0.19
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	9	0.19
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	9	0.19
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	9	0.19
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	9	0.19
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	12	0.19
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	4	0.19
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	12	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	5	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	5	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	7	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	7	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	8	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	8	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	12	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	12	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	14	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	14	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	17	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	17	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	19	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	19	0.19
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	20	0.19
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	20	0.19
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD11	4	0.19
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD12	4	0.19
(1,825)	1:250:B:HIS:HB2	1:281:B:LEU:HD13	4	0.19
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	1	0.19
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	6	0.19
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	19	0.19
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	6	0.19
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	6	0.19
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	6	0.19
(1,554)	1:237:B:GLU:HA	1:290:B:ARG:H	6	0.19
(1,554)	1:237:B:GLU:HA	1:290:B:ARG:H	18	0.19
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG21	10	0.19
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG22	10	0.19
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG23	10	0.19
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	12	0.19
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	12	0.19
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	12	0.19
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	12	0.19
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	12	0.19
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	7	0.19
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	7	0.19
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	7	0.19
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB2	11	0.18
(1,6955)	1:208:B:PRO:HB3	1:54:A:PHE:HB3	11	0.18
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	19	0.18
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	8	0.18
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	8	0.18
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	8	0.18
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	8	0.18
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	8	0.18
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	8	0.18
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	8	0.18
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	8	0.18
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	8	0.18
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD21	11	0.18
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD22	11	0.18
(1,6559)	1:190:A:LEU:HD11	1:194:A:LEU:HD23	11	0.18
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD21	11	0.18
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD22	11	0.18
(1,6559)	1:190:A:LEU:HD12	1:194:A:LEU:HD23	11	0.18
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD21	11	0.18
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD22	11	0.18
(1,6559)	1:190:A:LEU:HD13	1:194:A:LEU:HD23	11	0.18
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD11	11	0.18
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD12	11	0.18
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD13	11	0.18
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD11	11	0.18
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD12	11	0.18
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD13	11	0.18
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD11	11	0.18
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD12	11	0.18
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD13	11	0.18
(1,6479)	1:184:A:GLN:HB2	1:184:A:GLN:HE21	20	0.18
(1,6479)	1:184:A:GLN:HB3	1:184:A:GLN:HE21	20	0.18
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	18	0.18
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	2	0.18
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	2	0.18
(1,6335)	1:174:A:GLN:H	1:175:A:PRO:HD2	18	0.18
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	12	0.18
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	16	0.18
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	12	0.18
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	12	0.18
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	12	0.18
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	12	0.18
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	12	0.18
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	12	0.18
(1,6157)	1:162:A:TRP:HZ2	1:171:A:GLN:H	6	0.18
(1,6056)	1:155:A:TYR:H	1:179:A:LEU:HG	15	0.18
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	14	0.18
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	14	0.18
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	14	0.18
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD11	8	0.18
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD12	8	0.18
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD13	8	0.18
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD11	7	0.18
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD12	7	0.18
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD13	7	0.18
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	6	0.18
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	6	0.18
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	9	0.18
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	9	0.18
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	12	0.18
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	12	0.18
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	11	0.18
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	11	0.18
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	11	0.18
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	2	0.18
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	2	0.18
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	2	0.18
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	2	0.18
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	2	0.18
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	2	0.18
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	2	0.18
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	2	0.18
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	2	0.18
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	7	0.18
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	7	0.18
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	7	0.18
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	7	0.18
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	7	0.18
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	13	0.18
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	13	0.18
(1,5345)	1:113:A:PHE:HE1	1:113:A:PHE:H	14	0.18
(1,5345)	1:113:A:PHE:HE2	1:113:A:PHE:H	14	0.18
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	4	0.18
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	4	0.18
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	4	0.18
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	8	0.18
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	8	0.18
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	8	0.18
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	12	0.18
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	12	0.18
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	12	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	10	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	10	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	10	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	11	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	11	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	11	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	15	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	15	0.18
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	15	0.18
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	6	0.18
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	11	0.18
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	11	0.18
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	11	0.18
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	17	0.18
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	17	0.18
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	17	0.18
(1,4265)	1:52:A:ARG:HG3	1:53:A:GLY:H	6	0.18
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	10	0.18
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG21	10	0.18
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG22	10	0.18
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG23	10	0.18
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG21	10	0.18
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG22	10	0.18
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG23	10	0.18
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG21	10	0.18
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG22	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG23	10	0.18
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD11	1	0.18
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD12	1	0.18
(1,4021)	1:40:A:LEU:HA	1:40:A:LEU:HD13	1	0.18
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	7	0.18
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG21	3	0.18
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG22	3	0.18
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG23	3	0.18
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG21	3	0.18
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG22	3	0.18
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG23	3	0.18
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	18	0.18
(1,3579)	1:14:A:ASP:HB2	1:14:A:ASP:H	3	0.18
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	10	0.18
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	10	0.18
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	10	0.18
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	10	0.18
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	10	0.18
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	10	0.18
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	10	0.18
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	10	0.18
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	10	0.18
(1,3560)	1:13:A:MET:HE1	1:14:A:ASP:H	11	0.18
(1,3560)	1:13:A:MET:HE2	1:14:A:ASP:H	11	0.18
(1,3560)	1:13:A:MET:HE3	1:14:A:ASP:H	11	0.18
(1,3541)	1:12:A:LEU:HD21	1:169:A:GLN:HE21	15	0.18
(1,3541)	1:12:A:LEU:HD22	1:169:A:GLN:HE21	15	0.18
(1,3541)	1:12:A:LEU:HD23	1:169:A:GLN:HE21	15	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	1	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	2	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	3	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	4	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	6	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	7	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	8	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	9	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	10	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	11	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	12	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	13	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	14	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	16	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	18	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	19	0.18
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	20	0.18
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	3	0.18
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	3	0.18
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	3	0.18
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	3	0.18
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	3	0.18
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	3	0.18
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	3	0.18
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	3	0.18
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	3	0.18
(1,3089)	1:383:B:GLN:HA	1:386:B:SER:H	3	0.18
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	2	0.18
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	11	0.18
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	2	0.18
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	7	0.18
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	13	0.18
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	15	0.18
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	20	0.18
(1,2933)	1:373:B:GLN:H	1:374:B:PRO:HD2	8	0.18
(1,2727)	1:361:B:TRP:HB2	1:361:B:TRP:H	7	0.18
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD11	2	0.18
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD12	2	0.18
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD13	2	0.18
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	11	0.18
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	11	0.18
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	16	0.18
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	16	0.18
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	3	0.18
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD11	19	0.18
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD12	19	0.18
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD13	19	0.18
(1,2346)	1:335:B:TYR:HE1	1:335:B:TYR:H	7	0.18
(1,2346)	1:335:B:TYR:HE2	1:335:B:TYR:H	7	0.18
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	15	0.18
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	15	0.18
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	15	0.18
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	12	0.18
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	12	0.18
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	3	0.18
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	8	0.18
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	18	0.18
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	17	0.18
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG21	11	0.18
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG22	11	0.18
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG23	11	0.18
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG21	11	0.18
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG22	11	0.18
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG23	11	0.18
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG21	11	0.18
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG22	11	0.18
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG23	11	0.18
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG21	19	0.18
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG22	19	0.18
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG23	19	0.18
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG21	19	0.18
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG22	19	0.18
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG23	19	0.18
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG21	19	0.18
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG22	19	0.18
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG23	19	0.18
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD11	10	0.18
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD12	10	0.18
(1,1351)	1:280:B:SER:H	1:281:B:LEU:HD13	10	0.18
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	4	0.18
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	4	0.18
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	4	0.18
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	11	0.18
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	11	0.18
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	11	0.18
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	12	0.18
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	12	0.18
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	12	0.18
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	11	0.18
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	14	0.18
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD21	6	0.18
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD22	6	0.18
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD23	6	0.18
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD21	6	0.18
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD22	6	0.18
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD23	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	1	0.18
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	4	0.18
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	4	0.18
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	6	0.18
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	6	0.18
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	15	0.18
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	15	0.18
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	3	0.18
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	9	0.18
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	10	0.18
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	13	0.18
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	7	0.18
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	7	0.18
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	7	0.18
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	17	0.18
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	8	0.18
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	8	0.18
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	8	0.18
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	8	0.18
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	8	0.18
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	8	0.18
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	17	0.18
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	17	0.18
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	17	0.18
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB1	6	0.17
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB2	6	0.17
(1,6990)	1:215:B:HIS:HD1	1:59:A:ALA:HB3	6	0.17
(1,6650)	1:194:A:LEU:HB2	1:195:A:GLN:H	20	0.17
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD11	14	0.17
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD12	14	0.17
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD13	14	0.17
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	5	0.17
(1,6576)	1:191:A:ARG:HB2	1:191:A:ARG:HD3	13	0.17
(1,6479)	1:184:A:GLN:HB2	1:184:A:GLN:HE21	5	0.17
(1,6479)	1:184:A:GLN:HB3	1:184:A:GLN:HE21	5	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	1	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	2	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	5	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	8	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	11	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	13	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	14	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	17	0.17
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	19	0.17
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	13	0.17
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	13	0.17
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	13	0.17
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	17	0.17
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	17	0.17
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	17	0.17
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD11	14	0.17
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD12	14	0.17
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD13	14	0.17
(1,6367)	1:176:A:TRP:HB2	1:177:A:ASP:H	14	0.17
(1,6367)	1:176:A:TRP:HB2	1:177:A:ASP:H	18	0.17
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	3	0.17
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	7	0.17
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	18	0.17
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	12	0.17
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	12	0.17
(1,6035)	1:155:A:TYR:HE1	1:155:A:TYR:H	6	0.17
(1,6035)	1:155:A:TYR:HE2	1:155:A:TYR:H	6	0.17
(1,6035)	1:155:A:TYR:HE1	1:155:A:TYR:H	15	0.17
(1,6035)	1:155:A:TYR:HE2	1:155:A:TYR:H	15	0.17
(1,6032)	1:155:A:TYR:HB2	1:155:A:TYR:H	3	0.17
(1,6032)	1:155:A:TYR:HB2	1:155:A:TYR:H	12	0.17
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	7	0.17
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	7	0.17
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	7	0.17
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	7	0.17
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	7	0.17
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	7	0.17
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	7	0.17
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	7	0.17
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	7	0.17
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	15	0.17
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	15	0.17
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	15	0.17
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	15	0.17
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	15	0.17
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	15	0.17
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	15	0.17
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	15	0.17
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5856)	1:143:A:LEU:HD21	1:146:A:ALA:H	16	0.17
(1,5856)	1:143:A:LEU:HD22	1:146:A:ALA:H	16	0.17
(1,5856)	1:143:A:LEU:HD23	1:146:A:ALA:H	16	0.17
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD11	11	0.17
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD12	11	0.17
(1,5819)	1:141:A:GLN:HE21	1:194:A:LEU:HD13	11	0.17
(1,5683)	1:129:A:ILE:HG21	1:193:A:ILE:HG21	20	0.17
(1,5683)	1:129:A:ILE:HG22	1:193:A:ILE:HG21	20	0.17
(1,5683)	1:129:A:ILE:HG23	1:193:A:ILE:HG21	20	0.17
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	6	0.17
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	6	0.17
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	6	0.17
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	20	0.17
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	20	0.17
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	20	0.17
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD11	2	0.17
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD12	2	0.17
(1,5675)	1:129:A:ILE:HB	1:186:A:LEU:HD13	2	0.17
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	12	0.17
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	12	0.17
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	12	0.17
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	12	0.17
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	12	0.17
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	12	0.17
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	12	0.17
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	12	0.17
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	12	0.17
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	2	0.17
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	2	0.17
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	2	0.17
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	2	0.17
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	2	0.17
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	2	0.17
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	6	0.17
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	6	0.17
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	6	0.17
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	20	0.17
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	20	0.17
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	20	0.17
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	2	0.17
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	2	0.17
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4968)	1:91:A:ARG:HB3	1:91:A:ARG:H	17	0.17
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	6	0.17
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	6	0.17
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	6	0.17
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	7	0.17
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	7	0.17
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	7	0.17
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	19	0.17
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	20	0.17
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	15	0.17
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	15	0.17
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	15	0.17
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	18	0.17
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	18	0.17
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	18	0.17
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	20	0.17
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	20	0.17
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	20	0.17
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	13	0.17
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	13	0.17
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	13	0.17
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	15	0.17
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	19	0.17
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	11	0.17
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD21	11	0.17
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD22	11	0.17
(1,4383)	1:60:A:LYS:HA	1:62:A:LEU:HD23	11	0.17
(1,4265)	1:52:A:ARG:HG3	1:53:A:GLY:H	20	0.17
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	14	0.17
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	14	0.17
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	1	0.17
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	5	0.17
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	5	0.17
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	5	0.17
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	5	0.17
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	4	0.17
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	10	0.17
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	17	0.17
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG21	12	0.17
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG22	12	0.17
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG23	12	0.17
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG21	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG22	12	0.17
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG23	12	0.17
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	5	0.17
(1,3385)	2:416:D:DA:H1'	2:416:D:DA:H5''	17	0.17
(1,3292)	1:396:B:GLN:HA	1:396:B:GLN:HG2	19	0.17
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	18	0.17
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	18	0.17
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	18	0.17
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	18	0.17
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	18	0.17
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	18	0.17
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	18	0.17
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	18	0.17
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	18	0.17
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	14	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	1	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	3	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	4	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	5	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	8	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	11	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	12	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	18	0.17
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	19	0.17
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	9	0.17
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	16	0.17
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	19	0.17
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	9	0.17
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	6	0.17
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	6	0.17
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	12	0.17
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	12	0.17
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	13	0.17
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	13	0.17
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	15	0.17
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	15	0.17
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	20	0.17
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	20	0.17
(1,2594)	1:351:B:ILE:HD11	1:352:B:MET:H	3	0.17
(1,2594)	1:351:B:ILE:HD12	1:352:B:MET:H	3	0.17
(1,2594)	1:351:B:ILE:HD13	1:352:B:MET:H	3	0.17
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	6	0.17
(1,2397)	1:339:B:LEU:H	1:392:B:ILE:HG22	15	0.17
(1,2346)	1:335:B:TYR:HE1	1:335:B:TYR:H	11	0.17
(1,2346)	1:335:B:TYR:HE2	1:335:B:TYR:H	11	0.17
(1,2275)	1:328:B:ILE:HG21	1:330:B:ASP:H	13	0.17
(1,2275)	1:328:B:ILE:HG22	1:330:B:ASP:H	13	0.17
(1,2275)	1:328:B:ILE:HG23	1:330:B:ASP:H	13	0.17
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	8	0.17
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	8	0.17
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	8	0.17
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	9	0.17
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	9	0.17
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	9	0.17
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	9	0.17
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	9	0.17
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	9	0.17
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	9	0.17
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	9	0.17
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	9	0.17
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	9	0.17
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	9	0.17
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	9	0.17
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	9	0.17
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	9	0.17
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	9	0.17
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	9	0.17
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	9	0.17
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	9	0.17
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	8	0.17
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	8	0.17
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	8	0.17
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	10	0.17
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	10	0.17
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	10	0.17
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	14	0.17
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	14	0.17
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	14	0.17
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	14	0.17
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	14	0.17
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	14	0.17
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	17	0.17
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	17	0.17
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	12	0.17
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	18	0.17
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	7	0.17
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	6	0.17
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	14	0.17
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	6	0.17
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	6	0.17
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	6	0.17
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	7	0.17
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	7	0.17
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	7	0.17
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	14	0.17
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	14	0.17
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	14	0.17
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	15	0.17
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	15	0.17
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	15	0.17
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	6	0.17
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	9	0.17
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	13	0.17
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	17	0.17
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	18	0.17
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	20	0.17
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	14	0.17
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	15	0.17
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	2	0.17
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	17	0.17
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	20	0.17
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	20	0.17
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	20	0.17
(1,655)	1:239:B:LEU:HD11	1:289:B:TYR:HD1	8	0.17
(1,655)	1:239:B:LEU:HD11	1:289:B:TYR:HD2	8	0.17
(1,655)	1:239:B:LEU:HD12	1:289:B:TYR:HD1	8	0.17
(1,655)	1:239:B:LEU:HD12	1:289:B:TYR:HD2	8	0.17
(1,655)	1:239:B:LEU:HD13	1:289:B:TYR:HD1	8	0.17
(1,655)	1:239:B:LEU:HD13	1:289:B:TYR:HD2	8	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG21	1	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG22	1	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG23	1	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG21	1	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG22	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG23	1	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG21	1	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG22	1	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG23	1	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG21	19	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG22	19	0.17
(1,652)	1:239:B:LEU:HD21	1:288:B:ILE:HG23	19	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG21	19	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG22	19	0.17
(1,652)	1:239:B:LEU:HD22	1:288:B:ILE:HG23	19	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG21	19	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG22	19	0.17
(1,652)	1:239:B:LEU:HD23	1:288:B:ILE:HG23	19	0.17
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	2	0.17
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	2	0.17
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	2	0.17
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	8	0.17
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	8	0.17
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	8	0.17
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	15	0.17
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	15	0.17
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	15	0.17
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	17	0.17
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	17	0.17
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	17	0.17
(1,574)	1:237:B:GLU:HG2	1:290:B:ARG:HB2	20	0.17
(1,532)	1:236:B:VAL:HG21	1:291:B:VAL:HG11	1	0.17
(1,532)	1:236:B:VAL:HG21	1:291:B:VAL:HG12	1	0.17
(1,532)	1:236:B:VAL:HG21	1:291:B:VAL:HG13	1	0.17
(1,532)	1:236:B:VAL:HG22	1:291:B:VAL:HG11	1	0.17
(1,532)	1:236:B:VAL:HG22	1:291:B:VAL:HG12	1	0.17
(1,532)	1:236:B:VAL:HG22	1:291:B:VAL:HG13	1	0.17
(1,532)	1:236:B:VAL:HG23	1:291:B:VAL:HG11	1	0.17
