



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 07:03 pm BST

PDB ID : 3ZTG  
BMRB ID : 17772  
Title : Solution structure of the RING finger-like domain of Retinoblastoma Binding Protein-6 (RBBP6)  
Authors : Kappo, M.A.; Ab, E.; Atkinson, R.A.; Faro, A.; Muleya, V.; Mulaudzi, T.; Poole, J.O.; McKenzie, J.M.; Pugh, D.J.R.  
Deposited on : 2011-07-07

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

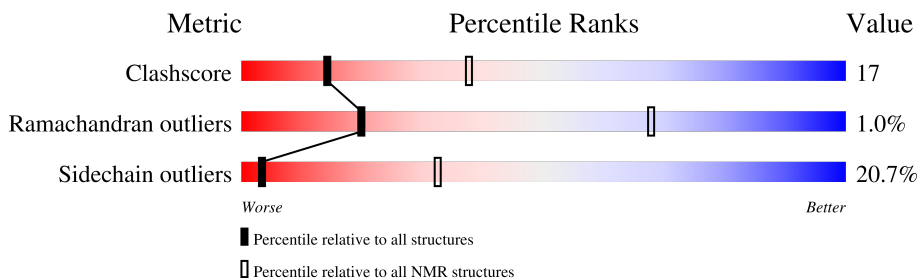
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 45%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	92	
1	B	92	

## 2 Ensemble composition and analysis i

This entry contains 32 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:253-A:322, B:255-B:319 (135)	0.30	17

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

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

The models can be grouped into 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 6, 12, 15, 16, 17, 18, 19, 21, 24, 29, 30, 31, 32
2	3, 7, 8, 9, 11, 23, 25, 26, 27, 28
3	10, 20, 22
4	2, 13
Single-model clusters	14

### 3 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2674 atoms, of which 1252 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBBP6.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	92	1335	435	626	122	143	9	0
1	B	92	1335	435	626	122	143	9	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP Q7Z6E9
A	245	PRO	-	expression tag	UNP Q7Z6E9
A	246	LEU	-	expression tag	UNP Q7Z6E9
A	247	GLY	-	expression tag	UNP Q7Z6E9
A	248	SER	-	expression tag	UNP Q7Z6E9
B	244	GLY	-	expression tag	UNP Q7Z6E9
B	245	PRO	-	expression tag	UNP Q7Z6E9
B	246	LEU	-	expression tag	UNP Q7Z6E9
B	247	GLY	-	expression tag	UNP Q7Z6E9
B	248	SER	-	expression tag	UNP Q7Z6E9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

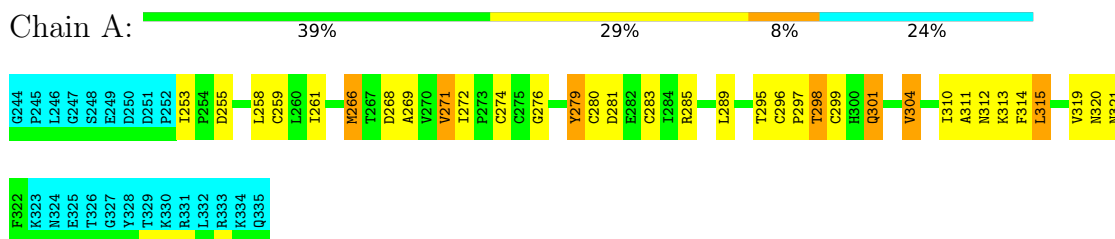
Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2
2	B	2	2	2

## 4 Residue-property plots [i](#)

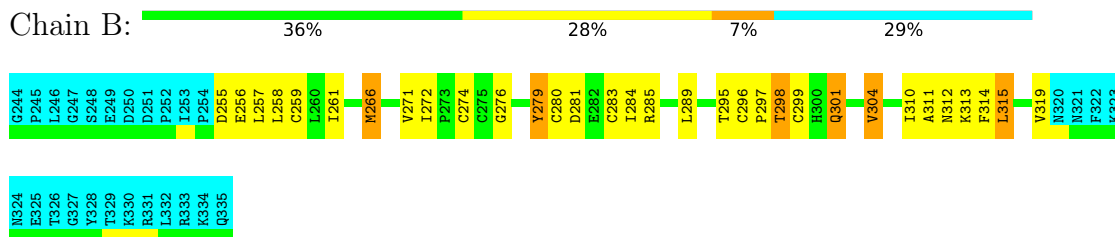
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

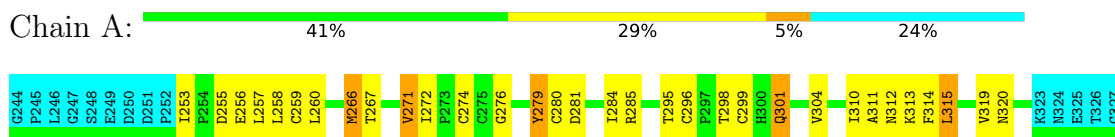


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

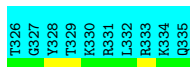
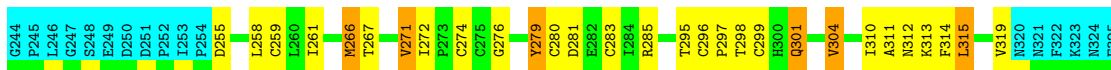
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6





- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

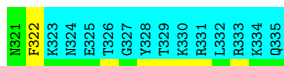
Chain B: 39% 25% 7% 29%



#### 4.2.2 Score per residue for model 2

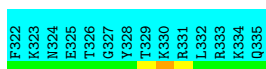
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A: 38% 29% 9% 24%