(1,532)	1:236:B:VAL:HG23	1:291:B:VAL:HG12	1	0.17
(1,532)	1:236:B:VAL:HG23	1:291:B:VAL:HG13	1	0.17
(1,523)	1:236:B:VAL:HG21	1:289:B:TYR:HA	14	0.17
(1,523)	1:236:B:VAL:HG22	1:289:B:TYR:HA	14	0.17
(1,523)	1:236:B:VAL:HG23	1:289:B:TYR:HA	14	0.17
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG11	18	0.17
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG12	18	0.17
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG13	18	0.17
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG11	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG12	7	0.17
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG13	7	0.17
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB2	11	0.16
(1,6956)	1:208:B:PRO:HB2	1:54:A:PHE:HB3	11	0.16
(1,6694)	1:197:A:GLN:HA	1:197:A:GLN:HG2	7	0.16
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	3	0.16
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	18	0.16
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	19	0.16
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	8	0.16
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	8	0.16
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	8	0.16
(1,6591)	1:191:A:ARG:HD3	1:192:A:ALA:H	14	0.16
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	20	0.16
(1,6570)	1:191:A:ARG:HB3	1:191:A:ARG:HD3	13	0.16
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD11	2	0.16
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD12	2	0.16
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD13	2	0.16
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD11	2	0.16
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD12	2	0.16
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD13	2	0.16
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD11	2	0.16
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD12	2	0.16
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD13	2	0.16
(1,6491)	1:184:A:GLN:HA	1:187:A:SER:H	18	0.16
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	3	0.16
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	7	0.16
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	12	0.16
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	20	0.16
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	19	0.16
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	19	0.16
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	19	0.16
(1,6348)	1:175:A:PRO:HA	1:179:A:LEU:HG	11	0.16
(1,6321)	1:174:A:GLN:HB3	1:174:A:GLN:H	12	0.16
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	7	0.16
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	7	0.16
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	15	0.16
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	15	0.16
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	4	0.16
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	17	0.16
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	15	0.16
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	15	0.16
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	15	0.16
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	15	0.16
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	15	0.16
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	15	0.16
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	15	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	2	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	2	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	2	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	2	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	2	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	2	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	2	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	2	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	2	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	6	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	6	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	6	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	6	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	6	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	6	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	6	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	6	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	6	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	19	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	19	0.16
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	19	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	19	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	19	0.16
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	19	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	19	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	19	0.16
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	19	0.16
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	5	0.16
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	8	0.16
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	8	0.16
(1,5806)	1:141:A:GLN:HB2	1:141:A:GLN:HE21	17	0.16
(1,5806)	1:141:A:GLN:HB3	1:141:A:GLN:HE21	17	0.16
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB1	7	0.16
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB2	7	0.16
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB3	7	0.16
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB1	7	0.16
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB2	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB3	7	0.16
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB1	7	0.16
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB2	7	0.16
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB3	7	0.16
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	17	0.16
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	17	0.16
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	8	0.16
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	9	0.16
(1,5575)	1:122:A:LEU:HD11	1:148:A:ALA:HB1	3	0.16
(1,5575)	1:122:A:LEU:HD11	1:148:A:ALA:HB2	3	0.16
(1,5575)	1:122:A:LEU:HD11	1:148:A:ALA:HB3	3	0.16
(1,5575)	1:122:A:LEU:HD12	1:148:A:ALA:HB1	3	0.16
(1,5575)	1:122:A:LEU:HD12	1:148:A:ALA:HB2	3	0.16
(1,5575)	1:122:A:LEU:HD12	1:148:A:ALA:HB3	3	0.16
(1,5575)	1:122:A:LEU:HD13	1:148:A:ALA:HB1	3	0.16
(1,5575)	1:122:A:LEU:HD13	1:148:A:ALA:HB2	3	0.16
(1,5575)	1:122:A:LEU:HD13	1:148:A:ALA:HB3	3	0.16
(1,5575)	1:122:A:LEU:HD21	1:148:A:ALA:HB1	3	0.16
(1,5575)	1:122:A:LEU:HD21	1:148:A:ALA:HB2	3	0.16
(1,5575)	1:122:A:LEU:HD21	1:148:A:ALA:HB3	3	0.16
(1,5575)	1:122:A:LEU:HD22	1:148:A:ALA:HB1	3	0.16
(1,5575)	1:122:A:LEU:HD22	1:148:A:ALA:HB2	3	0.16
(1,5575)	1:122:A:LEU:HD22	1:148:A:ALA:HB3	3	0.16
(1,5575)	1:122:A:LEU:HD23	1:148:A:ALA:HB1	3	0.16
(1,5575)	1:122:A:LEU:HD23	1:148:A:ALA:HB2	3	0.16
(1,5575)	1:122:A:LEU:HD23	1:148:A:ALA:HB3	3	0.16
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD11	15	0.16
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD12	15	0.16
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD13	15	0.16
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD21	15	0.16
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD22	15	0.16
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD23	15	0.16
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD11	15	0.16
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD12	15	0.16
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD13	15	0.16
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD21	15	0.16
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD22	15	0.16
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD23	15	0.16
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD11	15	0.16
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD12	15	0.16
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD13	15	0.16
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD21	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD22	15	0.16
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD23	15	0.16
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	12	0.16
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	19	0.16
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	8	0.16
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	8	0.16
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	8	0.16
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	8	0.16
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	8	0.16
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	8	0.16
(1,5286)	1:111:A:ARG:HA	1:111:A:ARG:HD2	16	0.16
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	1	0.16
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	1	0.16
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	1	0.16
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	8	0.16
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	8	0.16
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	8	0.16
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	5	0.16
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	5	0.16
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	5	0.16
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	11	0.16
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	6	0.16
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	6	0.16
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	6	0.16
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	6	0.16
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	6	0.16
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	6	0.16
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	18	0.16
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	18	0.16
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	18	0.16
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	18	0.16
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	18	0.16
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	18	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	2	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	2	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	2	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	8	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	8	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	8	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	18	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	18	0.16
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	7	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	1	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	1	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	1	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	2	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	2	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	2	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	4	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	4	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	4	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	5	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	5	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	5	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	6	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	6	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	6	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	7	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	7	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	7	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	8	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	8	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	8	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	9	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	9	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	9	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	10	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	10	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	10	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	12	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	12	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	12	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	14	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	14	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	14	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	16	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	16	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	16	0.16
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	19	0.16
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	19	0.16
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	19	0.16
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	8	0.16
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	8	0.16
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	8	0.16
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	8	0.16
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	2	0.16
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	4	0.16
(1,4265)	1:52:A:ARG:HG3	1:53:A:GLY:H	5	0.16
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	16	0.16
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	16	0.16
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	16	0.16
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	19	0.16
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	19	0.16
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	19	0.16
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	14	0.16
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	14	0.16
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	14	0.16
(1,4015)	1:39:A:ARG:H	1:47:A:LYS:HA	9	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	3	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	3	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	3	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	4	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	4	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	4	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	16	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	16	0.16
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	16	0.16
(1,3886)	1:36:A:GLU:HA	1:93:A:THR:HB	2	0.16
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	11	0.16
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG21	5	0.16
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG22	5	0.16
(1,3608)	1:15:A:PRO:HG2	1:166:A:VAL:HG23	5	0.16
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG21	5	0.16
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG22	5	0.16
(1,3608)	1:15:A:PRO:HG3	1:166:A:VAL:HG23	5	0.16
(1,3292)	1:396:B:GLN:HA	1:396:B:GLN:HG2	12	0.16
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	13	0.16
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	19	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	9	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	9	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	9	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	9	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	9	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	9	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	9	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	9	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	16	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	16	0.16
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	16	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	16	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	16	0.16
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	16	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	16	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	16	0.16
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	16	0.16
(1,3089)	1:383:B:GLN:HA	1:386:B:SER:H	12	0.16
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	9	0.16
(1,2962)	1:375:B:TRP:HZ3	1:375:B:TRP:H	6	0.16
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	14	0.16
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	20	0.16
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	10	0.16
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	10	0.16
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	17	0.16
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	17	0.16
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	9	0.16
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	17	0.16
(1,2580)	1:351:B:ILE:HG12	1:351:B:ILE:H	19	0.16
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD11	9	0.16
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD12	9	0.16
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD13	9	0.16
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD11	12	0.16
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD12	12	0.16
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD13	12	0.16
(1,2403)	1:340:B:GLN:HB2	1:340:B:GLN:HE21	5	0.16
(1,2403)	1:340:B:GLN:HB3	1:340:B:GLN:HE21	5	0.16
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE1	16	0.16
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE2	16	0.16
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE3	16	0.16
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE1	16	0.16
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE2	16	0.16
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE3	16	0.16
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE1	16	0.16
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE2	16	0.16
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE3	16	0.16
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	6	0.16
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	6	0.16
(1,2104)	1:318:B:HIS:HE1	1:318:B:HIS:H	7	0.16
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	1	0.16
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	1	0.16
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	1	0.16
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	1	0.16
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	1	0.16
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	1	0.16
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	1	0.16
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	1	0.16
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	1	0.16
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	20	0.16
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	20	0.16
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	20	0.16
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	20	0.16
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	20	0.16
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	20	0.16
(1,1750)	1:300:B:CYS:H	1:301:B:PHE:H	6	0.16
(1,1708)	1:295:B:ILE:HD11	1:296:B:SER:H	4	0.16
(1,1708)	1:295:B:ILE:HD12	1:296:B:SER:H	4	0.16
(1,1708)	1:295:B:ILE:HD13	1:296:B:SER:H	4	0.16
(1,1708)	1:295:B:ILE:HD11	1:296:B:SER:H	11	0.16
(1,1708)	1:295:B:ILE:HD12	1:296:B:SER:H	11	0.16
(1,1708)	1:295:B:ILE:HD13	1:296:B:SER:H	11	0.16
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	14	0.16
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	15	0.16
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	2	0.16
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	2	0.16
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE1	5	0.16
(1,1671)	1:294:B:PHE:HA	1:324:B:PHE:HE2	5	0.16
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	6	0.16
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	6	0.16
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	6	0.16
(1,1447)	1:283:B:LEU:HD21	1:318:B:HIS:HD2	4	0.16
(1,1447)	1:283:B:LEU:HD22	1:318:B:HIS:HD2	4	0.16
(1,1447)	1:283:B:LEU:HD23	1:318:B:HIS:HD2	4	0.16
(1,1447)	1:283:B:LEU:HD21	1:318:B:HIS:HD2	20	0.16
(1,1447)	1:283:B:LEU:HD22	1:318:B:HIS:HD2	20	0.16
(1,1447)	1:283:B:LEU:HD23	1:318:B:HIS:HD2	20	0.16
(1,1446)	1:283:B:LEU:HD11	1:318:B:HIS:HD2	12	0.16
(1,1446)	1:283:B:LEU:HD12	1:318:B:HIS:HD2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1446)	1:283:B:LEU:HD13	1:318:B:HIS:HD2	12	0.16
(1,1406)	1:282:B:GLN:HB2	1:282:B:GLN:H	3	0.16
(1,1337)	1:279:B:PRO:HA	1:282:B:GLN:HB3	6	0.16
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	7	0.16
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	12	0.16
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	8	0.16
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	8	0.16
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	8	0.16
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	7	0.16
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	15	0.16
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD21	14	0.16
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD22	14	0.16
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD23	14	0.16
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD21	14	0.16
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD22	14	0.16
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD23	14	0.16
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	10	0.16
(1,1147)	1:274:B:PHE:HE1	1:274:B:PHE:H	11	0.16
(1,1147)	1:274:B:PHE:HE2	1:274:B:PHE:H	11	0.16
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	4	0.16
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD1	16	0.16
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD2	16	0.16
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD1	16	0.16
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD2	16	0.16
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD1	16	0.16
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD2	16	0.16
(1,884)	1:253:B:PHE:HD1	1:253:B:PHE:H	2	0.16
(1,884)	1:253:B:PHE:HD2	1:253:B:PHE:H	2	0.16
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	4	0.16
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	18	0.16
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	20	0.16
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	5	0.16
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	5	0.16
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	5	0.16
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	12	0.16
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	12	0.16
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	12	0.16
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	20	0.16
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	20	0.16
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	20	0.16
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	10	0.16
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	10	0.16
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	16	0.16
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	16	0.16
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	16	0.16
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG11	16	0.16
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG12	16	0.16
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG13	16	0.16
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG11	16	0.16
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG12	16	0.16
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG13	16	0.16
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG11	16	0.16
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG12	16	0.16
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG13	16	0.16
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB2	7	0.15
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB3	7	0.15
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	4	0.15
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	7	0.15
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD11	19	0.15
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD12	19	0.15
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD13	19	0.15
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	4	0.15
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD21	18	0.15
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD22	18	0.15
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD23	18	0.15
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD21	18	0.15
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD22	18	0.15
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD23	18	0.15
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD21	18	0.15
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD22	18	0.15
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD23	18	0.15
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	10	0.15
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	14	0.15
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	17	0.15
(1,6479)	1:184:A:GLN:HB2	1:184:A:GLN:HE21	18	0.15
(1,6479)	1:184:A:GLN:HB3	1:184:A:GLN:HE21	18	0.15
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	4	0.15
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	18	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	3	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	3	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	3	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	8	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	8	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	20	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	20	0.15
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	20	0.15
(1,6367)	1:176:A:TRP:HB2	1:177:A:ASP:H	10	0.15
(1,6348)	1:175:A:PRO:HA	1:179:A:LEU:HG	20	0.15
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	13	0.15
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	1	0.15
(1,6120)	1:161:A:CYS:HG	1:161:A:CYS:H	12	0.15
(1,6035)	1:155:A:TYR:HE1	1:155:A:TYR:H	13	0.15
(1,6035)	1:155:A:TYR:HE2	1:155:A:TYR:H	13	0.15
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	11	0.15
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	11	0.15
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	11	0.15
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	11	0.15
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	11	0.15
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	11	0.15
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	11	0.15
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	11	0.15
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	11	0.15
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	20	0.15
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	20	0.15
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	20	0.15
(1,5856)	1:143:A:LEU:HD21	1:146:A:ALA:H	15	0.15
(1,5856)	1:143:A:LEU:HD22	1:146:A:ALA:H	15	0.15
(1,5856)	1:143:A:LEU:HD23	1:146:A:ALA:H	15	0.15
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD11	12	0.15
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD12	12	0.15
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD13	12	0.15
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	1	0.15
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	1	0.15
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	7	0.15
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	7	0.15
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	7	0.15
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	19	0.15
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	19	0.15
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	19	0.15
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	3	0.15
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	12	0.15
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	17	0.15
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	20	0.15
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD11	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD12	16	0.15
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD13	16	0.15
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD21	16	0.15
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD22	16	0.15
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD23	16	0.15
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD11	16	0.15
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD12	16	0.15
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD13	16	0.15
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD21	16	0.15
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD22	16	0.15
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD23	16	0.15
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD11	16	0.15
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD12	16	0.15
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD13	16	0.15
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD21	16	0.15
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD22	16	0.15
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD23	16	0.15
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	6	0.15
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	6	0.15
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	6	0.15
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	12	0.15
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	12	0.15
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	12	0.15
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	15	0.15
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	15	0.15
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	15	0.15
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	19	0.15
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	19	0.15
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	19	0.15
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	20	0.15
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	20	0.15
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	20	0.15
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	3	0.15
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	6	0.15
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	8	0.15
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	17	0.15
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	15	0.15
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	15	0.15
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	15	0.15
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	15	0.15
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	15	0.15
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	15	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	15	0.15
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	15	0.15
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	15	0.15
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	10	0.15
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	14	0.15
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	14	0.15
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	14	0.15
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	7	0.15
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	7	0.15
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	7	0.15
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	16	0.15
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	16	0.15
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	16	0.15
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	18	0.15
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	18	0.15
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	18	0.15
(1,4968)	1:91:A:ARG:HB3	1:91:A:ARG:H	5	0.15
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	2	0.15
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	2	0.15
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	2	0.15
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	2	0.15
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	2	0.15
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	2	0.15
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	19	0.15
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	19	0.15
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	19	0.15
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	14	0.15
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	15	0.15
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	17	0.15
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	3	0.15
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	3	0.15
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	3	0.15
(1,4697)	1:79:A:VAL:HG11	1:79:A:VAL:H	13	0.15
(1,4697)	1:79:A:VAL:HG12	1:79:A:VAL:H	13	0.15
(1,4697)	1:79:A:VAL:HG13	1:79:A:VAL:H	13	0.15
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	11	0.15
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	11	0.15
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	11	0.15
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	20	0.15
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	5	0.15
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	5	0.15
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	16	0.15
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	14	0.15
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	15	0.15
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	18	0.15
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	7	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	3	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	6	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	9	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	11	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	12	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	16	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	18	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	19	0.15
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	20	0.15
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	8	0.15
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	8	0.15
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	8	0.15
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	17	0.15
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	17	0.15
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	17	0.15
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG21	15	0.15
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG22	15	0.15
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG23	15	0.15
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG21	15	0.15
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG22	15	0.15
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG23	15	0.15
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG21	15	0.15
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG22	15	0.15
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG23	15	0.15
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	13	0.15
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	13	0.15
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	13	0.15
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	14	0.15
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	14	0.15
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	14	0.15
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	1	0.15
(1,3624)	1:16:A:HIS:HD1	1:17:A:ILE:HD11	8	0.15
(1,3624)	1:16:A:HIS:HD1	1:17:A:ILE:HD12	8	0.15
(1,3624)	1:16:A:HIS:HD1	1:17:A:ILE:HD13	8	0.15
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	2	0.15
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	12	0.15
(1,3541)	1:12:A:LEU:HD21	1:169:A:GLN:HE21	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3541)	1:12:A:LEU:HD22	1:169:A:GLN:HE21	1	0.15
(1,3541)	1:12:A:LEU:HD23	1:169:A:GLN:HE21	1	0.15
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD21	11	0.15
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD22	11	0.15
(1,3517)	1:11:A:HIS:HD2	1:12:A:LEU:HD23	11	0.15
(1,3292)	1:396:B:GLN:HA	1:396:B:GLN:HG2	8	0.15
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	1	0.15
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	7	0.15
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	8	0.15
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	15	0.15
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	7	0.15
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	12	0.15
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	6	0.15
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	10	0.15
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	5	0.15
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	5	0.15
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	5	0.15
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	8	0.15
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	8	0.15
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	8	0.15
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	13	0.15
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	6	0.15
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	11	0.15
(1,2901)	1:372:B:PHE:HZ	1:375:B:TRP:H	18	0.15
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	11	0.15
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	17	0.15
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	20	0.15
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	5	0.15
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	16	0.15
(1,2782)	1:363:B:THR:HG21	1:365:B:VAL:H	10	0.15
(1,2782)	1:363:B:THR:HG22	1:365:B:VAL:H	10	0.15
(1,2782)	1:363:B:THR:HG23	1:365:B:VAL:H	10	0.15
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	3	0.15
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	3	0.15
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	4	0.15
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	4	0.15
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	7	0.15
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	7	0.15
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	9	0.15
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	9	0.15
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	14	0.15
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	18	0.15
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	18	0.15
(1,2594)	1:351:B:ILE:HD11	1:352:B:MET:H	2	0.15
(1,2594)	1:351:B:ILE:HD12	1:352:B:MET:H	2	0.15
(1,2594)	1:351:B:ILE:HD13	1:352:B:MET:H	2	0.15
(1,2586)	1:351:B:ILE:HG21	1:352:B:MET:H	7	0.15
(1,2586)	1:351:B:ILE:HG22	1:352:B:MET:H	7	0.15
(1,2586)	1:351:B:ILE:HG23	1:352:B:MET:H	7	0.15
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG11	2	0.15
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG12	2	0.15
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG13	2	0.15
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD21	4	0.15
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD22	4	0.15
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD23	4	0.15
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD21	4	0.15
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD22	4	0.15
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD23	4	0.15
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD21	4	0.15
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD22	4	0.15
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD23	4	0.15
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	14	0.15
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	14	0.15
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	14	0.15
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	15	0.15
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	15	0.15
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	15	0.15
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	18	0.15
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	18	0.15
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	18	0.15
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	19	0.15
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	19	0.15
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	19	0.15
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	20	0.15
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	20	0.15
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	20	0.15
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	6	0.15
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	6	0.15
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	6	0.15
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	8	0.15
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	8	0.15
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	8	0.15
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	17	0.15
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	17	0.15
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	17	0.15
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	17	0.15
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	17	0.15
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	17	0.15
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	17	0.15
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	17	0.15
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	17	0.15
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	4	0.15
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	4	0.15
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	4	0.15
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	4	0.15
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	4	0.15
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	4	0.15
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	5	0.15
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	15	0.15
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	15	0.15
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	15	0.15
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	15	0.15
(1,1447)	1:283:B:LEU:HD21	1:318:B:HIS:HD2	15	0.15
(1,1447)	1:283:B:LEU:HD22	1:318:B:HIS:HD2	15	0.15
(1,1447)	1:283:B:LEU:HD23	1:318:B:HIS:HD2	15	0.15
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG21	19	0.15
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG22	19	0.15
(1,1389)	1:281:B:LEU:HD21	1:291:B:VAL:HG23	19	0.15
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG21	19	0.15
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG22	19	0.15
(1,1389)	1:281:B:LEU:HD22	1:291:B:VAL:HG23	19	0.15
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG21	19	0.15
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG22	19	0.15
(1,1389)	1:281:B:LEU:HD23	1:291:B:VAL:HG23	19	0.15
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	1	0.15
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	1	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	1	0.15
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	2	0.15
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	2	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	2	0.15
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	5	0.15
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	5	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	5	0.15
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	10	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	10	0.15
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	16	0.15
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	16	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	16	0.15
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	17	0.15
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	17	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	17	0.15
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	20	0.15
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	20	0.15
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	20	0.15
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	2	0.15
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	2	0.15
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	2	0.15
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	17	0.15
(1,1231)	1:275:B:LEU:HD11	1:312:B:PHE:HZ	8	0.15
(1,1231)	1:275:B:LEU:HD12	1:312:B:PHE:HZ	8	0.15
(1,1231)	1:275:B:LEU:HD13	1:312:B:PHE:HZ	8	0.15
(1,1231)	1:275:B:LEU:HD11	1:312:B:PHE:HZ	9	0.15
(1,1231)	1:275:B:LEU:HD12	1:312:B:PHE:HZ	9	0.15
(1,1231)	1:275:B:LEU:HD13	1:312:B:PHE:HZ	9	0.15
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	3	0.15
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	5	0.15
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	8	0.15
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	12	0.15
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	16	0.15
(1,789)	1:246:B:LYS:HE2	1:247:B:MET:H	6	0.15
(1,789)	1:246:B:LYS:HE3	1:247:B:MET:H	6	0.15
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	2	0.15
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	5	0.15
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	5	0.15
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	8	0.15
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	15	0.15
(1,660)	1:239:B:LEU:HD21	1:244:B:SER:HB2	15	0.15
(1,660)	1:239:B:LEU:HD22	1:244:B:SER:HB2	15	0.15
(1,660)	1:239:B:LEU:HD23	1:244:B:SER:HB2	15	0.15
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	2	0.15
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	2	0.15
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	2	0.15
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	9	0.15
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	9	0.15
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	13	0.15
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	13	0.15
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	13	0.15
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	16	0.15
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	16	0.15
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	16	0.15
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	3	0.15
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	3	0.15
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	3	0.15
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	5	0.15
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	5	0.15
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	5	0.15
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	10	0.15
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	10	0.15
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	10	0.15
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	18	0.15
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	18	0.15
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	18	0.15
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	8	0.15
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	13	0.15
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG21	14	0.15
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG22	14	0.15
(1,488)	1:235:B:GLU:HG2	1:363:B:THR:HG23	14	0.15
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	7	0.15
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	7	0.15
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	7	0.15
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	7	0.15
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	7	0.15
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	7	0.15
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	3	0.15
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	3	0.15
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	3	0.15
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	3	0.15
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	3	0.15
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	3	0.15
(1,456)	1:234:B:TYR:HB3	1:252:B:GLY:H	12	0.15
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	20	0.15
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	20	0.15
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	20	0.15
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE1	7	0.15
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE2	7	0.15
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE1	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE2	7	0.15
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE1	7	0.15
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE2	7	0.15
(1,361)	1:227:B:ARG:HE	1:227:B:ARG:H	4	0.15
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	3	0.15
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	3	0.15
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	3	0.15
(1,316)	1:221:B:PHE:HD1	1:296:B:SER:H	12	0.15
(1,316)	1:221:B:PHE:HD2	1:296:B:SER:H	12	0.15
(1,7000)	1:11:A:HIS:HB2	1:253:B:PHE:HE1	14	0.14
(1,7000)	1:11:A:HIS:HB2	1:253:B:PHE:HE2	14	0.14
(1,7000)	1:11:A:HIS:HB3	1:253:B:PHE:HE1	14	0.14
(1,7000)	1:11:A:HIS:HB3	1:253:B:PHE:HE2	14	0.14
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB2	18	0.14
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB3	18	0.14
(1,6962)	1:208:B:PRO:HB2	1:165:A:PHE:HE1	20	0.14
(1,6962)	1:208:B:PRO:HB3	1:165:A:PHE:HE1	20	0.14
(1,6694)	1:197:A:GLN:HA	1:197:A:GLN:HG2	5	0.14
(1,6694)	1:197:A:GLN:HA	1:197:A:GLN:HG2	18	0.14
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	7	0.14
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	8	0.14
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	13	0.14
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	14	0.14
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	15	0.14
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	17	0.14
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	13	0.14
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	18	0.14
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	1	0.14
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	9	0.14
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	11	0.14
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	12	0.14
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	14	0.14
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	6	0.14
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	16	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	1	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	1	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	1	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	5	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	5	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	5	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD11	11	0.14
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD12	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6386)	1:177:A:ASP:HB2	1:179:A:LEU:HD13	11	0.14
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD21	10	0.14
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD22	10	0.14
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD23	10	0.14
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD21	15	0.14
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD22	15	0.14
(1,6350)	1:175:A:PRO:HA	1:179:A:LEU:HD23	15	0.14
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	4	0.14
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	10	0.14
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	10	0.14
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	16	0.14
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	16	0.14
(1,6251)	1:169:A:GLN:HB3	1:169:A:GLN:HE22	3	0.14
(1,6249)	1:169:A:GLN:HB2	1:169:A:GLN:H	15	0.14
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	20	0.14
(1,6224)	1:168:A:HIS:HA	1:168:A:HIS:HD2	6	0.14
(1,6224)	1:168:A:HIS:HA	1:168:A:HIS:HD2	16	0.14
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	5	0.14
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	9	0.14
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	20	0.14
(1,6050)	1:155:A:TYR:HE1	1:173:A:PHE:HZ	3	0.14
(1,6050)	1:155:A:TYR:HE2	1:173:A:PHE:HZ	3	0.14
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	12	0.14
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	12	0.14
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	16	0.14
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	16	0.14
(1,6032)	1:155:A:TYR:HB2	1:155:A:TYR:H	16	0.14
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	11	0.14
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	11	0.14
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	11	0.14
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	18	0.14
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	18	0.14
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	18	0.14
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD11	6	0.14
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD12	6	0.14
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD13	6	0.14
(1,5859)	1:143:A:LEU:HD11	1:148:A:ALA:H	17	0.14
(1,5859)	1:143:A:LEU:HD12	1:148:A:ALA:H	17	0.14
(1,5859)	1:143:A:LEU:HD13	1:148:A:ALA:H	17	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD11	2	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD12	2	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD13	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD11	15	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD12	15	0.14
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD13	15	0.14
(1,5815)	1:141:A:GLN:HE21	1:193:A:ILE:HG21	7	0.14
(1,5815)	1:141:A:GLN:HE21	1:193:A:ILE:HG21	20	0.14
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	10	0.14
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	10	0.14
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	19	0.14
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	19	0.14
(1,5693)	1:129:A:ILE:HD11	1:189:A:ARG:H	13	0.14
(1,5693)	1:129:A:ILE:HD12	1:189:A:ARG:H	13	0.14
(1,5693)	1:129:A:ILE:HD13	1:189:A:ARG:H	13	0.14
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD21	12	0.14
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD22	12	0.14
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD23	12	0.14
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD21	12	0.14
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD22	12	0.14
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD23	12	0.14
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD21	12	0.14
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD22	12	0.14
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD23	12	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	4	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	4	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	4	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	12	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	12	0.14
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	12	0.14
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	7	0.14
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	15	0.14
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	19	0.14
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	1	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	1	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	1	0.14
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	2	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	2	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	2	0.14
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	3	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	3	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	3	0.14
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	4	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	4	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	8	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	8	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	8	0.14
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	9	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	9	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	9	0.14
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	10	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	10	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	10	0.14
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	11	0.14
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	11	0.14
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	11	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	1	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	2	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	7	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	9	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	10	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	13	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	14	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	18	0.14
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	20	0.14
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	14	0.14
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	14	0.14
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	14	0.14
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	14	0.14
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	14	0.14
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	14	0.14
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	14	0.14
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	14	0.14
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	14	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	3	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	3	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	3	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	3	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	3	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	3	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	5	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	5	0.14
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	5	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	5	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	5	0.14
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5312)	1:111:A:ARG:HD2	1:142:A:MET:HE1	8	0.14
(1,5312)	1:111:A:ARG:HD2	1:142:A:MET:HE2	8	0.14
(1,5312)	1:111:A:ARG:HD2	1:142:A:MET:HE3	8	0.14
(1,5308)	1:111:A:ARG:HD3	1:115:A:GLN:HG2	8	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	5	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	5	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	5	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	8	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	8	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	8	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	12	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	12	0.14
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	12	0.14
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	1	0.14
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	4	0.14
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	5	0.14
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	17	0.14
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	18	0.14
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	20	0.14
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	3	0.14
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	3	0.14
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	3	0.14
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	17	0.14
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	17	0.14
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	17	0.14
(1,5105)	1:96:A:ILE:HG21	1:126:A:ALA:HA	10	0.14
(1,5105)	1:96:A:ILE:HG22	1:126:A:ALA:HA	10	0.14
(1,5105)	1:96:A:ILE:HG23	1:126:A:ALA:HA	10	0.14
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	7	0.14
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	7	0.14
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	7	0.14
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	10	0.14
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	10	0.14
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	10	0.14
(1,4968)	1:91:A:ARG:HB3	1:91:A:ARG:H	8	0.14
(1,4968)	1:91:A:ARG:HB3	1:91:A:ARG:H	12	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	8	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	8	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	8	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	8	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	8	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	12	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	12	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	12	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	12	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	12	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	12	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	16	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	16	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	16	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	16	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	16	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	16	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	19	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	19	0.14
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	19	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	19	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	19	0.14
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	19	0.14
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	16	0.14
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	16	0.14
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	16	0.14
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	20	0.14
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	20	0.14
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	20	0.14
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	5	0.14
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	1	0.14
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	1	0.14
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	1	0.14
(1,4619)	1:76:A:LEU:HD11	1:94:A:TRP:HZ3	11	0.14
(1,4619)	1:76:A:LEU:HD12	1:94:A:TRP:HZ3	11	0.14
(1,4619)	1:76:A:LEU:HD13	1:94:A:TRP:HZ3	11	0.14
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	2	0.14
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	5	0.14
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	8	0.14
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	9	0.14
(1,4412)	1:62:A:LEU:HD21	1:67:A:TYR:HD1	14	0.14
(1,4412)	1:62:A:LEU:HD21	1:67:A:TYR:HD2	14	0.14
(1,4412)	1:62:A:LEU:HD22	1:67:A:TYR:HD1	14	0.14
(1,4412)	1:62:A:LEU:HD22	1:67:A:TYR:HD2	14	0.14
(1,4412)	1:62:A:LEU:HD23	1:67:A:TYR:HD1	14	0.14
(1,4412)	1:62:A:LEU:HD23	1:67:A:TYR:HD2	14	0.14
(1,4091)	1:41:A:ASP:HB2	1:44:A:THR:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4091)	1:41:A:ASP:HB3	1:44:A:THR:H	13	0.14
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	4	0.14
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	8	0.14
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	13	0.14
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	11	0.14
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	11	0.14
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	11	0.14
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	4	0.14
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	4	0.14
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	4	0.14
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	11	0.14
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	11	0.14
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	11	0.14
(1,4015)	1:39:A:ARG:H	1:47:A:LYS:HA	14	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	5	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	5	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	5	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	7	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	7	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	7	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	19	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	19	0.14
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	19	0.14
(1,3940)	1:37:A:VAL:HG11	1:93:A:THR:H	3	0.14
(1,3940)	1:37:A:VAL:HG12	1:93:A:THR:H	3	0.14
(1,3940)	1:37:A:VAL:HG13	1:93:A:THR:H	3	0.14
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE1	3	0.14
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE2	3	0.14
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE3	3	0.14
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE1	3	0.14
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE2	3	0.14
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE3	3	0.14
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE1	3	0.14
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE2	3	0.14
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE3	3	0.14
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	20	0.14
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	19	0.14
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	11	0.14
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	5	0.14
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	5	0.14
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	5	0.14
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	5	0.14
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	5	0.14
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	5	0.14
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	5	0.14
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	5	0.14
(1,3541)	1:12:A:LEU:HD21	1:169:A:GLN:HE21	2	0.14
(1,3541)	1:12:A:LEU:HD22	1:169:A:GLN:HE21	2	0.14
(1,3541)	1:12:A:LEU:HD23	1:169:A:GLN:HE21	2	0.14
(1,3292)	1:396:B:GLN:HA	1:396:B:GLN:HG2	2	0.14
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	8	0.14
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	15	0.14
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	4	0.14
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	6	0.14
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	10	0.14
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	17	0.14
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	20	0.14
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	4	0.14
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD11	20	0.14
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD12	20	0.14
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD13	20	0.14
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	5	0.14
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	5	0.14
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	5	0.14
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	5	0.14
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	5	0.14
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	5	0.14
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	5	0.14
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	5	0.14
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	5	0.14
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	13	0.14
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	13	0.14
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	13	0.14
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	13	0.14
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	13	0.14
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	13	0.14
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	13	0.14
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	13	0.14
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	13	0.14
(1,3156)	1:389:B:LEU:HD21	1:392:B:ILE:HD11	16	0.14
(1,3156)	1:389:B:LEU:HD21	1:392:B:ILE:HD12	16	0.14
(1,3156)	1:389:B:LEU:HD21	1:392:B:ILE:HD13	16	0.14
(1,3156)	1:389:B:LEU:HD22	1:392:B:ILE:HD11	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3156)	1:389:B:LEU:HD22	1:392:B:ILE:HD12	16	0.14
(1,3156)	1:389:B:LEU:HD22	1:392:B:ILE:HD13	16	0.14
(1,3156)	1:389:B:LEU:HD23	1:392:B:ILE:HD11	16	0.14
(1,3156)	1:389:B:LEU:HD23	1:392:B:ILE:HD12	16	0.14
(1,3156)	1:389:B:LEU:HD23	1:392:B:ILE:HD13	16	0.14
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	3	0.14
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	20	0.14
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	20	0.14
(1,2994)	1:377:B:GLY:H	1:378:B:LEU:H	17	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	1	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	1	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	1	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	3	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	3	0.14
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	3	0.14
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	2	0.14
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	15	0.14
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	16	0.14
(1,2901)	1:372:B:PHE:HZ	1:375:B:TRP:H	15	0.14
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	4	0.14
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	10	0.14
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	12	0.14
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	1	0.14
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	17	0.14
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD11	19	0.14
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD12	19	0.14
(1,2654)	1:354:B:TYR:H	1:378:B:LEU:HD13	19	0.14
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	15	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD11	11	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD12	11	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD13	11	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD11	14	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD12	14	0.14
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD13	14	0.14
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	2	0.14
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	2	0.14
(1,2600)	1:351:B:ILE:HD11	1:389:B:LEU:H	10	0.14
(1,2600)	1:351:B:ILE:HD12	1:389:B:LEU:H	10	0.14
(1,2600)	1:351:B:ILE:HD13	1:389:B:LEU:H	10	0.14
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD11	8	0.14
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD12	8	0.14
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD13	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD11	8	0.14
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD12	8	0.14
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD13	8	0.14
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD11	8	0.14
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD12	8	0.14
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD13	8	0.14
(1,2590)	1:351:B:ILE:HG21	1:385:B:LEU:H	3	0.14
(1,2590)	1:351:B:ILE:HG22	1:385:B:LEU:H	3	0.14
(1,2590)	1:351:B:ILE:HG23	1:385:B:LEU:H	3	0.14
(1,2586)	1:351:B:ILE:HG21	1:352:B:MET:H	1	0.14
(1,2586)	1:351:B:ILE:HG22	1:352:B:MET:H	1	0.14
(1,2586)	1:351:B:ILE:HG23	1:352:B:MET:H	1	0.14
(1,2586)	1:351:B:ILE:HG21	1:352:B:MET:H	15	0.14
(1,2586)	1:351:B:ILE:HG22	1:352:B:MET:H	15	0.14
(1,2586)	1:351:B:ILE:HG23	1:352:B:MET:H	15	0.14
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG11	4	0.14
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG12	4	0.14
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG13	4	0.14
(1,2346)	1:335:B:TYR:HE1	1:335:B:TYR:H	15	0.14
(1,2346)	1:335:B:TYR:HE2	1:335:B:TYR:H	15	0.14
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD21	6	0.14
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD22	6	0.14
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD23	6	0.14
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD21	6	0.14
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD22	6	0.14
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD23	6	0.14
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD21	6	0.14
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD22	6	0.14
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD23	6	0.14
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	17	0.14
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	17	0.14
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	17	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	14	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	14	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	14	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	14	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	14	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	14	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	14	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	14	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	14	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	14	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	14	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	14	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	14	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	14	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	14	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	14	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	14	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	18	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	18	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	18	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	18	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	18	0.14
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	18	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	18	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	18	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	18	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	18	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	18	0.14
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	18	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	18	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	18	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	18	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	18	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	18	0.14
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	18	0.14
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	12	0.14
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	12	0.14
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	12	0.14
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	17	0.14
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	17	0.14
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	17	0.14
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	3	0.14
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	7	0.14
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	8	0.14
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	10	0.14
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	12	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	7	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	7	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	7	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	7	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	7	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	7	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	7	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	7	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	8	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	8	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	8	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	8	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	8	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	8	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	8	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	8	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	8	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	11	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	11	0.14
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	11	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	11	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	11	0.14
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	11	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	11	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	11	0.14
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	11	0.14
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	2	0.14
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	2	0.14
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	2	0.14
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	2	0.14
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	2	0.14
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	2	0.14
(1,1910)	1:310:B:ARG:HD2	1:341:B:MET:HE1	14	0.14
(1,1910)	1:310:B:ARG:HD2	1:341:B:MET:HE2	14	0.14
(1,1910)	1:310:B:ARG:HD2	1:341:B:MET:HE3	14	0.14
(1,1750)	1:300:B:CYS:H	1:301:B:PHE:H	4	0.14
(1,1711)	1:295:B:ILE:HD11	1:326:B:ALA:H	15	0.14
(1,1711)	1:295:B:ILE:HD12	1:326:B:ALA:H	15	0.14
(1,1711)	1:295:B:ILE:HD13	1:326:B:ALA:H	15	0.14
(1,1704)	1:295:B:ILE:HG21	1:296:B:SER:H	7	0.14
(1,1704)	1:295:B:ILE:HG22	1:296:B:SER:H	7	0.14
(1,1704)	1:295:B:ILE:HG23	1:296:B:SER:H	7	0.14
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	13	0.14
(1,1667)	1:294:B:PHE:HB2	1:294:B:PHE:H	7	0.14
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	13	0.14
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	13	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	13	0.14
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	20	0.14
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	20	0.14
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	20	0.14
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	1	0.14
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	1	0.14
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	1	0.14
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG11	4	0.14
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG12	4	0.14
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG13	4	0.14
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG11	4	0.14
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG12	4	0.14
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG13	4	0.14
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG21	5	0.14
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG22	5	0.14
(1,1550)	1:289:B:TYR:HB2	1:291:B:VAL:HG23	5	0.14
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG21	5	0.14
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG22	5	0.14
(1,1550)	1:289:B:TYR:HB3	1:291:B:VAL:HG23	5	0.14
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD11	6	0.14
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD12	6	0.14
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD13	6	0.14
(1,1400)	1:282:B:GLN:HA	1:282:B:GLN:HE22	7	0.14
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	4	0.14
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	9	0.14
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	9	0.14
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	9	0.14
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	13	0.14
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	13	0.14
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	13	0.14
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	18	0.14
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	18	0.14
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	18	0.14
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	17	0.14
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	17	0.14
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	17	0.14
(1,1231)	1:275:B:LEU:HD11	1:312:B:PHE:HZ	1	0.14
(1,1231)	1:275:B:LEU:HD12	1:312:B:PHE:HZ	1	0.14
(1,1231)	1:275:B:LEU:HD13	1:312:B:PHE:HZ	1	0.14
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD21	4	0.14
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD22	4	0.14
(1,1177)	1:274:B:PHE:HE1	1:321:B:LEU:HD23	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD21	4	0.14
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD22	4	0.14
(1,1177)	1:274:B:PHE:HE2	1:321:B:LEU:HD23	4	0.14
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	2	0.14
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	9	0.14
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	10	0.14
(1,910)	1:254:B:LEU:HD21	1:274:B:PHE:HA	8	0.14
(1,910)	1:254:B:LEU:HD22	1:274:B:PHE:HA	8	0.14
(1,910)	1:254:B:LEU:HD23	1:274:B:PHE:HA	8	0.14
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	16	0.14
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	12	0.14
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	14	0.14
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	3	0.14
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	3	0.14
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	3	0.14
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	10	0.14
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	12	0.14
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	18	0.14
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	18	0.14
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	18	0.14
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	12	0.14
(1,529)	1:236:B:VAL:HG21	1:290:B:ARG:H	12	0.14
(1,529)	1:236:B:VAL:HG22	1:290:B:ARG:H	12	0.14
(1,529)	1:236:B:VAL:HG23	1:290:B:ARG:H	12	0.14
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG11	17	0.14
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG12	17	0.14
(1,490)	1:235:B:GLU:H	1:291:B:VAL:HG13	17	0.14
(1,472)	1:234:B:TYR:H	1:364:B:PHE:HD1	3	0.14
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	1	0.14
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	1	0.14
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	1	0.14
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	1	0.14
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	1	0.14
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	1	0.14
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	9	0.14
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	9	0.14
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	9	0.14
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	9	0.14
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	9	0.14
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	9	0.14
(1,411)	1:232:B:LEU:HD11	1:274:B:PHE:HZ	16	0.14
(1,411)	1:232:B:LEU:HD12	1:274:B:PHE:HZ	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,411)	1:232:B:LEU:HD13	1:274:B:PHE:HZ	16	0.14
(1,411)	1:232:B:LEU:HD21	1:274:B:PHE:HZ	16	0.14
(1,411)	1:232:B:LEU:HD22	1:274:B:PHE:HZ	16	0.14
(1,411)	1:232:B:LEU:HD23	1:274:B:PHE:HZ	16	0.14
(1,411)	1:232:B:LEU:HD11	1:274:B:PHE:HZ	19	0.14
(1,411)	1:232:B:LEU:HD12	1:274:B:PHE:HZ	19	0.14
(1,411)	1:232:B:LEU:HD13	1:274:B:PHE:HZ	19	0.14
(1,411)	1:232:B:LEU:HD21	1:274:B:PHE:HZ	19	0.14
(1,411)	1:232:B:LEU:HD22	1:274:B:PHE:HZ	19	0.14
(1,411)	1:232:B:LEU:HD23	1:274:B:PHE:HZ	19	0.14
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	6	0.14
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	6	0.14
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	6	0.14
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	10	0.14
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	10	0.14
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	10	0.14
(1,292)	1:218:B:THR:HG21	1:375:B:TRP:HZ2	6	0.14
(1,292)	1:218:B:THR:HG22	1:375:B:TRP:HZ2	6	0.14
(1,292)	1:218:B:THR:HG23	1:375:B:TRP:HZ2	6	0.14
(1,157)	1:212:B:MET:HE1	1:233:B:CYS:HB3	9	0.14
(1,157)	1:212:B:MET:HE2	1:233:B:CYS:HB3	9	0.14
(1,157)	1:212:B:MET:HE3	1:233:B:CYS:HB3	9	0.14
(1,6687)	1:196:A:ASN:HD22	1:196:A:ASN:H	9	0.13
(1,6687)	1:196:A:ASN:HD22	1:196:A:ASN:H	15	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	1	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	2	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	5	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	6	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	9	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	10	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	12	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	16	0.13
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	20	0.13
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	1	0.13
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	2	0.13
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	10	0.13
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	11	0.13
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	6	0.13
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	8	0.13
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	9	0.13
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	12	0.13
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	16	0.13
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	19	0.13
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD11	15	0.13
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD12	15	0.13
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD13	15	0.13
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	13	0.13
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	8	0.13
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	7	0.13
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	12	0.13
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	16	0.13
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	19	0.13
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	1	0.13
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	5	0.13
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	10	0.13
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	13	0.13
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	18	0.13
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	19	0.13
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	20	0.13
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	9	0.13
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	15	0.13
(1,6321)	1:174:A:GLN:HB3	1:174:A:GLN:H	7	0.13
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	6	0.13
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	6	0.13
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	11	0.13
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	13	0.13
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	14	0.13
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	17	0.13
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	18	0.13
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	20	0.13
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	5	0.13
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	18	0.13
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	19	0.13
(1,6157)	1:162:A:TRP:HZ2	1:171:A:GLN:H	16	0.13
(1,6120)	1:161:A:CYS:HG	1:161:A:CYS:H	7	0.13
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	7	0.13
(1,6056)	1:155:A:TYR:H	1:179:A:LEU:HG	10	0.13
(1,6056)	1:155:A:TYR:H	1:179:A:LEU:HG	18	0.13
(1,6050)	1:155:A:TYR:HE1	1:173:A:PHE:HZ	16	0.13
(1,6050)	1:155:A:TYR:HE2	1:173:A:PHE:HZ	16	0.13
(1,6035)	1:155:A:TYR:HE1	1:155:A:TYR:H	5	0.13
(1,6035)	1:155:A:TYR:HE2	1:155:A:TYR:H	5	0.13
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	8	0.13
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	8	0.13
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	8	0.13
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	8	0.13
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	8	0.13
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	8	0.13
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	8	0.13
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	8	0.13
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD11	10	0.13
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD12	10	0.13
(1,5995)	1:152:A:ILE:HG21	1:190:A:LEU:HD13	10	0.13
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD11	10	0.13
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD12	10	0.13
(1,5995)	1:152:A:ILE:HG22	1:190:A:LEU:HD13	10	0.13
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD11	10	0.13
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD12	10	0.13
(1,5995)	1:152:A:ILE:HG23	1:190:A:LEU:HD13	10	0.13
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD11	19	0.13
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD12	19	0.13
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD13	19	0.13
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD11	19	0.13
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD12	19	0.13
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD13	19	0.13
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD11	19	0.13
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD12	19	0.13
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD13	19	0.13
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	20	0.13
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	20	0.13
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	20	0.13
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD11	10	0.13
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD12	10	0.13
(1,5823)	1:141:A:GLN:HE22	1:194:A:LEU:HD13	10	0.13
(1,5815)	1:141:A:GLN:HE21	1:193:A:ILE:HG21	14	0.13
(1,5800)	1:140:A:LEU:H	1:193:A:ILE:HG22	12	0.13
(1,5800)	1:140:A:LEU:H	1:193:A:ILE:HG22	15	0.13
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	2	0.13
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	2	0.13
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	5	0.13
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	5	0.13
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	6	0.13
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	6	0.13
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	13	0.13
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	20	0.13
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	20	0.13
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	15	0.13
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	15	0.13
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	15	0.13
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	16	0.13
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	16	0.13
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	16	0.13
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	4	0.13
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	5	0.13
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD11	9	0.13
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD12	9	0.13
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD13	9	0.13
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD21	9	0.13
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD22	9	0.13
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD23	9	0.13
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD11	9	0.13
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD12	9	0.13
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD13	9	0.13
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD21	9	0.13
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD22	9	0.13
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD23	9	0.13
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD11	9	0.13
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD12	9	0.13
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD13	9	0.13
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD21	9	0.13
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD22	9	0.13
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD23	9	0.13
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	5	0.13
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	5	0.13
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	5	0.13
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	14	0.13
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	14	0.13
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	14	0.13
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	16	0.13
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	16	0.13
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	16	0.13
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	18	0.13
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	18	0.13
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	18	0.13
(1,5506)	1:119:A:HIS:HE1	1:119:A:HIS:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	2	0.13
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	13	0.13
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	4	0.13
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	5	0.13
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	11	0.13
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	15	0.13
(1,5424)	1:115:A:GLN:HB3	1:115:A:GLN:HE22	16	0.13
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	19	0.13
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	19	0.13
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	19	0.13
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	19	0.13
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	19	0.13
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	19	0.13
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	19	0.13
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	19	0.13
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	19	0.13
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	20	0.13
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	20	0.13
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	20	0.13
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	20	0.13
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	20	0.13
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	20	0.13
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	20	0.13
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	20	0.13
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	20	0.13
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	20	0.13
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	20	0.13
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	20	0.13
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	20	0.13
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	20	0.13
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	20	0.13
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	19	0.13
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	8	0.13
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	11	0.13
(1,5118)	1:97:A:SER:HB3	1:97:A:SER:H	16	0.13
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	9	0.13
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	9	0.13
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	9	0.13
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	15	0.13
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	15	0.13
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	15	0.13
(1,5103)	1:96:A:ILE:HG21	1:97:A:SER:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5103)	1:96:A:ILE:HG22	1:97:A:SER:H	3	0.13
(1,5103)	1:96:A:ILE:HG23	1:97:A:SER:H	3	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	2	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	2	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	2	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	17	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	17	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	17	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	19	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	19	0.13
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	19	0.13
(1,4968)	1:91:A:ARG:HB3	1:91:A:ARG:H	9	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	3	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	3	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	3	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	3	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	3	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	3	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	5	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	5	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	5	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	5	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	5	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	5	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	10	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	10	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	10	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	10	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	10	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	10	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	17	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	17	0.13
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	17	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	17	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	17	0.13
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	17	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	6	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	6	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	6	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	9	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	9	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	20	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	20	0.13
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	20	0.13
(1,4908)	1:88:A:GLN:HB3	1:89:A:ILE:H	7	0.13
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	18	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	1	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	1	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	1	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	8	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	8	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	8	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	20	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	20	0.13
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	20	0.13
(1,4651)	1:77:A:ASP:HA	1:80:A:PRO:HB2	11	0.13
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	1	0.13
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	13	0.13
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	1	0.13
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	4	0.13
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	7	0.13
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	5	0.13
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	6	0.13
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	10	0.13
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	16	0.13
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	19	0.13
(1,4346)	1:57:A:ASN:HB2	1:57:A:ASN:H	7	0.13
(1,4265)	1:52:A:ARG:HG3	1:53:A:GLY:H	19	0.13
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	1	0.13
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	1	0.13
(1,4195)	1:47:A:LYS:HE2	1:48:A:MET:H	4	0.13
(1,4195)	1:47:A:LYS:HE3	1:48:A:MET:H	4	0.13
(1,4125)	1:44:A:THR:HG1	1:44:A:THR:H	2	0.13
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	2	0.13
(1,4089)	1:41:A:ASP:HB2	1:45:A:SER:H	14	0.13
(1,4066)	1:40:A:LEU:HD21	1:45:A:SER:HB2	12	0.13
(1,4066)	1:40:A:LEU:HD22	1:45:A:SER:HB2	12	0.13
(1,4066)	1:40:A:LEU:HD23	1:45:A:SER:HB2	12	0.13
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	13	0.13
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	13	0.13
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	13	0.13
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	5	0.13
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	5	0.13
(1,4045)	1:40:A:LEU:HD11	1:42:A:ASN:H	20	0.13
(1,4045)	1:40:A:LEU:HD12	1:42:A:ASN:H	20	0.13
(1,4045)	1:40:A:LEU:HD13	1:42:A:ASN:H	20	0.13
(1,4015)	1:39:A:ARG:H	1:47:A:LYS:HA	18	0.13
(1,4009)	1:39:A:ARG:HG2	1:88:A:GLN:HB2	14	0.13
(1,3960)	1:38:A:GLU:HA	1:91:A:ARG:H	15	0.13
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	19	0.13
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	10	0.13
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE1	20	0.13
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE2	20	0.13
(1,3913)	1:37:A:VAL:HG21	1:48:A:MET:HE3	20	0.13
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE1	20	0.13
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE2	20	0.13
(1,3913)	1:37:A:VAL:HG22	1:48:A:MET:HE3	20	0.13
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE1	20	0.13
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE2	20	0.13
(1,3913)	1:37:A:VAL:HG23	1:48:A:MET:HE3	20	0.13
(1,3809)	1:33:A:LEU:HD11	1:35:A:TYR:HE1	10	0.13
(1,3809)	1:33:A:LEU:HD11	1:35:A:TYR:HE2	10	0.13
(1,3809)	1:33:A:LEU:HD12	1:35:A:TYR:HE1	10	0.13
(1,3809)	1:33:A:LEU:HD12	1:35:A:TYR:HE2	10	0.13
(1,3809)	1:33:A:LEU:HD13	1:35:A:TYR:HE1	10	0.13
(1,3809)	1:33:A:LEU:HD13	1:35:A:TYR:HE2	10	0.13
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	13	0.13
(1,3609)	1:15:A:PRO:HG2	1:168:A:HIS:H	1	0.13
(1,3609)	1:15:A:PRO:HG3	1:168:A:HIS:H	1	0.13
(1,3581)	1:14:A:ASP:HA	1:17:A:ILE:HB	13	0.13
(1,3568)	1:13:A:MET:HE1	1:34:A:CYS:HB2	15	0.13
(1,3568)	1:13:A:MET:HE2	1:34:A:CYS:HB2	15	0.13
(1,3568)	1:13:A:MET:HE3	1:34:A:CYS:HB2	15	0.13
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	16	0.13
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	16	0.13
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	16	0.13
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	16	0.13
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	16	0.13
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	16	0.13
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	16	0.13
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	16	0.13
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	16	0.13
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	15	0.13
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	18	0.13
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	1	0.13
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	3	0.13
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	12	0.13
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	18	0.13
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	6	0.13
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	8	0.13
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	10	0.13
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	11	0.13
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	14	0.13
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	18	0.13
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	2	0.13
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	6	0.13
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	8	0.13
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	9	0.13
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	15	0.13
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	19	0.13
(1,3086)	1:383:B:GLN:H	1:383:B:GLN:HE21	6	0.13
(1,3086)	1:383:B:GLN:H	1:383:B:GLN:HE21	13	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	2	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	4	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	6	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	7	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	8	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	9	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	12	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	15	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	16	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	17	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	18	0.13
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	19	0.13
(1,3009)	1:378:B:LEU:HD11	1:381:B:HIS:HB3	20	0.13
(1,3009)	1:378:B:LEU:HD12	1:381:B:HIS:HB3	20	0.13
(1,3009)	1:378:B:LEU:HD13	1:381:B:HIS:HB3	20	0.13
(1,3009)	1:378:B:LEU:HD21	1:381:B:HIS:HB3	20	0.13
(1,3009)	1:378:B:LEU:HD22	1:381:B:HIS:HB3	20	0.13
(1,3009)	1:378:B:LEU:HD23	1:381:B:HIS:HB3	20	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	4	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	4	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	4	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	7	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	7	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	9	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	9	0.13
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	9	0.13
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	6	0.13
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	14	0.13
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	20	0.13
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	13	0.13
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	15	0.13
(1,2919)	1:373:B:GLN:HB3	1:373:B:GLN:H	4	0.13
(1,2919)	1:373:B:GLN:HB3	1:373:B:GLN:H	14	0.13
(1,2901)	1:372:B:PHE:HZ	1:375:B:TRP:H	9	0.13
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	11	0.13
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	14	0.13
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	17	0.13
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	20	0.13
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	1	0.13
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	4	0.13
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	6	0.13
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	18	0.13
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	8	0.13
(1,2727)	1:361:B:TRP:HB2	1:361:B:TRP:H	14	0.13
(1,2697)	1:358:B:LYS:H	1:372:B:PHE:HD1	8	0.13
(1,2697)	1:358:B:LYS:H	1:372:B:PHE:HD2	8	0.13
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	16	0.13
(1,2638)	1:354:B:TYR:HD1	1:355:B:ASP:H	1	0.13
(1,2638)	1:354:B:TYR:HD2	1:355:B:ASP:H	1	0.13
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	19	0.13
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	19	0.13
(1,2600)	1:351:B:ILE:HD11	1:389:B:LEU:H	7	0.13
(1,2600)	1:351:B:ILE:HD12	1:389:B:LEU:H	7	0.13
(1,2600)	1:351:B:ILE:HD13	1:389:B:LEU:H	7	0.13
(1,2594)	1:351:B:ILE:HD11	1:352:B:MET:H	12	0.13
(1,2594)	1:351:B:ILE:HD12	1:352:B:MET:H	12	0.13
(1,2594)	1:351:B:ILE:HD13	1:352:B:MET:H	12	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD11	3	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD12	3	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD13	3	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD11	3	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD12	3	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD13	3	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD11	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD12	3	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD13	3	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD11	4	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD12	4	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD13	4	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD11	4	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD12	4	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD13	4	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD11	4	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD12	4	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD13	4	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD11	13	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD12	13	0.13
(1,2592)	1:351:B:ILE:HG21	1:389:B:LEU:HD13	13	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD11	13	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD12	13	0.13
(1,2592)	1:351:B:ILE:HG22	1:389:B:LEU:HD13	13	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD11	13	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD12	13	0.13
(1,2592)	1:351:B:ILE:HG23	1:389:B:LEU:HD13	13	0.13
(1,2590)	1:351:B:ILE:HG21	1:385:B:LEU:H	7	0.13
(1,2590)	1:351:B:ILE:HG22	1:385:B:LEU:H	7	0.13
(1,2590)	1:351:B:ILE:HG23	1:385:B:LEU:H	7	0.13
(1,2586)	1:351:B:ILE:HG21	1:352:B:MET:H	20	0.13
(1,2586)	1:351:B:ILE:HG22	1:352:B:MET:H	20	0.13
(1,2586)	1:351:B:ILE:HG23	1:352:B:MET:H	20	0.13
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD21	2	0.13
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD22	2	0.13
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD23	2	0.13
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD21	2	0.13
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD22	2	0.13
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD23	2	0.13
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD21	2	0.13
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD22	2	0.13
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD23	2	0.13
(1,2275)	1:328:B:ILE:HG21	1:330:B:ASP:H	5	0.13
(1,2275)	1:328:B:ILE:HG22	1:330:B:ASP:H	5	0.13
(1,2275)	1:328:B:ILE:HG23	1:330:B:ASP:H	5	0.13
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	1	0.13
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	1	0.13
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	1	0.13
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	10	0.13
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	10	0.13
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	12	0.13
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	12	0.13
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	12	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	7	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	7	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	7	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	7	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	7	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	7	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	7	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	7	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	7	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	7	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	7	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	7	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	7	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	7	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	7	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	7	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	7	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	7	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	8	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	8	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	8	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	8	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	8	0.13
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	8	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	8	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	8	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	8	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	8	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	8	0.13
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	8	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	8	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	8	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	8	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	8	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	8	0.13
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	8	0.13
(1,2104)	1:318:B:HIS:HE1	1:318:B:HIS:H	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	5	0.13
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	6	0.13
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	14	0.13
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	1	0.13
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	2	0.13
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	7	0.13
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	8	0.13
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	13	0.13
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	13	0.13
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	13	0.13
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	13	0.13
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	13	0.13
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	13	0.13
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	13	0.13
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	13	0.13
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	13	0.13
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	16	0.13
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	16	0.13
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	16	0.13
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	16	0.13
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	16	0.13
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	16	0.13
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	16	0.13
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	16	0.13
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	16	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	12	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	12	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	12	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	12	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	12	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	12	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	13	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	13	0.13
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	13	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	13	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	13	0.13
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	13	0.13
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	11	0.13
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	17	0.13
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	17	0.13
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	17	0.13
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	18	0.13
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	18	0.13
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	7	0.13
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	7	0.13
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	7	0.13
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	20	0.13
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG11	1	0.13
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG12	1	0.13
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG13	1	0.13
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG11	1	0.13
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG12	1	0.13
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG13	1	0.13
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD11	6	0.13
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD12	6	0.13
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD13	6	0.13
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	15	0.13
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	20	0.13
(1,1295)	1:278:B:VAL:HG11	1:278:B:VAL:H	3	0.13
(1,1295)	1:278:B:VAL:HG12	1:278:B:VAL:H	3	0.13
(1,1295)	1:278:B:VAL:HG13	1:278:B:VAL:H	3	0.13
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	10	0.13
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	14	0.13
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	16	0.13
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	7	0.13
(1,1019)	1:262:B:ASN:HB2	1:263:B:SER:H	11	0.13
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD1	8	0.13
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD2	8	0.13
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD1	8	0.13
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD2	8	0.13
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD1	8	0.13
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD2	8	0.13
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD1	9	0.13
(1,1007)	1:261:B:LEU:HD11	1:266:B:TYR:HD2	9	0.13
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD1	9	0.13
(1,1007)	1:261:B:LEU:HD12	1:266:B:TYR:HD2	9	0.13
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD1	9	0.13
(1,1007)	1:261:B:LEU:HD13	1:266:B:TYR:HD2	9	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	1	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	2	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	3	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	4	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	7	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	8	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	9	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	10	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	11	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	12	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	13	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	14	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	16	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	17	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	18	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	19	0.13
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	20	0.13
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	20	0.13
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD1	19	0.13
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD2	19	0.13
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD1	19	0.13
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD2	19	0.13
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	8	0.13
(1,774)	1:246:B:LYS:HG2	1:246:B:LYS:H	11	0.13
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	1	0.13
(1,719)	1:243:B:THR:HG1	1:243:B:THR:H	6	0.13
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	13	0.13
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	11	0.13
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	11	0.13
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	11	0.13
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	18	0.13
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	18	0.13
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	18	0.13
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	11	0.13
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	11	0.13
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	11	0.13
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	16	0.13
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	16	0.13
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	16	0.13
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	3	0.13
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	20	0.13
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	5	0.13
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	6	0.13
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	8	0.13
(1,534)	1:236:B:VAL:HG11	1:292:B:THR:H	19	0.13
(1,534)	1:236:B:VAL:HG12	1:292:B:THR:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	1:236:B:VAL:HG13	1:292:B:THR:H	19	0.13
(1,529)	1:236:B:VAL:HG21	1:290:B:ARG:H	8	0.13
(1,529)	1:236:B:VAL:HG22	1:290:B:ARG:H	8	0.13
(1,529)	1:236:B:VAL:HG23	1:290:B:ARG:H	8	0.13
(1,403)	1:232:B:LEU:HD11	1:234:B:TYR:HE1	14	0.13
(1,403)	1:232:B:LEU:HD11	1:234:B:TYR:HE2	14	0.13
(1,403)	1:232:B:LEU:HD12	1:234:B:TYR:HE1	14	0.13
(1,403)	1:232:B:LEU:HD12	1:234:B:TYR:HE2	14	0.13
(1,403)	1:232:B:LEU:HD13	1:234:B:TYR:HE1	14	0.13
(1,403)	1:232:B:LEU:HD13	1:234:B:TYR:HE2	14	0.13
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	13	0.13
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	13	0.13
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	13	0.13
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	14	0.13
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	14	0.13
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	14	0.13
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	15	0.13
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	15	0.13
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	15	0.13
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	19	0.13
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	19	0.13
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	19	0.13
(1,321)	1:221:B:PHE:HZ	1:233:B:CYS:H	4	0.13
(1,286)	1:218:B:THR:HG21	1:361:B:TRP:HZ2	5	0.13
(1,286)	1:218:B:THR:HG22	1:361:B:TRP:HZ2	5	0.13
(1,286)	1:218:B:THR:HG23	1:361:B:TRP:HZ2	5	0.13
(1,286)	1:218:B:THR:HG21	1:361:B:TRP:HZ2	17	0.13
(1,286)	1:218:B:THR:HG22	1:361:B:TRP:HZ2	17	0.13
(1,286)	1:218:B:THR:HG23	1:361:B:TRP:HZ2	17	0.13
(1,214)	1:215:B:HIS:HD1	1:216:B:ILE:HD11	15	0.13
(1,214)	1:215:B:HIS:HD1	1:216:B:ILE:HD12	15	0.13
(1,214)	1:215:B:HIS:HD1	1:216:B:ILE:HD13	15	0.13
(1,199)	1:214:B:PRO:HG2	1:367:B:HIS:H	18	0.13
(1,199)	1:214:B:PRO:HG3	1:367:B:HIS:H	18	0.13
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	1	0.13
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	8	0.13
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	15	0.13
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	3	0.13
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB2	19	0.12
(1,6997)	1:11:A:HIS:HB2	1:253:B:PHE:HB3	19	0.12
(1,6975)	1:210:B:HIS:HD2	1:54:A:PHE:HD2	10	0.12
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB2	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB3	11	0.12
(1,6687)	1:196:A:ASN:HD22	1:196:A:ASN:H	4	0.12
(1,6672)	1:195:A:GLN:HB3	1:196:A:ASN:H	11	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	3	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	5	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	6	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	8	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	14	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	15	0.12
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	20	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	1	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	2	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	3	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	4	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	5	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	7	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	10	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	11	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	13	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	14	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	17	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	18	0.12
(1,6658)	1:195:A:GLN:HA	1:195:A:GLN:HE22	20	0.12
(1,6650)	1:194:A:LEU:HB2	1:195:A:GLN:H	6	0.12
(1,6650)	1:194:A:LEU:HB2	1:195:A:GLN:H	14	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	1	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	2	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	3	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	6	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	7	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	9	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	10	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	12	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	14	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	16	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	17	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	18	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	19	0.12
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	20	0.12
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD11	20	0.12
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD12	20	0.12
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD13	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD11	20	0.12
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD12	20	0.12
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD13	20	0.12
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD11	20	0.12
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD12	20	0.12
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD13	20	0.12
(1,6518)	1:186:A:LEU:HA	1:189:A:ARG:H	7	0.12
(1,6489)	1:184:A:GLN:H	1:184:A:GLN:HE22	6	0.12
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	13	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	3	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	4	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	7	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	8	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	9	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	11	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	15	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	16	0.12
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	17	0.12
(1,6421)	1:180:A:ASP:HA	1:183:A:SER:H	19	0.12
(1,6412)	1:179:A:LEU:HD11	1:182:A:HIS:HB2	15	0.12
(1,6412)	1:179:A:LEU:HD12	1:182:A:HIS:HB2	15	0.12
(1,6412)	1:179:A:LEU:HD13	1:182:A:HIS:HB2	15	0.12
(1,6412)	1:179:A:LEU:HD21	1:182:A:HIS:HB2	15	0.12
(1,6412)	1:179:A:LEU:HD22	1:182:A:HIS:HB2	15	0.12
(1,6412)	1:179:A:LEU:HD23	1:182:A:HIS:HB2	15	0.12
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	15	0.12
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	4	0.12
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	6	0.12
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	9	0.12
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	10	0.12
(1,6348)	1:175:A:PRO:HA	1:179:A:LEU:HG	9	0.12
(1,6321)	1:174:A:GLN:HB3	1:174:A:GLN:H	2	0.12
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	4	0.12
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	4	0.12
(1,6251)	1:169:A:GLN:HB3	1:169:A:GLN:HE22	10	0.12
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	5	0.12
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	9	0.12
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	10	0.12
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	11	0.12
(1,6243)	1:169:A:GLN:HA	1:169:A:GLN:HE22	14	0.12
(1,6221)	1:167:A:ASP:H	1:168:A:HIS:H	18	0.12
(1,6164)	1:162:A:TRP:HH2	1:166:A:VAL:HG21	16	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6164)	1:162:A:TRP:HH2	1:166:A:VAL:HG22	16	0.12
(1,6164)	1:162:A:TRP:HH2	1:166:A:VAL:HG23	16	0.12
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	16	0.12
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	17	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	1	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	2	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	3	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	4	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	5	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	6	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	8	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	9	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	10	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	11	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	12	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	13	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	14	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	15	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	16	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	17	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	18	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	19	0.12
(1,6114)	1:161:A:CYS:HA	1:161:A:CYS:HB2	20	0.12
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	1	0.12
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	1	0.12
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	9	0.12
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	9	0.12
(1,6035)	1:155:A:TYR:HE1	1:155:A:TYR:H	14	0.12
(1,6035)	1:155:A:TYR:HE2	1:155:A:TYR:H	14	0.12
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	12	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	2	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	2	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	2	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	7	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	7	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	7	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	9	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	9	0.12
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	9	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	1	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	1	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	2	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	2	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	2	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	3	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	3	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	3	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	5	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	5	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	5	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	6	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	6	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	6	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	7	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	7	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	7	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	8	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	8	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	8	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	9	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	9	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	9	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	10	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	10	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	10	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	12	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	12	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	12	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	13	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	13	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	13	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	14	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	14	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	14	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	15	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	15	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	15	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	16	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	16	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	16	0.12
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	18	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	18	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	19	0.12
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	19	0.12
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	19	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG11	1	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG12	1	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG13	1	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG21	1	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG22	1	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG23	1	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG11	4	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG12	4	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG13	4	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG21	4	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG22	4	0.12
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG23	4	0.12
(1,5800)	1:140:A:LEU:H	1:193:A:ILE:HG22	13	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	3	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	3	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	4	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	4	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	7	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	7	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	8	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	8	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	11	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	11	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	12	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	12	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	14	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	14	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	15	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	15	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	16	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	16	0.12
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	18	0.12
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	18	0.12
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD21	7	0.12
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD22	7	0.12
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD23	7	0.12
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD21	7	0.12
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD22	7	0.12
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD23	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD21	7	0.12
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD22	7	0.12
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD23	7	0.12
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	1	0.12
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	6	0.12
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	16	0.12
(1,5668)	1:129:A:ILE:HG13	1:129:A:ILE:H	18	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD11	10	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD12	10	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD13	10	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD21	10	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD22	10	0.12
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD23	10	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD11	10	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD12	10	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD13	10	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD21	10	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD22	10	0.12
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD23	10	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD11	10	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD12	10	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD13	10	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD21	10	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD22	10	0.12
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD23	10	0.12
(1,5521)	1:120:A:VAL:HG21	1:120:A:VAL:H	13	0.12
(1,5521)	1:120:A:VAL:HG22	1:120:A:VAL:H	13	0.12
(1,5521)	1:120:A:VAL:HG23	1:120:A:VAL:H	13	0.12
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	12	0.12
(1,5453)	1:116:A:GLU:HB3	1:116:A:GLU:HG2	1	0.12
(1,5453)	1:116:A:GLU:HB3	1:116:A:GLU:HG2	20	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	2	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	3	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	4	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	5	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	6	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	7	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	8	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	9	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	10	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	11	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	13	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	14	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	15	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	16	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	17	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	18	0.12
(1,5452)	1:116:A:GLU:HB3	1:116:A:GLU:HG3	19	0.12
(1,5446)	1:116:A:GLU:HA	1:116:A:GLU:HB3	5	0.12
(1,5446)	1:116:A:GLU:HA	1:116:A:GLU:HB3	6	0.12
(1,5446)	1:116:A:GLU:HA	1:116:A:GLU:HB3	8	0.12
(1,5446)	1:116:A:GLU:HA	1:116:A:GLU:HB3	12	0.12
(1,5446)	1:116:A:GLU:HA	1:116:A:GLU:HB3	16	0.12
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	4	0.12
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	6	0.12
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	7	0.12
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	8	0.12
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	10	0.12
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	11	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	4	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	4	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	4	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	4	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	4	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	4	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	4	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	4	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	4	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	11	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	11	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	11	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	11	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	11	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	11	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	11	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	11	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	11	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB1	13	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB2	13	0.12
(1,5404)	1:114:A:LEU:HD21	1:146:A:ALA:HB3	13	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB1	13	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB2	13	0.12
(1,5404)	1:114:A:LEU:HD22	1:146:A:ALA:HB3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB1	13	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB2	13	0.12
(1,5404)	1:114:A:LEU:HD23	1:146:A:ALA:HB3	13	0.12
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	1	0.12
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	1	0.12
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	1	0.12
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	1	0.12
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	1	0.12
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	1	0.12
(1,5330)	1:112:A:ALA:HB1	1:115:A:GLN:HE21	12	0.12
(1,5330)	1:112:A:ALA:HB2	1:115:A:GLN:HE21	12	0.12
(1,5330)	1:112:A:ALA:HB3	1:115:A:GLN:HE21	12	0.12
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	4	0.12
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	4	0.12
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	4	0.12
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG21	20	0.12
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG22	20	0.12
(1,5135)	1:99:A:SER:H	1:129:A:ILE:HG23	20	0.12
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	2	0.12
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	3	0.12
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	7	0.12
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	12	0.12
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	14	0.12
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	15	0.12
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	18	0.12
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	18	0.12
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	18	0.12
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	4	0.12
(1,4968)	1:91:A:ARG:HB3	1:91:A:ARG:H	2	0.12
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	15	0.12
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	15	0.12
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	15	0.12
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	15	0.12
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	15	0.12
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	15	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	1	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	1	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	1	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	7	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	7	0.12
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	7	0.12
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD11	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD12	4	0.12
(1,4792)	1:82:A:LEU:H	1:84:A:LEU:HD13	4	0.12
(1,4703)	1:79:A:VAL:HA	1:82:A:LEU:H	11	0.12
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	14	0.12
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	14	0.12
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	14	0.12
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	2	0.12
(1,4650)	1:77:A:ASP:HA	1:80:A:PRO:HB3	16	0.12
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	2	0.12
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	2	0.12
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	2	0.12
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	6	0.12
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	6	0.12
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	6	0.12
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	13	0.12
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	17	0.12
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD21	11	0.12
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD22	11	0.12
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD23	11	0.12
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD21	11	0.12
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD22	11	0.12
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD23	11	0.12
(1,4353)	1:58:A:GLN:HA	1:58:A:GLN:HB2	8	0.12
(1,4353)	1:58:A:GLN:HA	1:58:A:GLN:HB2	20	0.12
(1,4287)	1:54:A:PHE:HD1	1:54:A:PHE:H	15	0.12
(1,4287)	1:54:A:PHE:HD2	1:54:A:PHE:H	15	0.12
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	3	0.12
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	5	0.12
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	7	0.12
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	9	0.12
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	18	0.12
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	20	0.12
(1,4173)	1:47:A:LYS:HG3	1:47:A:LYS:HD3	1	0.12
(1,4173)	1:47:A:LYS:HG3	1:47:A:LYS:HD3	8	0.12
(1,4173)	1:47:A:LYS:HG3	1:47:A:LYS:HD3	10	0.12
(1,4173)	1:47:A:LYS:HG3	1:47:A:LYS:HD3	12	0.12
(1,4173)	1:47:A:LYS:HG3	1:47:A:LYS:HD3	13	0.12
(1,4062)	1:40:A:LEU:HD21	1:90:A:TYR:HD1	7	0.12
(1,4062)	1:40:A:LEU:HD21	1:90:A:TYR:HD2	7	0.12
(1,4062)	1:40:A:LEU:HD22	1:90:A:TYR:HD1	7	0.12
(1,4062)	1:40:A:LEU:HD22	1:90:A:TYR:HD2	7	0.12
(1,4062)	1:40:A:LEU:HD23	1:90:A:TYR:HD1	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4062)	1:40:A:LEU:HD23	1:90:A:TYR:HD2	7	0.12
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG21	1	0.12
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG22	1	0.12
(1,4058)	1:40:A:LEU:HD21	1:89:A:ILE:HG23	1	0.12
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG21	1	0.12
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG22	1	0.12
(1,4058)	1:40:A:LEU:HD22	1:89:A:ILE:HG23	1	0.12
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG21	1	0.12
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG22	1	0.12
(1,4058)	1:40:A:LEU:HD23	1:89:A:ILE:HG23	1	0.12
(1,4015)	1:39:A:ARG:H	1:47:A:LYS:HA	5	0.12
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	8	0.12
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	8	0.12
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	8	0.12
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG21	13	0.12
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG22	13	0.12
(1,4013)	1:39:A:ARG:H	1:46:A:VAL:HG23	13	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	2	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	4	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	7	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	9	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	12	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	13	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	14	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	15	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	16	0.12
(1,3951)	1:38:A:GLU:HB2	1:38:A:GLU:HG2	18	0.12
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	1	0.12
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	5	0.12
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	6	0.12
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	11	0.12
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	17	0.12
(1,3948)	1:38:A:GLU:HB3	1:38:A:GLU:HG2	20	0.12
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	3	0.12
(1,3817)	1:33:A:LEU:HD11	1:75:A:PHE:HZ	6	0.12
(1,3817)	1:33:A:LEU:HD12	1:75:A:PHE:HZ	6	0.12
(1,3817)	1:33:A:LEU:HD13	1:75:A:PHE:HZ	6	0.12
(1,3817)	1:33:A:LEU:HD21	1:75:A:PHE:HZ	6	0.12
(1,3817)	1:33:A:LEU:HD22	1:75:A:PHE:HZ	6	0.12
(1,3817)	1:33:A:LEU:HD23	1:75:A:PHE:HZ	6	0.12
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	7	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	2	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	3	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	4	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	5	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	6	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	7	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	9	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	11	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	12	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	13	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	14	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	15	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	17	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	18	0.12
(1,3502)	1:10:A:ARG:HG2	1:10:A:ARG:HD2	20	0.12
(1,3501)	1:10:A:ARG:HG3	1:10:A:ARG:HD2	10	0.12
(1,3501)	1:10:A:ARG:HG3	1:10:A:ARG:HD2	19	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	1	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	2	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	3	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	4	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	5	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	6	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	7	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	8	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	9	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	10	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	11	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	12	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	13	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	14	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	17	0.12
(1,3498)	1:10:A:ARG:HB2	1:10:A:ARG:HG2	20	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	1	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	2	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	3	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	4	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	5	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	6	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	7	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	8	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	10	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	11	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	12	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	13	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	14	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	15	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	16	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	17	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	18	0.12
(1,3492)	1:10:A:ARG:HB3	1:10:A:ARG:HG3	20	0.12
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	2	0.12
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	8	0.12
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	19	0.12
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	20	0.12
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	13	0.12
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	1	0.12
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	8	0.12
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	10	0.12
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	11	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	1	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	2	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	4	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	5	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	6	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	7	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	10	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	11	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	12	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	13	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	14	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	16	0.12
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	19	0.12
(1,3320)	2:410:D:DT:H1'	2:410:D:DT:H6	11	0.12
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	3	0.12
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	6	0.12
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	7	0.12
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	9	0.12
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	12	0.12
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	14	0.12
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	18	0.12
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	3	0.12
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	7	0.12
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	2	0.12
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	5	0.12
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	9	0.12
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	14	0.12
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	16	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	1	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	3	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	9	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	13	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	16	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	19	0.12
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	20	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	1	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	3	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	4	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	5	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	7	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	10	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	11	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	12	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	13	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	14	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	16	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	17	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	18	0.12
(1,3256)	1:394:B:GLN:HA	1:394:B:GLN:HE22	20	0.12
(1,3086)	1:383:B:GLN:H	1:383:B:GLN:HE21	4	0.12
(1,3086)	1:383:B:GLN:H	1:383:B:GLN:HE21	11	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	3	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	6	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	7	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	8	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	10	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	14	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	17	0.12
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	19	0.12
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	1	0.12
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	10	0.12
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	11	0.12
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	13	0.12
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	12	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	12	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	12	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	18	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	18	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	18	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD11	19	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD12	19	0.12
(1,2983)	1:376:B:ASP:HB3	1:378:B:LEU:HD13	19	0.12
(1,2980)	1:376:B:ASP:HA	1:378:B:LEU:H	11	0.12
(1,2978)	1:376:B:ASP:HB2	1:376:B:ASP:H	10	0.12
(1,2950)	1:374:B:PRO:HB2	1:375:B:TRP:H	8	0.12
(1,2919)	1:373:B:GLN:HB3	1:373:B:GLN:H	13	0.12
(1,2901)	1:372:B:PHE:HZ	1:375:B:TRP:H	8	0.12
(1,2901)	1:372:B:PHE:HZ	1:375:B:TRP:H	10	0.12
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	1	0.12
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	6	0.12
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	9	0.12
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	13	0.12
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	19	0.12
(1,2841)	1:368:B:GLN:HA	1:368:B:GLN:HE22	14	0.12
(1,2834)	1:367:B:HIS:HD2	1:370:B:GLN:H	8	0.12
(1,2834)	1:367:B:HIS:HD2	1:370:B:GLN:H	13	0.12
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	6	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	1	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	2	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	3	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	4	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	5	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	6	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	7	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	8	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	9	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	10	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	11	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	12	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	13	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	14	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	15	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	16	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	17	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	19	0.12
(1,2712)	1:360:B:CYS:HA	1:360:B:CYS:HB2	20	0.12
(1,2653)	1:354:B:TYR:H	1:378:B:LEU:HG	6	0.12
(1,2638)	1:354:B:TYR:HD1	1:355:B:ASP:H	11	0.12
(1,2638)	1:354:B:TYR:HD2	1:355:B:ASP:H	11	0.12
(1,2635)	1:354:B:TYR:HA	1:378:B:LEU:HD21	4	0.12
(1,2635)	1:354:B:TYR:HA	1:378:B:LEU:HD22	4	0.12
(1,2635)	1:354:B:TYR:HA	1:378:B:LEU:HD23	4	0.12
(1,2600)	1:351:B:ILE:HD11	1:389:B:LEU:H	18	0.12
(1,2600)	1:351:B:ILE:HD12	1:389:B:LEU:H	18	0.12
(1,2600)	1:351:B:ILE:HD13	1:389:B:LEU:H	18	0.12
(1,2583)	1:351:B:ILE:HD11	1:351:B:ILE:H	2	0.12
(1,2583)	1:351:B:ILE:HD12	1:351:B:ILE:H	2	0.12
(1,2583)	1:351:B:ILE:HD13	1:351:B:ILE:H	2	0.12
(1,2574)	1:351:B:ILE:HB	1:351:B:ILE:H	1	0.12
(1,2574)	1:351:B:ILE:HB	1:351:B:ILE:H	7	0.12
(1,2574)	1:351:B:ILE:HB	1:351:B:ILE:H	15	0.12
(1,2574)	1:351:B:ILE:HB	1:351:B:ILE:H	20	0.12
(1,2552)	1:349:B:VAL:H	1:393:B:LEU:HD11	4	0.12
(1,2552)	1:349:B:VAL:H	1:393:B:LEU:HD12	4	0.12
(1,2552)	1:349:B:VAL:H	1:393:B:LEU:HD13	4	0.12
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	3	0.12
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	3	0.12
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	3	0.12
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	7	0.12
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	7	0.12
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	7	0.12
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	9	0.12
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	9	0.12
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	9	0.12
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	14	0.12
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	14	0.12
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	14	0.12
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	16	0.12
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	16	0.12
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	16	0.12
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	17	0.12
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	17	0.12
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	17	0.12
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG11	8	0.12
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG12	8	0.12
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG13	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG11	19	0.12
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG12	19	0.12
(1,2471)	1:343:B:ARG:HB3	1:349:B:VAL:HG13	19	0.12
(1,2456)	1:342:B:LEU:HD11	1:347:B:ALA:H	2	0.12
(1,2456)	1:342:B:LEU:HD12	1:347:B:ALA:H	2	0.12
(1,2456)	1:342:B:LEU:HD13	1:347:B:ALA:H	2	0.12
(1,2456)	1:342:B:LEU:HD11	1:347:B:ALA:H	18	0.12
(1,2456)	1:342:B:LEU:HD12	1:347:B:ALA:H	18	0.12
(1,2456)	1:342:B:LEU:HD13	1:347:B:ALA:H	18	0.12
(1,2456)	1:342:B:LEU:HD11	1:347:B:ALA:H	19	0.12
(1,2456)	1:342:B:LEU:HD12	1:347:B:ALA:H	19	0.12
(1,2456)	1:342:B:LEU:HD13	1:347:B:ALA:H	19	0.12
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD11	16	0.12
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD12	16	0.12
(1,2387)	1:339:B:LEU:HD11	1:392:B:ILE:HD13	16	0.12
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD11	16	0.12
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD12	16	0.12
(1,2387)	1:339:B:LEU:HD12	1:392:B:ILE:HD13	16	0.12
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD11	16	0.12
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD12	16	0.12
(1,2387)	1:339:B:LEU:HD13	1:392:B:ILE:HD13	16	0.12
(1,2384)	1:339:B:LEU:HD21	1:392:B:ILE:HG12	5	0.12
(1,2384)	1:339:B:LEU:HD21	1:392:B:ILE:HG13	5	0.12
(1,2384)	1:339:B:LEU:HD22	1:392:B:ILE:HG12	5	0.12
(1,2384)	1:339:B:LEU:HD22	1:392:B:ILE:HG13	5	0.12
(1,2384)	1:339:B:LEU:HD23	1:392:B:ILE:HG12	5	0.12
(1,2384)	1:339:B:LEU:HD23	1:392:B:ILE:HG13	5	0.12
(1,2347)	1:335:B:TYR:HD1	1:336:B:LYS:H	11	0.12
(1,2347)	1:335:B:TYR:HD2	1:336:B:LYS:H	11	0.12
(1,2347)	1:335:B:TYR:HD1	1:336:B:LYS:H	18	0.12
(1,2347)	1:335:B:TYR:HD2	1:336:B:LYS:H	18	0.12
(1,2346)	1:335:B:TYR:HE1	1:335:B:TYR:H	1	0.12
(1,2346)	1:335:B:TYR:HE2	1:335:B:TYR:H	1	0.12
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	2	0.12
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	2	0.12
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	2	0.12
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	3	0.12
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	3	0.12
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	3	0.12
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	4	0.12
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	4	0.12
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	7	0.12
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	7	0.12
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	7	0.12
(1,2203)	1:323:B:ILE:HD11	1:324:B:PHE:H	16	0.12
(1,2203)	1:323:B:ILE:HD12	1:324:B:PHE:H	16	0.12
(1,2203)	1:323:B:ILE:HD13	1:324:B:PHE:H	16	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	10	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	10	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	10	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	10	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	10	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	10	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	10	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	10	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	10	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	10	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	10	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	10	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	10	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	10	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	10	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	10	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	10	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	10	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	20	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	20	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	20	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	20	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	20	0.12
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	20	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	20	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	20	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	20	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	20	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	20	0.12
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	20	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	20	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	20	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	20	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	20	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	20	0.12
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	11	0.12
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	11	0.12
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	11	0.12
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	14	0.12
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	14	0.12
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	14	0.12
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	18	0.12
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	18	0.12
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	18	0.12
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	1	0.12
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	7	0.12
(1,2051)	1:315:B:GLU:HB3	1:315:B:GLU:HG2	4	0.12
(1,2051)	1:315:B:GLU:HB3	1:315:B:GLU:HG2	9	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	1	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	2	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	3	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	5	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	6	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	7	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	8	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	10	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	11	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	12	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	13	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	14	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	15	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	16	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	17	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	18	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	19	0.12
(1,2050)	1:315:B:GLU:HB3	1:315:B:GLU:HG3	20	0.12
(1,2044)	1:315:B:GLU:HA	1:315:B:GLU:HB3	3	0.12
(1,2044)	1:315:B:GLU:HA	1:315:B:GLU:HB3	5	0.12
(1,2044)	1:315:B:GLU:HA	1:315:B:GLU:HB3	8	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	1	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	4	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	11	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	12	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	13	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	16	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	17	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	19	0.12
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	20	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	3	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	6	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	10	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	13	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	15	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	17	0.12
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	19	0.12
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	9	0.12
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	9	0.12
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	9	0.12
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	9	0.12
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	9	0.12
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	9	0.12
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	9	0.12
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	9	0.12
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	9	0.12
(1,1770)	1:301:B:PHE:HE1	1:341:B:MET:HE1	14	0.12
(1,1770)	1:301:B:PHE:HE1	1:341:B:MET:HE2	14	0.12
(1,1770)	1:301:B:PHE:HE1	1:341:B:MET:HE3	14	0.12
(1,1770)	1:301:B:PHE:HE2	1:341:B:MET:HE1	14	0.12
(1,1770)	1:301:B:PHE:HE2	1:341:B:MET:HE2	14	0.12
(1,1770)	1:301:B:PHE:HE2	1:341:B:MET:HE3	14	0.12
(1,1708)	1:295:B:ILE:HD11	1:296:B:SER:H	13	0.12
(1,1708)	1:295:B:ILE:HD12	1:296:B:SER:H	13	0.12
(1,1708)	1:295:B:ILE:HD13	1:296:B:SER:H	13	0.12
(1,1708)	1:295:B:ILE:HD11	1:296:B:SER:H	20	0.12
(1,1708)	1:295:B:ILE:HD12	1:296:B:SER:H	20	0.12
(1,1708)	1:295:B:ILE:HD13	1:296:B:SER:H	20	0.12
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	4	0.12
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	17	0.12
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	4	0.12
(1,1639)	1:293:B:TRP:HZ3	1:293:B:TRP:H	7	0.12
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	12	0.12
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	12	0.12
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	12	0.12
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	10	0.12
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	10	0.12
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	10	0.12
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	1	0.12
(1,1569)	1:290:B:ARG:HB3	1:290:B:ARG:H	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1556)	1:289:B:TYR:HD1	1:319:B:VAL:HG11	16	0.12
(1,1556)	1:289:B:TYR:HD1	1:319:B:VAL:HG12	16	0.12
(1,1556)	1:289:B:TYR:HD1	1:319:B:VAL:HG13	16	0.12
(1,1556)	1:289:B:TYR:HD2	1:319:B:VAL:HG11	16	0.12
(1,1556)	1:289:B:TYR:HD2	1:319:B:VAL:HG12	16	0.12
(1,1556)	1:289:B:TYR:HD2	1:319:B:VAL:HG13	16	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD11	1	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD12	1	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD13	1	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD11	13	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD12	13	0.12
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD13	13	0.12
(1,1474)	1:285:B:PRO:HB2	1:286:B:ALA:H	3	0.12
(1,1447)	1:283:B:LEU:HD21	1:318:B:HIS:HD2	2	0.12
(1,1447)	1:283:B:LEU:HD22	1:318:B:HIS:HD2	2	0.12
(1,1447)	1:283:B:LEU:HD23	1:318:B:HIS:HD2	2	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD21	15	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD22	15	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD23	15	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD21	20	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD22	20	0.12
(1,1394)	1:281:B:LEU:H	1:283:B:LEU:HD23	20	0.12
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	11	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	1	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	1	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	1	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	9	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	9	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	9	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD21	13	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD22	13	0.12
(1,1259)	1:277:B:LEU:HA	1:277:B:LEU:HD23	13	0.12
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	1	0.12
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	8	0.12
(1,1231)	1:275:B:LEU:HD11	1:312:B:PHE:HZ	17	0.12
(1,1231)	1:275:B:LEU:HD12	1:312:B:PHE:HZ	17	0.12
(1,1231)	1:275:B:LEU:HD13	1:312:B:PHE:HZ	17	0.12
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD11	8	0.12
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD12	8	0.12
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD13	8	0.12
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	11	0.12
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	6	0.12
(1,950)	1:257:B:GLN:HA	1:257:B:GLN:HB2	15	0.12
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	12	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	2	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	3	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	4	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	5	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	6	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	7	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	8	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	9	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	10	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	11	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	12	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	13	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	14	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	16	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	17	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	18	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	19	0.12
(1,767)	1:246:B:LYS:HG3	1:246:B:LYS:HD3	20	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG11	8	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG12	8	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG13	8	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG11	12	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG12	12	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG13	12	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG11	14	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG12	14	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG13	14	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG11	19	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG12	19	0.12
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG13	19	0.12
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	7	0.12
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	11	0.12
(1,683)	1:240:B:ASP:HB2	1:244:B:SER:H	16	0.12
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	10	0.12
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	10	0.12
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	10	0.12
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	17	0.12
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	17	0.12
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:239:B:LEU:HD11	1:289:B:TYR:HD1	3	0.12
(1,655)	1:239:B:LEU:HD11	1:289:B:TYR:HD2	3	0.12
(1,655)	1:239:B:LEU:HD12	1:289:B:TYR:HD1	3	0.12
(1,655)	1:239:B:LEU:HD12	1:289:B:TYR:HD2	3	0.12
(1,655)	1:239:B:LEU:HD13	1:289:B:TYR:HD1	3	0.12
(1,655)	1:239:B:LEU:HD13	1:289:B:TYR:HD2	3	0.12
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	9	0.12
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	9	0.12
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	9	0.12
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG21	4	0.12
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG22	4	0.12
(1,607)	1:238:B:ARG:H	1:245:B:VAL:HG23	4	0.12
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	6	0.12
(1,565)	1:237:B:GLU:HG2	1:244:B:SER:HB3	15	0.12
(1,565)	1:237:B:GLU:HG3	1:244:B:SER:HB3	15	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	1	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	2	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	4	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	7	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	9	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	11	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	12	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	15	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	16	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	18	0.12
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	19	0.12
(1,542)	1:237:B:GLU:HB3	1:237:B:GLU:HG2	14	0.12
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	19	0.12
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	19	0.12
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	19	0.12
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	19	0.12
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	19	0.12
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	19	0.12
(1,472)	1:234:B:TYR:H	1:364:B:PHE:HD1	4	0.12
(1,471)	1:234:B:TYR:H	1:254:B:LEU:H	16	0.12
(1,471)	1:234:B:TYR:H	1:254:B:LEU:H	17	0.12
(1,471)	1:234:B:TYR:H	1:254:B:LEU:H	20	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	7	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	7	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	7	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	7	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	7	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	10	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	10	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	10	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	10	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	10	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	10	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	16	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	16	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	16	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	16	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	16	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	16	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	20	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	20	0.12
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	20	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	20	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	20	0.12
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	20	0.12
(1,413)	1:232:B:LEU:HD11	1:293:B:TRP:HZ2	12	0.12
(1,413)	1:232:B:LEU:HD12	1:293:B:TRP:HZ2	12	0.12
(1,413)	1:232:B:LEU:HD13	1:293:B:TRP:HZ2	12	0.12
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	9	0.12
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	9	0.12
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	9	0.12
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	20	0.12
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	20	0.12
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	20	0.12
(1,157)	1:212:B:MET:HE1	1:233:B:CYS:HB3	1	0.12
(1,157)	1:212:B:MET:HE2	1:233:B:CYS:HB3	1	0.12
(1,157)	1:212:B:MET:HE3	1:233:B:CYS:HB3	1	0.12
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG11	5	0.12
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG12	5	0.12
(1,148)	1:212:B:MET:HG3	1:365:B:VAL:HG13	5	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	2	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	4	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	5	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	6	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	7	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	10	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	11	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	13	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	14	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	16	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	17	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	19	0.12
(1,92)	1:209:B:ARG:HG2	1:209:B:ARG:HD2	20	0.12
(1,91)	1:209:B:ARG:HG3	1:209:B:ARG:HD2	3	0.12
(1,91)	1:209:B:ARG:HG3	1:209:B:ARG:HD2	18	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	2	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	6	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	7	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	9	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	10	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	11	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	12	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	14	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	18	0.12
(1,88)	1:209:B:ARG:HB2	1:209:B:ARG:HG2	20	0.12
(1,87)	1:209:B:ARG:HB2	1:209:B:ARG:HG3	1	0.12
(1,87)	1:209:B:ARG:HB2	1:209:B:ARG:HG3	8	0.12
(1,83)	1:209:B:ARG:HB3	1:209:B:ARG:HG2	5	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	3	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	6	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	7	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	10	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	12	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	14	0.12
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	20	0.12
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	5	0.12
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	9	0.12
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	10	0.12
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	12	0.12
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	16	0.12
(1,6998)	1:11:A:HIS:HB3	1:253:B:PHE:HD1	14	0.11
(1,6998)	1:11:A:HIS:HB3	1:253:B:PHE:HD2	14	0.11
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB2	15	0.11
(1,6971)	1:210:B:HIS:HB2	1:54:A:PHE:HB3	15	0.11
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD1	13	0.11
(1,6954)	1:208:B:PRO:HA	1:54:A:PHE:HD2	13	0.11
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	7	0.11
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	8	0.11
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6687)	1:196:A:ASN:HD22	1:196:A:ASN:H	5	0.11
(1,6687)	1:196:A:ASN:HD22	1:196:A:ASN:H	8	0.11
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	9	0.11
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	16	0.11
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	19	0.11
(1,6650)	1:194:A:LEU:HB2	1:195:A:GLN:H	16	0.11
(1,6646)	1:194:A:LEU:HD11	1:194:A:LEU:H	7	0.11
(1,6646)	1:194:A:LEU:HD12	1:194:A:LEU:H	7	0.11
(1,6646)	1:194:A:LEU:HD13	1:194:A:LEU:H	7	0.11
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD11	12	0.11
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD12	12	0.11
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD13	12	0.11
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	10	0.11
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	4	0.11
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	5	0.11
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	11	0.11
(1,6575)	1:191:A:ARG:HB2	1:191:A:ARG:HG2	13	0.11
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD11	8	0.11
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD12	8	0.11
(1,6558)	1:190:A:LEU:HD21	1:193:A:ILE:HD13	8	0.11
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD11	8	0.11
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD12	8	0.11
(1,6558)	1:190:A:LEU:HD22	1:193:A:ILE:HD13	8	0.11
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD11	8	0.11
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD12	8	0.11
(1,6558)	1:190:A:LEU:HD23	1:193:A:ILE:HD13	8	0.11
(1,6491)	1:184:A:GLN:HA	1:187:A:SER:H	15	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	1	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	3	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	7	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	8	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	9	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	10	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	11	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	14	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	15	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	16	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	18	0.11
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	19	0.11
(1,6455)	1:182:A:HIS:HD1	1:182:A:HIS:H	8	0.11
(1,6453)	1:182:A:HIS:HB3	1:182:A:HIS:H	13	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	2	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	3	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	4	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	5	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	6	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	7	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	8	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	10	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	11	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	14	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	15	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	16	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	17	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	18	0.11
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	19	0.11
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	2	0.11
(1,6423)	1:180:A:ASP:HB2	1:181:A:GLU:H	6	0.11
(1,6412)	1:179:A:LEU:HD11	1:182:A:HIS:HB2	7	0.11
(1,6412)	1:179:A:LEU:HD12	1:182:A:HIS:HB2	7	0.11
(1,6412)	1:179:A:LEU:HD13	1:182:A:HIS:HB2	7	0.11
(1,6412)	1:179:A:LEU:HD21	1:182:A:HIS:HB2	7	0.11
(1,6412)	1:179:A:LEU:HD22	1:182:A:HIS:HB2	7	0.11
(1,6412)	1:179:A:LEU:HD23	1:182:A:HIS:HB2	7	0.11
(1,6411)	1:179:A:LEU:HD11	1:182:A:HIS:HB3	10	0.11
(1,6411)	1:179:A:LEU:HD12	1:182:A:HIS:HB3	10	0.11
(1,6411)	1:179:A:LEU:HD13	1:182:A:HIS:HB3	10	0.11
(1,6411)	1:179:A:LEU:HD21	1:182:A:HIS:HB3	10	0.11
(1,6411)	1:179:A:LEU:HD22	1:182:A:HIS:HB3	10	0.11
(1,6411)	1:179:A:LEU:HD23	1:182:A:HIS:HB3	10	0.11
(1,6396)	1:178:A:GLY:H	1:179:A:LEU:H	10	0.11
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD11	12	0.11
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD12	12	0.11
(1,6385)	1:177:A:ASP:HB3	1:179:A:LEU:HD13	12	0.11
(1,6382)	1:177:A:ASP:HA	1:179:A:LEU:H	7	0.11
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	7	0.11
(1,6380)	1:177:A:ASP:HB2	1:177:A:ASP:H	16	0.11
(1,6367)	1:176:A:TRP:HB2	1:177:A:ASP:H	20	0.11
(1,6348)	1:175:A:PRO:HA	1:179:A:LEU:HG	1	0.11
(1,6348)	1:175:A:PRO:HA	1:179:A:LEU:HG	8	0.11
(1,6303)	1:173:A:PHE:HZ	1:176:A:TRP:H	20	0.11
(1,6301)	1:173:A:PHE:HE1	1:179:A:LEU:HG	3	0.11
(1,6301)	1:173:A:PHE:HE2	1:179:A:LEU:HG	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	1	0.11
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	4	0.11
(1,6248)	1:169:A:GLN:HB3	1:169:A:GLN:H	19	0.11
(1,6213)	1:166:A:VAL:HG11	1:169:A:GLN:H	2	0.11
(1,6213)	1:166:A:VAL:HG12	1:169:A:GLN:H	2	0.11
(1,6213)	1:166:A:VAL:HG13	1:169:A:GLN:H	2	0.11
(1,6213)	1:166:A:VAL:HG21	1:169:A:GLN:H	2	0.11
(1,6213)	1:166:A:VAL:HG22	1:169:A:GLN:H	2	0.11
(1,6213)	1:166:A:VAL:HG23	1:169:A:GLN:H	2	0.11
(1,6184)	1:164:A:THR:HG21	1:166:A:VAL:H	9	0.11
(1,6184)	1:164:A:THR:HG22	1:166:A:VAL:H	9	0.11
(1,6184)	1:164:A:THR:HG23	1:166:A:VAL:H	9	0.11
(1,6162)	1:162:A:TRP:HZ3	1:173:A:PHE:H	3	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG21	3	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG22	3	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG23	3	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG21	9	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG22	9	0.11
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG23	9	0.11
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	7	0.11
(1,6045)	1:155:A:TYR:HD1	1:175:A:PRO:HG2	6	0.11
(1,6045)	1:155:A:TYR:HD2	1:175:A:PRO:HG2	6	0.11
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	3	0.11
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	3	0.11
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	8	0.11
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	8	0.11
(1,5983)	1:152:A:ILE:HG12	1:152:A:ILE:H	14	0.11
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	3	0.11
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	3	0.11
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	3	0.11
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	17	0.11
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	17	0.11
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	17	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD11	13	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD12	13	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD13	13	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD11	14	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD12	14	0.11
(1,5955)	1:150:A:VAL:H	1:194:A:LEU:HD13	14	0.11
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD11	11	0.11
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD12	11	0.11
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD13	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD11	11	0.11
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD12	11	0.11
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD13	11	0.11
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD11	11	0.11
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD12	11	0.11
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD13	11	0.11
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	4	0.11
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	4	0.11
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	4	0.11
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	11	0.11
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	11	0.11
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	11	0.11
(1,5911)	1:148:A:ALA:HB1	1:149:A:GLN:H	17	0.11
(1,5911)	1:148:A:ALA:HB2	1:149:A:GLN:H	17	0.11
(1,5911)	1:148:A:ALA:HB3	1:149:A:GLN:H	17	0.11
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG11	20	0.11
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG12	20	0.11
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG13	20	0.11
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG21	20	0.11
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG22	20	0.11
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG23	20	0.11
(1,5866)	1:144:A:ARG:HB3	1:144:A:ARG:H	16	0.11
(1,5856)	1:143:A:LEU:HD21	1:146:A:ALA:H	3	0.11
(1,5856)	1:143:A:LEU:HD22	1:146:A:ALA:H	3	0.11
(1,5856)	1:143:A:LEU:HD23	1:146:A:ALA:H	3	0.11
(1,5815)	1:141:A:GLN:HE21	1:193:A:ILE:HG21	16	0.11
(1,5800)	1:140:A:LEU:H	1:193:A:ILE:HG22	19	0.11
(1,5799)	1:140:A:LEU:H	1:193:A:ILE:HG21	17	0.11
(1,5708)	1:131:A:ASP:HB2	1:131:A:ASP:H	9	0.11
(1,5708)	1:131:A:ASP:HB3	1:131:A:ASP:H	9	0.11
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD21	20	0.11
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD22	20	0.11
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD23	20	0.11
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD21	20	0.11
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD22	20	0.11
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD23	20	0.11
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD21	20	0.11
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD22	20	0.11
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD23	20	0.11
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD21	5	0.11
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD22	5	0.11
(1,5676)	1:129:A:ILE:HB	1:186:A:LEU:HD23	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5652)	1:126:A:ALA:H	1:190:A:LEU:HD21	18	0.11
(1,5652)	1:126:A:ALA:H	1:190:A:LEU:HD22	18	0.11
(1,5652)	1:126:A:ALA:H	1:190:A:LEU:HD23	18	0.11
(1,5612)	1:124:A:ILE:H	1:150:A:VAL:HA	17	0.11
(1,5606)	1:124:A:ILE:HD11	1:125:A:PHE:H	19	0.11
(1,5606)	1:124:A:ILE:HD12	1:125:A:PHE:H	19	0.11
(1,5606)	1:124:A:ILE:HD13	1:125:A:PHE:H	19	0.11
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB1	2	0.11
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB2	2	0.11
(1,5599)	1:124:A:ILE:HB	1:148:A:ALA:HB3	2	0.11
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD11	19	0.11
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD12	19	0.11
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD13	19	0.11
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD21	19	0.11
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD22	19	0.11
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD23	19	0.11
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD11	19	0.11
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD12	19	0.11
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD13	19	0.11
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD21	19	0.11
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD22	19	0.11
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD23	19	0.11
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD11	19	0.11
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD12	19	0.11
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD13	19	0.11
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD21	19	0.11
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD22	19	0.11
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD23	19	0.11
(1,5506)	1:119:A:HIS:HE1	1:119:A:HIS:H	14	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	1	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	2	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	3	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	5	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	6	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	7	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	8	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	9	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	10	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	11	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	13	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	14	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	16	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	17	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	18	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	19	0.11
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	20	0.11
(1,5464)	1:116:A:GLU:HG3	1:117:A:ASN:H	1	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	1	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	3	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	5	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	9	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	14	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	16	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	18	0.11
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	19	0.11
(1,5330)	1:112:A:ALA:HB1	1:115:A:GLN:HE21	3	0.11
(1,5330)	1:112:A:ALA:HB2	1:115:A:GLN:HE21	3	0.11
(1,5330)	1:112:A:ALA:HB3	1:115:A:GLN:HE21	3	0.11
(1,5330)	1:112:A:ALA:HB1	1:115:A:GLN:HE21	19	0.11
(1,5330)	1:112:A:ALA:HB2	1:115:A:GLN:HE21	19	0.11
(1,5330)	1:112:A:ALA:HB3	1:115:A:GLN:HE21	19	0.11
(1,5308)	1:111:A:ARG:HD3	1:115:A:GLN:HG2	6	0.11
(1,5172)	1:102:A:PHE:HE1	1:142:A:MET:HE1	11	0.11
(1,5172)	1:102:A:PHE:HE1	1:142:A:MET:HE2	11	0.11
(1,5172)	1:102:A:PHE:HE1	1:142:A:MET:HE3	11	0.11
(1,5172)	1:102:A:PHE:HE2	1:142:A:MET:HE1	11	0.11
(1,5172)	1:102:A:PHE:HE2	1:142:A:MET:HE2	11	0.11
(1,5172)	1:102:A:PHE:HE2	1:142:A:MET:HE3	11	0.11
(1,5106)	1:96:A:ILE:HG21	1:127:A:ALA:H	7	0.11
(1,5106)	1:96:A:ILE:HG22	1:127:A:ALA:H	7	0.11
(1,5106)	1:96:A:ILE:HG23	1:127:A:ALA:H	7	0.11
(1,5103)	1:96:A:ILE:HG21	1:97:A:SER:H	1	0.11
(1,5103)	1:96:A:ILE:HG22	1:97:A:SER:H	1	0.11
(1,5103)	1:96:A:ILE:HG23	1:97:A:SER:H	1	0.11
(1,5103)	1:96:A:ILE:HG21	1:97:A:SER:H	10	0.11
(1,5103)	1:96:A:ILE:HG22	1:97:A:SER:H	10	0.11
(1,5103)	1:96:A:ILE:HG23	1:97:A:SER:H	10	0.11
(1,5099)	1:96:A:ILE:HG13	1:126:A:ALA:HA	5	0.11
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	15	0.11
(1,5039)	1:94:A:TRP:HZ3	1:94:A:TRP:H	13	0.11
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	6	0.11
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	6	0.11
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG21	9	0.11
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG22	9	0.11
(1,4992)	1:92:A:VAL:HB	1:120:A:VAL:HG23	9	0.11
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG11	20	0.11
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG12	20	0.11
(1,4953)	1:90:A:TYR:HD1	1:92:A:VAL:HG13	20	0.11
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG11	20	0.11
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG12	20	0.11
(1,4953)	1:90:A:TYR:HD2	1:92:A:VAL:HG13	20	0.11
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	11	0.11
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	11	0.11
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	11	0.11
(1,4905)	1:88:A:GLN:HE22	1:88:A:GLN:H	7	0.11
(1,4890)	1:88:A:GLN:HA	1:88:A:GLN:HE22	13	0.11
(1,4858)	1:85:A:ASP:HB3	1:85:A:ASP:H	20	0.11
(1,4816)	1:83:A:GLN:H	1:84:A:LEU:H	14	0.11
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	16	0.11
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	16	0.11
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	16	0.11
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	4	0.11
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	4	0.11
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	4	0.11
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	1	0.11
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	4	0.11
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	5	0.11
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	6	0.11
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	8	0.11
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	16	0.11
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	20	0.11
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	9	0.11
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	20	0.11
(1,4523)	1:73:A:LEU:HD11	1:109:A:GLU:H	13	0.11
(1,4523)	1:73:A:LEU:HD12	1:109:A:GLU:H	13	0.11
(1,4523)	1:73:A:LEU:HD13	1:109:A:GLU:H	13	0.11
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	12	0.11
(1,4404)	1:62:A:LEU:HB3	1:62:A:LEU:H	3	0.11
(1,4404)	1:62:A:LEU:HB3	1:62:A:LEU:H	8	0.11
(1,4404)	1:62:A:LEU:HB3	1:62:A:LEU:H	12	0.11
(1,4404)	1:62:A:LEU:HB3	1:62:A:LEU:H	17	0.11
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD21	15	0.11
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD22	15	0.11
(1,4385)	1:60:A:LYS:HE2	1:62:A:LEU:HD23	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD21	15	0.11
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD22	15	0.11
(1,4385)	1:60:A:LYS:HE3	1:62:A:LEU:HD23	15	0.11
(1,4353)	1:58:A:GLN:HA	1:58:A:GLN:HB2	5	0.11
(1,4266)	1:52:A:ARG:HG2	1:53:A:GLY:H	14	0.11
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	15	0.11
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	2	0.11
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	2	0.11
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	2	0.11
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	9	0.11
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	9	0.11
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	9	0.11
(1,4060)	1:40:A:LEU:HD21	1:90:A:TYR:HA	7	0.11
(1,4060)	1:40:A:LEU:HD22	1:90:A:TYR:HA	7	0.11
(1,4060)	1:40:A:LEU:HD23	1:90:A:TYR:HA	7	0.11
(1,4046)	1:40:A:LEU:HD21	1:42:A:ASN:H	6	0.11
(1,4046)	1:40:A:LEU:HD22	1:42:A:ASN:H	6	0.11
(1,4046)	1:40:A:LEU:HD23	1:42:A:ASN:H	6	0.11
(1,4009)	1:39:A:ARG:HG2	1:88:A:GLN:HB2	3	0.11
(1,4009)	1:39:A:ARG:HG2	1:88:A:GLN:HB2	4	0.11
(1,3975)	1:38:A:GLU:HG3	1:91:A:ARG:HB3	2	0.11
(1,3950)	1:38:A:GLU:HB2	1:38:A:GLU:HG3	8	0.11
(1,3886)	1:36:A:GLU:HA	1:93:A:THR:HB	17	0.11
(1,3877)	1:35:A:TYR:H	1:55:A:LEU:H	16	0.11
(1,3732)	1:23:A:ASN:HB2	1:23:A:ASN:H	7	0.11
(1,3689)	1:19:A:THR:HB	1:19:A:THR:H	4	0.11
(1,3689)	1:19:A:THR:HB	1:19:A:THR:H	13	0.11
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	6	0.11
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	13	0.11
(1,3644)	1:17:A:ILE:HG12	1:17:A:ILE:H	18	0.11
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	9	0.11
(1,3620)	1:16:A:HIS:HA	1:19:A:THR:H	18	0.11
(1,3572)	1:13:A:MET:HE1	1:166:A:VAL:HG11	4	0.11
(1,3572)	1:13:A:MET:HE1	1:166:A:VAL:HG12	4	0.11
(1,3572)	1:13:A:MET:HE1	1:166:A:VAL:HG13	4	0.11
(1,3572)	1:13:A:MET:HE2	1:166:A:VAL:HG11	4	0.11
(1,3572)	1:13:A:MET:HE2	1:166:A:VAL:HG12	4	0.11
(1,3572)	1:13:A:MET:HE2	1:166:A:VAL:HG13	4	0.11
(1,3572)	1:13:A:MET:HE3	1:166:A:VAL:HG11	4	0.11
(1,3572)	1:13:A:MET:HE3	1:166:A:VAL:HG12	4	0.11
(1,3572)	1:13:A:MET:HE3	1:166:A:VAL:HG13	4	0.11
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	17	0.11
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	17	0.11
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	17	0.11
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	17	0.11
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	17	0.11
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	17	0.11
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	17	0.11
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	17	0.11
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG21	19	0.11
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG22	19	0.11
(1,3562)	1:13:A:MET:HE1	1:17:A:ILE:HG23	19	0.11
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG21	19	0.11
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG22	19	0.11
(1,3562)	1:13:A:MET:HE2	1:17:A:ILE:HG23	19	0.11
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG21	19	0.11
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG22	19	0.11
(1,3562)	1:13:A:MET:HE3	1:17:A:ILE:HG23	19	0.11
(1,3518)	1:11:A:HIS:HD2	1:12:A:LEU:H	6	0.11
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	5	0.11
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	7	0.11
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	10	0.11
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	12	0.11
(1,3487)	1:10:A:ARG:HA	1:10:A:ARG:HB2	17	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	1	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	3	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	4	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	9	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	11	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	13	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	14	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	15	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	16	0.11
(1,3486)	1:10:A:ARG:HA	1:10:A:ARG:HB3	18	0.11
(1,3456)	1:7:A:SER:HA	1:7:A:SER:HB2	1	0.11
(1,3456)	1:7:A:SER:HA	1:7:A:SER:HB2	4	0.11
(1,3456)	1:7:A:SER:HA	1:7:A:SER:HB2	7	0.11
(1,3456)	1:7:A:SER:HA	1:7:A:SER:HB2	8	0.11
(1,3456)	1:7:A:SER:HA	1:7:A:SER:HB2	15	0.11
(1,3456)	1:7:A:SER:HA	1:7:A:SER:HB2	18	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	2	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	3	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	5	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	6	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	7	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	9	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	12	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	13	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	14	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	15	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	16	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	17	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	18	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	19	0.11
(1,3332)	2:410:D:DT:H3'	2:410:D:DT:H4'	20	0.11
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	3	0.11
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	9	0.11
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	15	0.11
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	17	0.11
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	18	0.11
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	20	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	1	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	2	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	4	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	5	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	8	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	10	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	11	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	13	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	15	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	16	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	17	0.11
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	19	0.11
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	2	0.11
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	19	0.11
(1,3270)	1:394:B:GLN:HB3	1:395:B:ASN:H	11	0.11
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	2	0.11
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	15	0.11
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	17	0.11
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	2	0.11
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	2	0.11
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	2	0.11
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	2	0.11
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	2	0.11
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	2	0.11
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	2	0.11
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	2	0.11
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD21	20	0.11
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD22	20	0.11
(1,3157)	1:389:B:LEU:HD11	1:393:B:LEU:HD23	20	0.11
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD21	20	0.11
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD22	20	0.11
(1,3157)	1:389:B:LEU:HD12	1:393:B:LEU:HD23	20	0.11
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD21	20	0.11
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD22	20	0.11
(1,3157)	1:389:B:LEU:HD13	1:393:B:LEU:HD23	20	0.11
(1,3086)	1:383:B:GLN:H	1:383:B:GLN:HE21	16	0.11
(1,3077)	1:383:B:GLN:HB2	1:383:B:GLN:HE21	4	0.11
(1,3077)	1:383:B:GLN:HB3	1:383:B:GLN:HE21	4	0.11
(1,3077)	1:383:B:GLN:HB2	1:383:B:GLN:HE21	6	0.11
(1,3077)	1:383:B:GLN:HB3	1:383:B:GLN:HE21	6	0.11
(1,3077)	1:383:B:GLN:HB2	1:383:B:GLN:HE21	13	0.11
(1,3077)	1:383:B:GLN:HB3	1:383:B:GLN:HE21	13	0.11
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	15	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	1	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	2	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	4	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	5	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	9	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	11	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	12	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	13	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	15	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	16	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	18	0.11
(1,3033)	1:380:B:GLU:HB2	1:380:B:GLU:H	20	0.11
(1,3021)	1:379:B:ASP:HB2	1:380:B:GLU:H	5	0.11
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	4	0.11
(1,2978)	1:376:B:ASP:HB2	1:376:B:ASP:H	2	0.11
(1,2978)	1:376:B:ASP:HB2	1:376:B:ASP:H	13	0.11
(1,2978)	1:376:B:ASP:HB2	1:376:B:ASP:H	16	0.11
(1,2978)	1:376:B:ASP:HB2	1:376:B:ASP:H	17	0.11
(1,2946)	1:374:B:PRO:HA	1:378:B:LEU:HG	2	0.11
(1,2925)	1:373:B:GLN:HG2	1:373:B:GLN:HE21	12	0.11
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	2	0.11
(1,2819)	1:366:B:ASP:H	1:367:B:HIS:H	15	0.11
(1,2760)	1:361:B:TRP:HZ3	1:372:B:PHE:H	15	0.11
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	1	0.11
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	7	0.11
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	8	0.11
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	13	0.11
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	2	0.11
(1,2638)	1:354:B:TYR:HD1	1:355:B:ASP:H	7	0.11
(1,2638)	1:354:B:TYR:HD2	1:355:B:ASP:H	7	0.11
(1,2638)	1:354:B:TYR:HD1	1:355:B:ASP:H	17	0.11
(1,2638)	1:354:B:TYR:HD2	1:355:B:ASP:H	17	0.11
(1,2638)	1:354:B:TYR:HD1	1:355:B:ASP:H	19	0.11
(1,2638)	1:354:B:TYR:HD2	1:355:B:ASP:H	19	0.11
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD11	6	0.11
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD12	6	0.11
(1,2634)	1:354:B:TYR:HA	1:378:B:LEU:HD13	6	0.11
(1,2632)	1:354:B:TYR:HE1	1:354:B:TYR:H	5	0.11
(1,2632)	1:354:B:TYR:HE2	1:354:B:TYR:H	5	0.11
(1,2583)	1:351:B:ILE:HD11	1:351:B:ILE:H	12	0.11
(1,2583)	1:351:B:ILE:HD12	1:351:B:ILE:H	12	0.11
(1,2583)	1:351:B:ILE:HD13	1:351:B:ILE:H	12	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	1	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	1	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	1	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	2	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	2	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	2	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	4	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	4	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	4	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	5	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	5	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	5	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	6	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	6	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	6	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	8	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	8	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	8	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	10	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	10	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	11	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	11	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	11	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	12	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	12	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	12	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	13	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	13	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	13	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	15	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	15	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	15	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	18	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	18	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	18	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	19	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	19	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	19	0.11
(1,2508)	1:347:B:ALA:HB1	1:348:B:GLN:H	20	0.11
(1,2508)	1:347:B:ALA:HB2	1:348:B:GLN:H	20	0.11
(1,2508)	1:347:B:ALA:HB3	1:348:B:GLN:H	20	0.11
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD11	13	0.11
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD12	13	0.11
(1,2420)	1:340:B:GLN:HE22	1:393:B:LEU:HD13	13	0.11
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD11	16	0.11
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD12	16	0.11
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD13	16	0.11
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD11	18	0.11
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD12	18	0.11
(1,2416)	1:340:B:GLN:HE21	1:393:B:LEU:HD13	18	0.11
(1,2347)	1:335:B:TYR:HD1	1:336:B:LYS:H	1	0.11
(1,2347)	1:335:B:TYR:HD2	1:336:B:LYS:H	1	0.11
(1,2347)	1:335:B:TYR:HD1	1:336:B:LYS:H	7	0.11
(1,2347)	1:335:B:TYR:HD2	1:336:B:LYS:H	7	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE1	3	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE2	3	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE3	3	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE1	3	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE2	3	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE3	3	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE1	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE2	3	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE3	3	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE1	17	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE2	17	0.11
(1,2341)	1:334:B:LEU:HD11	1:341:B:MET:HE3	17	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE1	17	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE2	17	0.11
(1,2341)	1:334:B:LEU:HD12	1:341:B:MET:HE3	17	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE1	17	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE2	17	0.11
(1,2341)	1:334:B:LEU:HD13	1:341:B:MET:HE3	17	0.11
(1,2321)	1:333:B:PRO:HB2	1:334:B:LEU:H	20	0.11
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD21	7	0.11
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD22	7	0.11
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD23	7	0.11
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD21	7	0.11
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD22	7	0.11
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD23	7	0.11
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD21	7	0.11
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD22	7	0.11
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD23	7	0.11
(1,2241)	1:325:B:ALA:HB1	1:327:B:ARG:H	3	0.11
(1,2241)	1:325:B:ALA:HB2	1:327:B:ARG:H	3	0.11
(1,2241)	1:325:B:ALA:HB3	1:327:B:ARG:H	3	0.11
(1,2228)	1:324:B:PHE:HA	1:350:B:SER:H	20	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	17	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	17	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	17	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	17	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	17	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	17	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	17	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	17	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	17	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	17	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	17	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	17	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	17	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	17	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	17	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	17	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	17	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	19	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	19	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	19	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	19	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	19	0.11
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	19	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	19	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	19	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	19	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	19	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	19	0.11
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	19	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	19	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	19	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	19	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	19	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	19	0.11
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	19	0.11
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	1	0.11
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	1	0.11
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	1	0.11
(1,2119)	1:319:B:VAL:HG21	1:319:B:VAL:H	20	0.11
(1,2119)	1:319:B:VAL:HG22	1:319:B:VAL:H	20	0.11
(1,2119)	1:319:B:VAL:HG23	1:319:B:VAL:H	20	0.11
(1,2107)	1:318:B:HIS:HE1	1:319:B:VAL:HG21	12	0.11
(1,2107)	1:318:B:HIS:HE1	1:319:B:VAL:HG22	12	0.11
(1,2107)	1:318:B:HIS:HE1	1:319:B:VAL:HG23	12	0.11
(1,2104)	1:318:B:HIS:HE1	1:318:B:HIS:H	4	0.11
(1,2104)	1:318:B:HIS:HE1	1:318:B:HIS:H	20	0.11
(1,2103)	1:318:B:HIS:HB2	1:318:B:HIS:H	2	0.11
(1,2103)	1:318:B:HIS:HB2	1:318:B:HIS:H	10	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	2	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	3	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	4	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	5	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	6	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	8	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	9	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	10	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	11	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	13	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	14	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	15	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	16	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	17	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	18	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	19	0.11
(1,2090)	1:317:B:THR:HB	1:317:B:THR:H	20	0.11
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	2	0.11
(1,2028)	1:314:B:GLN:HG3	1:314:B:GLN:HE21	15	0.11
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	4	0.11
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	9	0.11
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	11	0.11
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	16	0.11
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	18	0.11
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	20	0.11
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB1	15	0.11
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB2	15	0.11
(1,2002)	1:313:B:LEU:HD21	1:345:B:ALA:HB3	15	0.11
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB1	15	0.11
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB2	15	0.11
(1,2002)	1:313:B:LEU:HD22	1:345:B:ALA:HB3	15	0.11
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB1	15	0.11
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB2	15	0.11
(1,2002)	1:313:B:LEU:HD23	1:345:B:ALA:HB3	15	0.11
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	8	0.11
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	8	0.11
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	8	0.11
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	8	0.11
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	8	0.11
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	8	0.11
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG21	15	0.11
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG22	15	0.11
(1,1953)	1:312:B:PHE:HD1	1:319:B:VAL:HG23	15	0.11
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG21	15	0.11
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG22	15	0.11
(1,1953)	1:312:B:PHE:HD2	1:319:B:VAL:HG23	15	0.11
(1,1776)	1:302:B:SER:H	1:334:B:LEU:HD11	6	0.11
(1,1776)	1:302:B:SER:H	1:334:B:LEU:HD12	6	0.11
(1,1776)	1:302:B:SER:H	1:334:B:LEU:HD13	6	0.11
(1,1769)	1:301:B:PHE:HD1	1:338:B:ALA:HB1	1	0.11
(1,1769)	1:301:B:PHE:HD1	1:338:B:ALA:HB2	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	1:301:B:PHE:HD1	1:338:B:ALA:HB3	1	0.11
(1,1769)	1:301:B:PHE:HD2	1:338:B:ALA:HB1	1	0.11
(1,1769)	1:301:B:PHE:HD2	1:338:B:ALA:HB2	1	0.11
(1,1769)	1:301:B:PHE:HD2	1:338:B:ALA:HB3	1	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	4	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	6	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	7	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	10	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	12	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	13	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	15	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	19	0.11
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	20	0.11
(1,1719)	1:296:B:SER:HB3	1:296:B:SER:H	8	0.11
(1,1719)	1:296:B:SER:HB3	1:296:B:SER:H	16	0.11
(1,1719)	1:296:B:SER:HB3	1:296:B:SER:H	17	0.11
(1,1708)	1:295:B:ILE:HD11	1:296:B:SER:H	10	0.11
(1,1708)	1:295:B:ILE:HD12	1:296:B:SER:H	10	0.11
(1,1708)	1:295:B:ILE:HD13	1:296:B:SER:H	10	0.11
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	3	0.11
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	19	0.11
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	20	0.11
(1,1699)	1:295:B:ILE:HB	1:297:B:TRP:H	15	0.11
(1,1642)	1:293:B:TRP:HA	1:295:B:ILE:HG21	11	0.11
(1,1642)	1:293:B:TRP:HA	1:295:B:ILE:HG22	11	0.11
(1,1642)	1:293:B:TRP:HA	1:295:B:ILE:HG23	11	0.11
(1,1639)	1:293:B:TRP:HZ3	1:293:B:TRP:H	20	0.11
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	4	0.11
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	4	0.11
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	4	0.11
(1,1609)	1:291:B:VAL:HG11	1:322:B:ARG:H	7	0.11
(1,1609)	1:291:B:VAL:HG12	1:322:B:ARG:H	7	0.11
(1,1609)	1:291:B:VAL:HG13	1:322:B:ARG:H	7	0.11
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	5	0.11
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	5	0.11
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	5	0.11
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG11	12	0.11
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG12	12	0.11
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG13	12	0.11
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG11	12	0.11
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG12	12	0.11
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG13	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD11	16	0.11
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD12	16	0.11
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD13	16	0.11
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD11	20	0.11
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD12	20	0.11
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD13	20	0.11
(1,1491)	1:287:B:GLN:HA	1:287:B:GLN:HE22	7	0.11
(1,1427)	1:283:B:LEU:HB3	1:283:B:LEU:H	8	0.11
(1,1301)	1:278:B:VAL:HA	1:281:B:LEU:H	19	0.11
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	2	0.11
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	5	0.11
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	9	0.11
(1,1248)	1:276:B:ASP:HA	1:279:B:PRO:HB3	18	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	4	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	6	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	7	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	9	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	10	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	11	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	12	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	14	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	15	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	17	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	18	0.11
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	19	0.11
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD11	6	0.11
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD12	6	0.11
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD13	6	0.11
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	4	0.11
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	6	0.11
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	7	0.11
(1,1151)	1:274:B:PHE:HA	1:277:B:LEU:H	15	0.11
(1,1120)	1:272:B:LEU:HD11	1:308:B:GLU:H	8	0.11
(1,1120)	1:272:B:LEU:HD12	1:308:B:GLU:H	8	0.11
(1,1120)	1:272:B:LEU:HD13	1:308:B:GLU:H	8	0.11
(1,1120)	1:272:B:LEU:HD11	1:308:B:GLU:H	20	0.11
(1,1120)	1:272:B:LEU:HD12	1:308:B:GLU:H	20	0.11
(1,1120)	1:272:B:LEU:HD13	1:308:B:GLU:H	20	0.11
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	1	0.11
(1,1060)	1:269:B:HIS:HA	1:273:B:ARG:H	11	0.11
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	1	0.11
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	13	0.11
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	14	0.11
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	17	0.11
(1,910)	1:254:B:LEU:HD21	1:274:B:PHE:HA	2	0.11
(1,910)	1:254:B:LEU:HD22	1:274:B:PHE:HA	2	0.11
(1,910)	1:254:B:LEU:HD23	1:274:B:PHE:HA	2	0.11
(1,910)	1:254:B:LEU:HD21	1:274:B:PHE:HA	16	0.11
(1,910)	1:254:B:LEU:HD22	1:274:B:PHE:HA	16	0.11
(1,910)	1:254:B:LEU:HD23	1:274:B:PHE:HA	16	0.11
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD1	11	0.11
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD2	11	0.11
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD1	11	0.11
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD2	11	0.11
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	4	0.11
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	5	0.11
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	7	0.11
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	14	0.11
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	15	0.11
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	17	0.11
(1,813)	1:248:B:ASP:HB2	1:248:B:ASP:H	12	0.11
(1,771)	1:246:B:LYS:HG2	1:246:B:LYS:HD3	15	0.11
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG11	1	0.11
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG12	1	0.11
(1,721)	1:243:B:THR:HA	1:245:B:VAL:HG13	1	0.11
(1,660)	1:239:B:LEU:HD21	1:244:B:SER:HB2	8	0.11
(1,660)	1:239:B:LEU:HD22	1:244:B:SER:HB2	8	0.11
(1,660)	1:239:B:LEU:HD23	1:244:B:SER:HB2	8	0.11
(1,660)	1:239:B:LEU:HD21	1:244:B:SER:HB2	14	0.11
(1,660)	1:239:B:LEU:HD22	1:244:B:SER:HB2	14	0.11
(1,660)	1:239:B:LEU:HD23	1:244:B:SER:HB2	14	0.11
(1,649)	1:239:B:LEU:HD11	1:288:B:ILE:HB	4	0.11
(1,649)	1:239:B:LEU:HD12	1:288:B:ILE:HB	4	0.11
(1,649)	1:239:B:LEU:HD13	1:288:B:ILE:HB	4	0.11
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	6	0.11
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	17	0.11
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	8	0.11
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	14	0.11
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	16	0.11
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	17	0.11
(1,545)	1:237:B:GLU:HB2	1:237:B:GLU:HG2	20	0.11
(1,544)	1:237:B:GLU:HB2	1:237:B:GLU:HG3	3	0.11
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG21	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG22	16	0.11
(1,482)	1:235:B:GLU:HB2	1:363:B:THR:HG23	16	0.11
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG21	16	0.11
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG22	16	0.11
(1,482)	1:235:B:GLU:HB3	1:363:B:THR:HG23	16	0.11
(1,472)	1:234:B:TYR:H	1:364:B:PHE:HD1	17	0.11
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD21	2	0.11
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD22	2	0.11
(1,464)	1:234:B:TYR:HD1	1:281:B:LEU:HD23	2	0.11
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD21	2	0.11
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD22	2	0.11
(1,464)	1:234:B:TYR:HD2	1:281:B:LEU:HD23	2	0.11
(1,417)	1:232:B:LEU:HD21	1:295:B:ILE:HG21	2	0.11
(1,417)	1:232:B:LEU:HD21	1:295:B:ILE:HG22	2	0.11
(1,417)	1:232:B:LEU:HD21	1:295:B:ILE:HG23	2	0.11
(1,417)	1:232:B:LEU:HD22	1:295:B:ILE:HG21	2	0.11
(1,417)	1:232:B:LEU:HD22	1:295:B:ILE:HG22	2	0.11
(1,417)	1:232:B:LEU:HD22	1:295:B:ILE:HG23	2	0.11
(1,417)	1:232:B:LEU:HD23	1:295:B:ILE:HG21	2	0.11
(1,417)	1:232:B:LEU:HD23	1:295:B:ILE:HG22	2	0.11
(1,417)	1:232:B:LEU:HD23	1:295:B:ILE:HG23	2	0.11
(1,411)	1:232:B:LEU:HD11	1:274:B:PHE:HZ	3	0.11
(1,411)	1:232:B:LEU:HD12	1:274:B:PHE:HZ	3	0.11
(1,411)	1:232:B:LEU:HD13	1:274:B:PHE:HZ	3	0.11
(1,411)	1:232:B:LEU:HD21	1:274:B:PHE:HZ	3	0.11
(1,411)	1:232:B:LEU:HD22	1:274:B:PHE:HZ	3	0.11
(1,411)	1:232:B:LEU:HD23	1:274:B:PHE:HZ	3	0.11
(1,411)	1:232:B:LEU:HD11	1:274:B:PHE:HZ	10	0.11
(1,411)	1:232:B:LEU:HD12	1:274:B:PHE:HZ	10	0.11
(1,411)	1:232:B:LEU:HD13	1:274:B:PHE:HZ	10	0.11
(1,411)	1:232:B:LEU:HD21	1:274:B:PHE:HZ	10	0.11
(1,411)	1:232:B:LEU:HD22	1:274:B:PHE:HZ	10	0.11
(1,411)	1:232:B:LEU:HD23	1:274:B:PHE:HZ	10	0.11
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE1	12	0.11
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE2	12	0.11
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE1	12	0.11
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE2	12	0.11
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE1	12	0.11
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE2	12	0.11
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	11	0.11
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	11	0.11
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	16	0.11
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	16	0.11
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	16	0.11
(1,292)	1:218:B:THR:HG21	1:375:B:TRP:HZ2	14	0.11
(1,292)	1:218:B:THR:HG22	1:375:B:TRP:HZ2	14	0.11
(1,292)	1:218:B:THR:HG23	1:375:B:TRP:HZ2	14	0.11
(1,286)	1:218:B:THR:HG21	1:361:B:TRP:HZ2	19	0.11
(1,286)	1:218:B:THR:HG22	1:361:B:TRP:HZ2	19	0.11
(1,286)	1:218:B:THR:HG23	1:361:B:TRP:HZ2	19	0.11
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	4	0.11
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG11	8	0.11
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG12	8	0.11
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG13	8	0.11
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG11	8	0.11
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG12	8	0.11
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG13	8	0.11
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG11	8	0.11
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG12	8	0.11
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG13	8	0.11
(1,138)	1:212:B:MET:HB2	1:212:B:MET:H	11	0.11
(1,138)	1:212:B:MET:HB2	1:212:B:MET:H	14	0.11
(1,138)	1:212:B:MET:HB2	1:212:B:MET:H	15	0.11
(1,138)	1:212:B:MET:HB2	1:212:B:MET:H	20	0.11
(1,132)	1:211:B:LEU:HD21	1:368:B:GLN:HE22	7	0.11
(1,132)	1:211:B:LEU:HD22	1:368:B:GLN:HE22	7	0.11
(1,132)	1:211:B:LEU:HD23	1:368:B:GLN:HE22	7	0.11
(1,103)	1:210:B:HIS:HB3	1:210:B:HIS:H	12	0.11
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	2	0.11
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	9	0.11
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	11	0.11
(1,82)	1:209:B:ARG:HB3	1:209:B:ARG:HG3	18	0.11
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	6	0.11
(1,77)	1:209:B:ARG:HA	1:209:B:ARG:HB2	20	0.11
(1,76)	1:209:B:ARG:HA	1:209:B:ARG:HB3	3	0.11
(1,76)	1:209:B:ARG:HA	1:209:B:ARG:HB3	13	0.11
(1,76)	1:209:B:ARG:HA	1:209:B:ARG:HB3	18	0.11
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	8	0.11
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	10	0.11
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	12	0.11
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	13	0.11
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	14	0.11
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	20	0.11
(1,46)	1:206:B:SER:HA	1:206:B:SER:HB2	4	0.11
(1,46)	1:206:B:SER:HA	1:206:B:SER:HB2	11	0.11
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	2	0.1
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	3	0.1
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	6	0.1
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	9	0.1
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	13	0.1
(1,6814)	2:402:C:DT:H1'	2:402:C:DT:H6	19	0.1
(1,6697)	1:197:A:GLN:HB3	1:197:A:GLN:H	6	0.1
(1,6697)	1:197:A:GLN:HB3	1:197:A:GLN:H	9	0.1
(1,6697)	1:197:A:GLN:HB3	1:197:A:GLN:H	11	0.1
(1,6697)	1:197:A:GLN:HB3	1:197:A:GLN:H	14	0.1
(1,6697)	1:197:A:GLN:HB3	1:197:A:GLN:H	19	0.1
(1,6697)	1:197:A:GLN:HB3	1:197:A:GLN:H	20	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	4	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	5	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	7	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	8	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	9	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	15	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	17	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	18	0.1
(1,6685)	1:196:A:ASN:HD21	1:196:A:ASN:HD22	20	0.1
(1,6683)	1:196:A:ASN:HB2	1:196:A:ASN:HD21	3	0.1
(1,6683)	1:196:A:ASN:HB2	1:196:A:ASN:HD21	14	0.1
(1,6683)	1:196:A:ASN:HB2	1:196:A:ASN:HD21	16	0.1
(1,6683)	1:196:A:ASN:HB2	1:196:A:ASN:HD21	18	0.1
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	4	0.1
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	12	0.1
(1,6671)	1:195:A:GLN:HE22	1:195:A:GLN:H	17	0.1
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD11	13	0.1
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD12	13	0.1
(1,6607)	1:192:A:ALA:H	1:193:A:ILE:HD13	13	0.1
(1,6581)	1:191:A:ARG:HG3	1:191:A:ARG:H	18	0.1
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD21	14	0.1
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD22	14	0.1
(1,6560)	1:190:A:LEU:HD21	1:194:A:LEU:HD23	14	0.1
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD21	14	0.1
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD22	14	0.1
(1,6560)	1:190:A:LEU:HD22	1:194:A:LEU:HD23	14	0.1
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD21	14	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD22	14	0.1
(1,6560)	1:190:A:LEU:HD23	1:194:A:LEU:HD23	14	0.1
(1,6487)	1:184:A:GLN:HE21	1:184:A:GLN:HE22	7	0.1
(1,6487)	1:184:A:GLN:HE21	1:184:A:GLN:HE22	9	0.1
(1,6487)	1:184:A:GLN:HE21	1:184:A:GLN:HE22	10	0.1
(1,6487)	1:184:A:GLN:HE21	1:184:A:GLN:HE22	11	0.1
(1,6487)	1:184:A:GLN:HE21	1:184:A:GLN:HE22	16	0.1
(1,6487)	1:184:A:GLN:HE21	1:184:A:GLN:HE22	19	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	2	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	4	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	5	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	6	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	12	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	13	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	17	0.1
(1,6464)	1:183:A:SER:HB3	1:183:A:SER:H	20	0.1
(1,6444)	1:181:A:GLU:HG3	1:182:A:HIS:H	13	0.1
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	9	0.1
(1,6435)	1:181:A:GLU:HB2	1:181:A:GLU:H	20	0.1
(1,6406)	1:179:A:LEU:HG	1:179:A:LEU:H	7	0.1
(1,6327)	1:174:A:GLN:HG2	1:174:A:GLN:HE21	7	0.1
(1,6251)	1:169:A:GLN:HB3	1:169:A:GLN:HE22	16	0.1
(1,6210)	1:166:A:VAL:HG21	1:168:A:HIS:HA	17	0.1
(1,6210)	1:166:A:VAL:HG22	1:168:A:HIS:HA	17	0.1
(1,6210)	1:166:A:VAL:HG23	1:168:A:HIS:HA	17	0.1
(1,6136)	1:162:A:TRP:HA	1:163:A:ASP:H	8	0.1
(1,6118)	1:161:A:CYS:HB3	1:161:A:CYS:H	2	0.1
(1,6118)	1:161:A:CYS:HB3	1:161:A:CYS:H	6	0.1
(1,6118)	1:161:A:CYS:HB3	1:161:A:CYS:H	7	0.1
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG21	15	0.1
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG22	15	0.1
(1,6109)	1:160:A:HIS:HD1	1:164:A:THR:HG23	15	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	2	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	3	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	4	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	5	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	8	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	10	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	12	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	13	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	17	0.1
(1,6071)	1:157:A:GLU:HB3	1:157:A:GLU:H	20	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	4	0.1
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	4	0.1
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	6	0.1
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	6	0.1
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	10	0.1
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	10	0.1
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	11	0.1
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	11	0.1
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	19	0.1
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	19	0.1
(1,6041)	1:155:A:TYR:HD1	1:156:A:ASP:H	20	0.1
(1,6041)	1:155:A:TYR:HD2	1:156:A:ASP:H	20	0.1
(1,6035)	1:155:A:TYR:HE1	1:155:A:TYR:H	8	0.1
(1,6035)	1:155:A:TYR:HE2	1:155:A:TYR:H	8	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	4	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	4	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	4	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	12	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	12	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	12	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	13	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	13	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	13	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD21	19	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD22	19	0.1
(1,5965)	1:151:A:SER:HA	1:190:A:LEU:HD23	19	0.1
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD11	3	0.1
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD12	3	0.1
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD13	3	0.1
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD11	3	0.1
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD12	3	0.1
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD13	3	0.1
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD11	3	0.1
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD12	3	0.1
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD13	3	0.1
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD11	10	0.1
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD12	10	0.1
(1,5951)	1:150:A:VAL:HG21	1:190:A:LEU:HD13	10	0.1
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD11	10	0.1
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD12	10	0.1
(1,5951)	1:150:A:VAL:HG22	1:190:A:LEU:HD13	10	0.1
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD11	10	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD12	10	0.1
(1,5951)	1:150:A:VAL:HG23	1:190:A:LEU:HD13	10	0.1
(1,5887)	1:145:A:ASP:HB3	1:145:A:ASP:H	4	0.1
(1,5887)	1:145:A:ASP:HB3	1:145:A:ASP:H	10	0.1
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG11	5	0.1
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG12	5	0.1
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG13	5	0.1
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG21	5	0.1
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG22	5	0.1
(1,5882)	1:144:A:ARG:H	1:150:A:VAL:HG23	5	0.1
(1,5812)	1:141:A:GLN:HE21	1:141:A:GLN:HE22	6	0.1
(1,5812)	1:141:A:GLN:HE21	1:141:A:GLN:HE22	7	0.1
(1,5812)	1:141:A:GLN:HE21	1:141:A:GLN:HE22	11	0.1
(1,5812)	1:141:A:GLN:HE21	1:141:A:GLN:HE22	14	0.1
(1,5787)	1:140:A:LEU:HD21	1:193:A:ILE:HG12	15	0.1
(1,5787)	1:140:A:LEU:HD21	1:193:A:ILE:HG13	15	0.1
(1,5787)	1:140:A:LEU:HD22	1:193:A:ILE:HG12	15	0.1
(1,5787)	1:140:A:LEU:HD22	1:193:A:ILE:HG13	15	0.1
(1,5787)	1:140:A:LEU:HD23	1:193:A:ILE:HG12	15	0.1
(1,5787)	1:140:A:LEU:HD23	1:193:A:ILE:HG13	15	0.1
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB1	8	0.1
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB2	8	0.1
(1,5742)	1:135:A:LEU:HD11	1:139:A:ALA:HB3	8	0.1
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB1	8	0.1
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB2	8	0.1
(1,5742)	1:135:A:LEU:HD12	1:139:A:ALA:HB3	8	0.1
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB1	8	0.1
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB2	8	0.1
(1,5742)	1:135:A:LEU:HD13	1:139:A:ALA:HB3	8	0.1
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD21	5	0.1
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD22	5	0.1
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD23	5	0.1
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD21	5	0.1
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD22	5	0.1
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD23	5	0.1
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD21	5	0.1
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD22	5	0.1
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD23	5	0.1
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD21	15	0.1
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD22	15	0.1
(1,5680)	1:129:A:ILE:HG21	1:186:A:LEU:HD23	15	0.1
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD21	15	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD22	15	0.1
(1,5680)	1:129:A:ILE:HG22	1:186:A:LEU:HD23	15	0.1
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD21	15	0.1
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD22	15	0.1
(1,5680)	1:129:A:ILE:HG23	1:186:A:LEU:HD23	15	0.1
(1,5631)	1:125:A:PHE:HA	1:151:A:SER:H	7	0.1
(1,5631)	1:125:A:PHE:HA	1:151:A:SER:H	20	0.1
(1,5606)	1:124:A:ILE:HD11	1:125:A:PHE:H	5	0.1
(1,5606)	1:124:A:ILE:HD12	1:125:A:PHE:H	5	0.1
(1,5606)	1:124:A:ILE:HD13	1:125:A:PHE:H	5	0.1
(1,5571)	1:122:A:LEU:HD11	1:143:A:LEU:HD11	7	0.1
(1,5571)	1:122:A:LEU:HD11	1:143:A:LEU:HD12	7	0.1
(1,5571)	1:122:A:LEU:HD11	1:143:A:LEU:HD13	7	0.1
(1,5571)	1:122:A:LEU:HD12	1:143:A:LEU:HD11	7	0.1
(1,5571)	1:122:A:LEU:HD12	1:143:A:LEU:HD12	7	0.1
(1,5571)	1:122:A:LEU:HD12	1:143:A:LEU:HD13	7	0.1
(1,5571)	1:122:A:LEU:HD13	1:143:A:LEU:HD11	7	0.1
(1,5571)	1:122:A:LEU:HD13	1:143:A:LEU:HD12	7	0.1
(1,5571)	1:122:A:LEU:HD13	1:143:A:LEU:HD13	7	0.1
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD11	2	0.1
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD12	2	0.1
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD13	2	0.1
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD21	2	0.1
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD22	2	0.1
(1,5524)	1:120:A:VAL:HG11	1:122:A:LEU:HD23	2	0.1
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD11	2	0.1
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD12	2	0.1
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD13	2	0.1
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD21	2	0.1
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD22	2	0.1
(1,5524)	1:120:A:VAL:HG12	1:122:A:LEU:HD23	2	0.1
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD11	2	0.1
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD12	2	0.1
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD13	2	0.1
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD21	2	0.1
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD22	2	0.1
(1,5524)	1:120:A:VAL:HG13	1:122:A:LEU:HD23	2	0.1
(1,5492)	1:118:A:THR:HB	1:118:A:THR:H	4	0.1
(1,5436)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	1	0.1
(1,5436)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	2	0.1
(1,5436)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	6	0.1
(1,5436)	1:115:A:GLN:HE21	1:115:A:GLN:HE22	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	12	0.1
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	17	0.1
(1,5430)	1:115:A:GLN:HG3	1:115:A:GLN:HE21	20	0.1
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG21	13	0.1
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG22	13	0.1
(1,5355)	1:113:A:PHE:HD1	1:120:A:VAL:HG23	13	0.1
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG21	13	0.1
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG22	13	0.1
(1,5355)	1:113:A:PHE:HD2	1:120:A:VAL:HG23	13	0.1
(1,5119)	1:97:A:SER:HB2	1:97:A:SER:H	13	0.1
(1,5103)	1:96:A:ILE:HG21	1:97:A:SER:H	8	0.1
(1,5103)	1:96:A:ILE:HG22	1:97:A:SER:H	8	0.1
(1,5103)	1:96:A:ILE:HG23	1:97:A:SER:H	8	0.1
(1,5087)	1:96:A:ILE:HB	1:96:A:ILE:H	14	0.1
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD11	4	0.1
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD12	4	0.1
(1,4919)	1:89:A:ILE:HA	1:89:A:ILE:HD13	4	0.1
(1,4883)	1:87:A:ALA:HB1	1:88:A:GLN:H	17	0.1
(1,4883)	1:87:A:ALA:HB2	1:88:A:GLN:H	17	0.1
(1,4883)	1:87:A:ALA:HB3	1:88:A:GLN:H	17	0.1
(1,4873)	1:86:A:PRO:HB2	1:87:A:ALA:H	4	0.1
(1,4826)	1:84:A:LEU:HB3	1:84:A:LEU:H	8	0.1
(1,4809)	1:83:A:GLN:HE21	1:83:A:GLN:H	19	0.1
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD21	2	0.1
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD22	2	0.1
(1,4661)	1:78:A:LEU:HA	1:78:A:LEU:HD23	2	0.1
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	7	0.1
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	7	0.1
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	7	0.1
(1,4633)	1:76:A:LEU:HD11	1:113:A:PHE:HZ	16	0.1
(1,4633)	1:76:A:LEU:HD12	1:113:A:PHE:HZ	16	0.1
(1,4633)	1:76:A:LEU:HD13	1:113:A:PHE:HZ	16	0.1
(1,4596)	1:76:A:LEU:HB3	1:76:A:LEU:H	2	0.1
(1,4554)	1:75:A:PHE:HA	1:78:A:LEU:H	11	0.1
(1,4486)	1:72:A:GLN:HB3	1:72:A:GLN:H	2	0.1
(1,4486)	1:72:A:GLN:HB3	1:72:A:GLN:H	12	0.1
(1,4463)	1:70:A:HIS:HA	1:74:A:ARG:H	7	0.1
(1,4384)	1:60:A:LYS:HE2	1:62:A:LEU:HD11	19	0.1
(1,4384)	1:60:A:LYS:HE2	1:62:A:LEU:HD12	19	0.1
(1,4384)	1:60:A:LYS:HE2	1:62:A:LEU:HD13	19	0.1
(1,4384)	1:60:A:LYS:HE3	1:62:A:LEU:HD11	19	0.1
(1,4384)	1:60:A:LYS:HE3	1:62:A:LEU:HD12	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4384)	1:60:A:LYS:HE3	1:62:A:LEU:HD13	19	0.1
(1,4347)	1:57:A:ASN:HD21	1:57:A:ASN:HD22	9	0.1
(1,4347)	1:57:A:ASN:HD21	1:57:A:ASN:HD22	10	0.1
(1,4347)	1:57:A:ASN:HD21	1:57:A:ASN:HD22	12	0.1
(1,4347)	1:57:A:ASN:HD21	1:57:A:ASN:HD22	19	0.1
(1,4346)	1:57:A:ASN:HB2	1:57:A:ASN:H	18	0.1
(1,4219)	1:49:A:ASP:HB2	1:49:A:ASP:H	7	0.1
(1,4218)	1:49:A:ASP:HB3	1:49:A:ASP:H	20	0.1
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	2	0.1
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	17	0.1
(1,4177)	1:47:A:LYS:HG2	1:47:A:LYS:HD3	19	0.1
(1,4065)	1:40:A:LEU:HD21	1:45:A:SER:HB3	12	0.1
(1,4065)	1:40:A:LEU:HD22	1:45:A:SER:HB3	12	0.1
(1,4065)	1:40:A:LEU:HD23	1:45:A:SER:HB3	12	0.1
(1,4057)	1:40:A:LEU:HD11	1:89:A:ILE:HG21	3	0.1
(1,4057)	1:40:A:LEU:HD11	1:89:A:ILE:HG22	3	0.1
(1,4057)	1:40:A:LEU:HD11	1:89:A:ILE:HG23	3	0.1
(1,4057)	1:40:A:LEU:HD12	1:89:A:ILE:HG21	3	0.1
(1,4057)	1:40:A:LEU:HD12	1:89:A:ILE:HG22	3	0.1
(1,4057)	1:40:A:LEU:HD12	1:89:A:ILE:HG23	3	0.1
(1,4057)	1:40:A:LEU:HD13	1:89:A:ILE:HG21	3	0.1
(1,4057)	1:40:A:LEU:HD13	1:89:A:ILE:HG22	3	0.1
(1,4057)	1:40:A:LEU:HD13	1:89:A:ILE:HG23	3	0.1
(1,4055)	1:40:A:LEU:HD11	1:89:A:ILE:HB	19	0.1
(1,4055)	1:40:A:LEU:HD12	1:89:A:ILE:HB	19	0.1
(1,4055)	1:40:A:LEU:HD13	1:89:A:ILE:HB	19	0.1
(1,4045)	1:40:A:LEU:HD11	1:42:A:ASN:H	1	0.1
(1,4045)	1:40:A:LEU:HD12	1:42:A:ASN:H	1	0.1
(1,4045)	1:40:A:LEU:HD13	1:42:A:ASN:H	1	0.1
(1,4014)	1:39:A:ARG:H	1:46:A:VAL:H	18	0.1
(1,4009)	1:39:A:ARG:HG2	1:88:A:GLN:HB2	11	0.1
(1,3767)	1:28:A:ARG:HE	1:28:A:ARG:H	19	0.1
(1,3689)	1:19:A:THR:HB	1:19:A:THR:H	5	0.1
(1,3689)	1:19:A:THR:HB	1:19:A:THR:H	8	0.1
(1,3689)	1:19:A:THR:HB	1:19:A:THR:H	14	0.1
(1,3597)	1:15:A:PRO:HA	1:19:A:THR:H	8	0.1
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	2	0.1
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	3	0.1
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	10	0.1
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	12	0.1
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	17	0.1
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3462)	1:7:A:SER:HB2	1:7:A:SER:H	20	0.1
(1,3327)	2:410:D:DT:H2''	2:410:D:DT:H3'	8	0.1
(1,3319)	2:410:D:DT:H1'	2:410:D:DT:H5''	20	0.1
(1,3295)	1:396:B:GLN:HB3	1:396:B:GLN:H	11	0.1
(1,3295)	1:396:B:GLN:HB3	1:396:B:GLN:H	14	0.1
(1,3295)	1:396:B:GLN:HB3	1:396:B:GLN:H	17	0.1
(1,3285)	1:395:B:ASN:HD22	1:395:B:ASN:H	20	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	1	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	2	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	3	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	4	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	6	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	7	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	8	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	9	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	10	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	12	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	13	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	15	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	19	0.1
(1,3283)	1:395:B:ASN:HD21	1:395:B:ASN:HD22	20	0.1
(1,3281)	1:395:B:ASN:HB2	1:395:B:ASN:HD21	17	0.1
(1,3281)	1:395:B:ASN:HB2	1:395:B:ASN:HD21	19	0.1
(1,3269)	1:394:B:GLN:HE22	1:394:B:GLN:H	5	0.1
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD11	6	0.1
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD12	6	0.1
(1,3205)	1:391:B:ALA:H	1:392:B:ILE:HD13	6	0.1
(1,3089)	1:383:B:GLN:HA	1:386:B:SER:H	7	0.1
(1,3089)	1:383:B:GLN:HA	1:386:B:SER:H	9	0.1
(1,3077)	1:383:B:GLN:HB2	1:383:B:GLN:HE21	11	0.1
(1,3077)	1:383:B:GLN:HB3	1:383:B:GLN:HE21	11	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	2	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	3	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	4	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	6	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	10	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	11	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	12	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	13	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	16	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	18	0.1
(1,3062)	1:382:B:SER:HB3	1:382:B:SER:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3009)	1:378:B:LEU:HD11	1:381:B:HIS:HB3	6	0.1
(1,3009)	1:378:B:LEU:HD12	1:381:B:HIS:HB3	6	0.1
(1,3009)	1:378:B:LEU:HD13	1:381:B:HIS:HB3	6	0.1
(1,3009)	1:378:B:LEU:HD21	1:381:B:HIS:HB3	6	0.1
(1,3009)	1:378:B:LEU:HD22	1:381:B:HIS:HB3	6	0.1
(1,3009)	1:378:B:LEU:HD23	1:381:B:HIS:HB3	6	0.1
(1,3004)	1:378:B:LEU:HG	1:378:B:LEU:H	3	0.1
(1,2962)	1:375:B:TRP:HZ3	1:375:B:TRP:H	2	0.1
(1,2901)	1:372:B:PHE:HZ	1:375:B:TRP:H	4	0.1
(1,2849)	1:368:B:GLN:HB3	1:368:B:GLN:HE22	15	0.1
(1,2846)	1:368:B:GLN:HB3	1:368:B:GLN:H	5	0.1
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	3	0.1
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	4	0.1
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	6	0.1
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	10	0.1
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	12	0.1
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	16	0.1
(1,2716)	1:360:B:CYS:HB3	1:360:B:CYS:H	19	0.1
(1,2707)	1:359:B:HIS:HD1	1:363:B:THR:HG21	2	0.1
(1,2707)	1:359:B:HIS:HD1	1:363:B:THR:HG22	2	0.1
(1,2707)	1:359:B:HIS:HD1	1:363:B:THR:HG23	2	0.1
(1,2673)	1:356:B:GLU:HA	1:359:B:HIS:H	10	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	4	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	5	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	7	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	9	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	10	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	12	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	16	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	18	0.1
(1,2668)	1:356:B:GLU:HB3	1:356:B:GLU:H	19	0.1
(1,2638)	1:354:B:TYR:HD1	1:355:B:ASP:H	6	0.1
(1,2638)	1:354:B:TYR:HD2	1:355:B:ASP:H	6	0.1
(1,2594)	1:351:B:ILE:HD11	1:352:B:MET:H	6	0.1
(1,2594)	1:351:B:ILE:HD12	1:352:B:MET:H	6	0.1
(1,2594)	1:351:B:ILE:HD13	1:352:B:MET:H	6	0.1
(1,2583)	1:351:B:ILE:HD11	1:351:B:ILE:H	3	0.1
(1,2583)	1:351:B:ILE:HD12	1:351:B:ILE:H	3	0.1
(1,2583)	1:351:B:ILE:HD13	1:351:B:ILE:H	3	0.1
(1,2583)	1:351:B:ILE:HD11	1:351:B:ILE:H	19	0.1
(1,2583)	1:351:B:ILE:HD12	1:351:B:ILE:H	19	0.1
(1,2583)	1:351:B:ILE:HD13	1:351:B:ILE:H	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2574)	1:351:B:ILE:HB	1:351:B:ILE:H	10	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD11	2	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD12	2	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD13	2	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD11	2	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD12	2	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD13	2	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD11	2	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD12	2	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD13	2	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD11	6	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD12	6	0.1
(1,2548)	1:349:B:VAL:HG21	1:389:B:LEU:HD13	6	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD11	6	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD12	6	0.1
(1,2548)	1:349:B:VAL:HG22	1:389:B:LEU:HD13	6	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD11	6	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD12	6	0.1
(1,2548)	1:349:B:VAL:HG23	1:389:B:LEU:HD13	6	0.1
(1,2456)	1:342:B:LEU:HD11	1:347:B:ALA:H	4	0.1
(1,2456)	1:342:B:LEU:HD12	1:347:B:ALA:H	4	0.1
(1,2456)	1:342:B:LEU:HD13	1:347:B:ALA:H	4	0.1
(1,2409)	1:340:B:GLN:HE21	1:340:B:GLN:HE22	7	0.1
(1,2409)	1:340:B:GLN:HE21	1:340:B:GLN:HE22	9	0.1
(1,2409)	1:340:B:GLN:HE21	1:340:B:GLN:HE22	12	0.1
(1,2409)	1:340:B:GLN:HE21	1:340:B:GLN:HE22	16	0.1
(1,2409)	1:340:B:GLN:HE21	1:340:B:GLN:HE22	18	0.1
(1,2347)	1:335:B:TYR:HD1	1:336:B:LYS:H	16	0.1
(1,2347)	1:335:B:TYR:HD2	1:336:B:LYS:H	16	0.1
(1,2346)	1:335:B:TYR:HE1	1:335:B:TYR:H	18	0.1
(1,2346)	1:335:B:TYR:HE2	1:335:B:TYR:H	18	0.1
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD21	11	0.1
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD22	11	0.1
(1,2288)	1:328:B:ILE:HD11	1:385:B:LEU:HD23	11	0.1
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD21	11	0.1
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD22	11	0.1
(1,2288)	1:328:B:ILE:HD12	1:385:B:LEU:HD23	11	0.1
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD21	11	0.1
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD22	11	0.1
(1,2288)	1:328:B:ILE:HD13	1:385:B:LEU:HD23	11	0.1
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD11	6	0.1
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD12	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD13	6	0.1
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD21	6	0.1
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD22	6	0.1
(1,2122)	1:319:B:VAL:HG11	1:321:B:LEU:HD23	6	0.1
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD11	6	0.1
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD12	6	0.1
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD13	6	0.1
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD21	6	0.1
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD22	6	0.1
(1,2122)	1:319:B:VAL:HG12	1:321:B:LEU:HD23	6	0.1
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD11	6	0.1
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD12	6	0.1
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD13	6	0.1
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD21	6	0.1
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD22	6	0.1
(1,2122)	1:319:B:VAL:HG13	1:321:B:LEU:HD23	6	0.1
(1,2079)	1:316:B:ASN:HB2	1:318:B:HIS:HD2	19	0.1
(1,2052)	1:315:B:GLU:HB3	1:315:B:GLU:H	4	0.1
(1,2034)	1:314:B:GLN:HE21	1:314:B:GLN:HE22	1	0.1
(1,2034)	1:314:B:GLN:HE21	1:314:B:GLN:HE22	4	0.1
(1,2034)	1:314:B:GLN:HE21	1:314:B:GLN:HE22	10	0.1
(1,2034)	1:314:B:GLN:HE21	1:314:B:GLN:HE22	12	0.1
(1,2022)	1:314:B:GLN:HB3	1:314:B:GLN:HE22	5	0.1
(1,1854)	1:309:B:VAL:HB	1:309:B:VAL:H	8	0.1
(1,1750)	1:300:B:CYS:H	1:301:B:PHE:H	12	0.1
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	1	0.1
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	2	0.1
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	3	0.1
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	11	0.1
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	14	0.1
(1,1720)	1:296:B:SER:HB2	1:296:B:SER:H	18	0.1
(1,1703)	1:295:B:ILE:HG12	1:326:B:ALA:H	12	0.1
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG21	18	0.1
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG22	18	0.1
(1,1593)	1:291:B:VAL:HB	1:319:B:VAL:HG23	18	0.1
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG11	8	0.1
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG12	8	0.1
(1,1554)	1:289:B:TYR:HD1	1:291:B:VAL:HG13	8	0.1
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG11	8	0.1
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG12	8	0.1
(1,1554)	1:289:B:TYR:HD2	1:291:B:VAL:HG13	8	0.1
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD11	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD12	11	0.1
(1,1520)	1:288:B:ILE:HA	1:288:B:ILE:HD13	11	0.1
(1,1484)	1:286:B:ALA:HB1	1:287:B:GLN:H	6	0.1
(1,1484)	1:286:B:ALA:HB2	1:287:B:GLN:H	6	0.1
(1,1484)	1:286:B:ALA:HB3	1:287:B:GLN:H	6	0.1
(1,1441)	1:283:B:LEU:HD11	1:289:B:TYR:HE1	13	0.1
(1,1441)	1:283:B:LEU:HD11	1:289:B:TYR:HE2	13	0.1
(1,1441)	1:283:B:LEU:HD12	1:289:B:TYR:HE1	13	0.1
(1,1441)	1:283:B:LEU:HD12	1:289:B:TYR:HE2	13	0.1
(1,1441)	1:283:B:LEU:HD13	1:289:B:TYR:HE1	13	0.1
(1,1441)	1:283:B:LEU:HD13	1:289:B:TYR:HE2	13	0.1
(1,1427)	1:283:B:LEU:HB3	1:283:B:LEU:H	1	0.1
(1,1427)	1:283:B:LEU:HB3	1:283:B:LEU:H	7	0.1
(1,1427)	1:283:B:LEU:HB3	1:283:B:LEU:H	12	0.1
(1,1427)	1:283:B:LEU:HB3	1:283:B:LEU:H	18	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD11	3	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD12	3	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD13	3	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD11	9	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD12	9	0.1
(1,1393)	1:281:B:LEU:H	1:283:B:LEU:HD13	9	0.1
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG21	16	0.1
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG22	16	0.1
(1,1388)	1:281:B:LEU:HD11	1:291:B:VAL:HG23	16	0.1
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG21	16	0.1
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG22	16	0.1
(1,1388)	1:281:B:LEU:HD12	1:291:B:VAL:HG23	16	0.1
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG21	16	0.1
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG22	16	0.1
(1,1388)	1:281:B:LEU:HD13	1:291:B:VAL:HG23	16	0.1
(1,1249)	1:276:B:ASP:HA	1:279:B:PRO:HB2	20	0.1
(1,1231)	1:275:B:LEU:HD11	1:312:B:PHE:HZ	13	0.1
(1,1231)	1:275:B:LEU:HD12	1:312:B:PHE:HZ	13	0.1
(1,1231)	1:275:B:LEU:HD13	1:312:B:PHE:HZ	13	0.1
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	8	0.1
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	13	0.1
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	16	0.1
(1,1195)	1:275:B:LEU:HB3	1:275:B:LEU:H	20	0.1
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD11	16	0.1
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD12	16	0.1
(1,1178)	1:274:B:PHE:HZ	1:277:B:LEU:HD13	16	0.1
(1,1155)	1:274:B:PHE:HB3	1:277:B:LEU:HD11	16	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1155)	1:274:B:PHE:HB3	1:277:B:LEU:HD12	16	0.1
(1,1155)	1:274:B:PHE:HB3	1:277:B:LEU:HD13	16	0.1
(1,1083)	1:271:B:GLN:HB3	1:271:B:GLN:H	7	0.1
(1,944)	1:256:B:ASN:HD21	1:256:B:ASN:HD22	2	0.1
(1,944)	1:256:B:ASN:HD21	1:256:B:ASN:HD22	3	0.1
(1,944)	1:256:B:ASN:HD21	1:256:B:ASN:HD22	4	0.1
(1,944)	1:256:B:ASN:HD21	1:256:B:ASN:HD22	18	0.1
(1,940)	1:256:B:ASN:HB3	1:256:B:ASN:H	18	0.1
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD1	5	0.1
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD2	5	0.1
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD1	5	0.1
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD2	5	0.1
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD1	20	0.1
(1,889)	1:253:B:PHE:HD1	1:364:B:PHE:HD2	20	0.1
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD1	20	0.1
(1,889)	1:253:B:PHE:HD2	1:364:B:PHE:HD2	20	0.1
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	1	0.1
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	2	0.1
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	10	0.1
(1,844)	1:251:B:ARG:HB3	1:251:B:ARG:H	19	0.1
(1,659)	1:239:B:LEU:HD21	1:244:B:SER:HB3	15	0.1
(1,659)	1:239:B:LEU:HD22	1:244:B:SER:HB3	15	0.1
(1,659)	1:239:B:LEU:HD23	1:244:B:SER:HB3	15	0.1
(1,609)	1:238:B:ARG:H	1:246:B:LYS:HA	7	0.1
(1,603)	1:238:B:ARG:HG2	1:287:B:GLN:HB2	15	0.1
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE1	1	0.1
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE2	1	0.1
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE1	1	0.1
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE2	1	0.1
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE1	1	0.1
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE2	1	0.1
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE1	20	0.1
(1,409)	1:232:B:LEU:HD11	1:274:B:PHE:HE2	20	0.1
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE1	20	0.1
(1,409)	1:232:B:LEU:HD12	1:274:B:PHE:HE2	20	0.1
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE1	20	0.1
(1,409)	1:232:B:LEU:HD13	1:274:B:PHE:HE2	20	0.1
(1,356)	1:225:B:ILE:HD11	1:226:B:GLY:H	1	0.1
(1,356)	1:225:B:ILE:HD12	1:226:B:GLY:H	1	0.1
(1,356)	1:225:B:ILE:HD13	1:226:B:GLY:H	1	0.1
(1,328)	1:222:B:ASN:HB2	1:222:B:ASN:H	3	0.1
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	6	0.1
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	13	0.1
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	15	0.1
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	16	0.1
(1,279)	1:218:B:THR:HB	1:218:B:THR:H	18	0.1
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG11	11	0.1
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG12	11	0.1
(1,162)	1:212:B:MET:HE1	1:365:B:VAL:HG13	11	0.1
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG11	11	0.1
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG12	11	0.1
(1,162)	1:212:B:MET:HE2	1:365:B:VAL:HG13	11	0.1
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG11	11	0.1
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG12	11	0.1
(1,162)	1:212:B:MET:HE3	1:365:B:VAL:HG13	11	0.1
(1,157)	1:212:B:MET:HE1	1:233:B:CYS:HB3	4	0.1
(1,157)	1:212:B:MET:HE2	1:233:B:CYS:HB3	4	0.1
(1,157)	1:212:B:MET:HE3	1:233:B:CYS:HB3	4	0.1
(1,157)	1:212:B:MET:HE1	1:233:B:CYS:HB3	17	0.1
(1,157)	1:212:B:MET:HE2	1:233:B:CYS:HB3	17	0.1
(1,157)	1:212:B:MET:HE3	1:233:B:CYS:HB3	17	0.1
(1,138)	1:212:B:MET:HB2	1:212:B:MET:H	1	0.1
(1,83)	1:209:B:ARG:HB3	1:209:B:ARG:HG2	16	0.1
(1,76)	1:209:B:ARG:HA	1:209:B:ARG:HB3	11	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	1	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	2	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	3	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	6	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	7	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	16	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	17	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	18	0.1
(1,52)	1:206:B:SER:HB2	1:206:B:SER:H	19	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found