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain B: 38% 27% 5% 29%



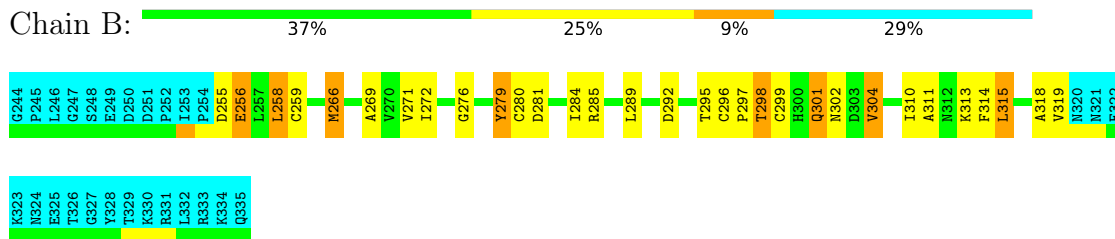
#### 4.2.3 Score per residue for model 3

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A: 41% 27% 8% 24%

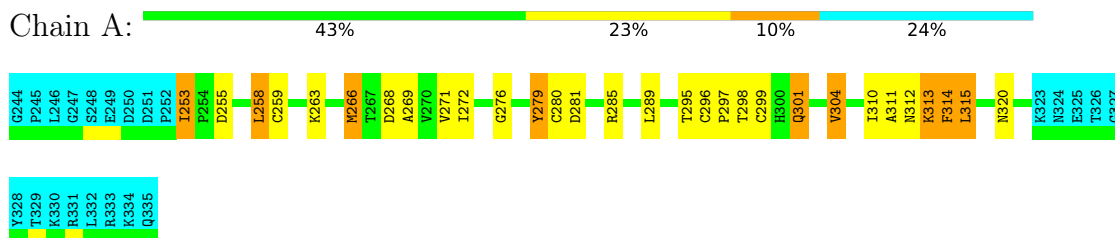


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

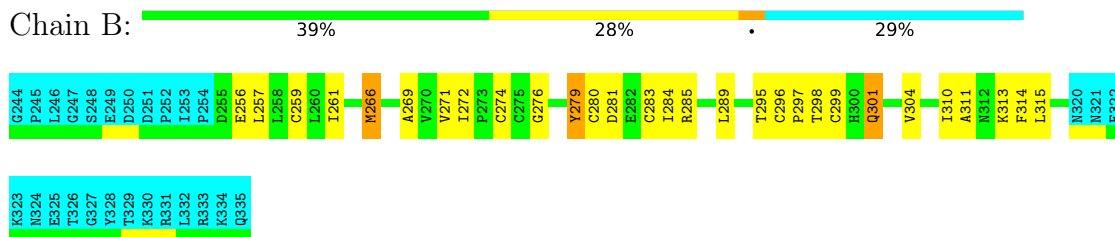


#### 4.2.4 Score per residue for model 4

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

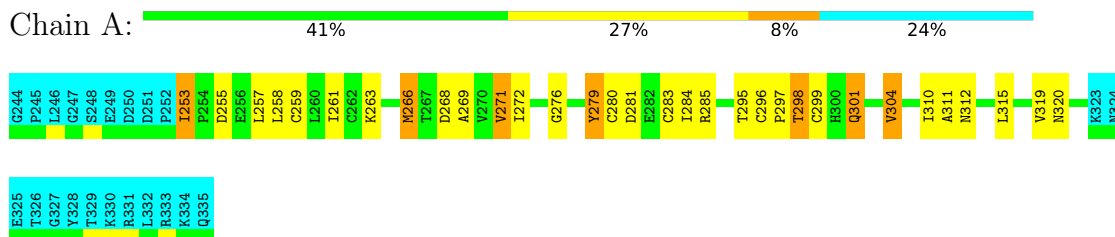


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

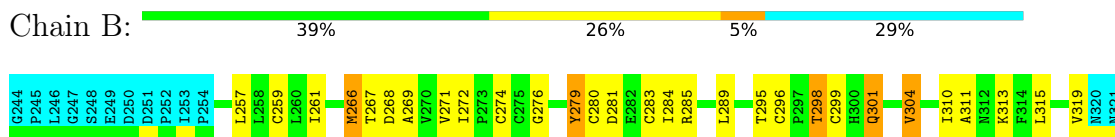


#### 4.2.5 Score per residue for model 5

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



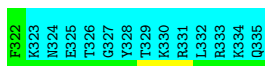
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



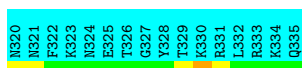
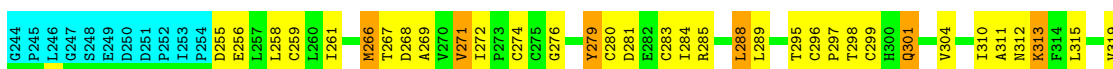


#### 4.2.6 Score per residue for model 6

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

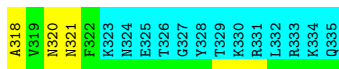
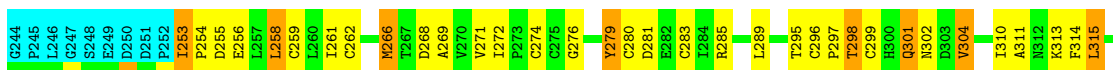


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



#### 4.2.7 Score per residue for model 7

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



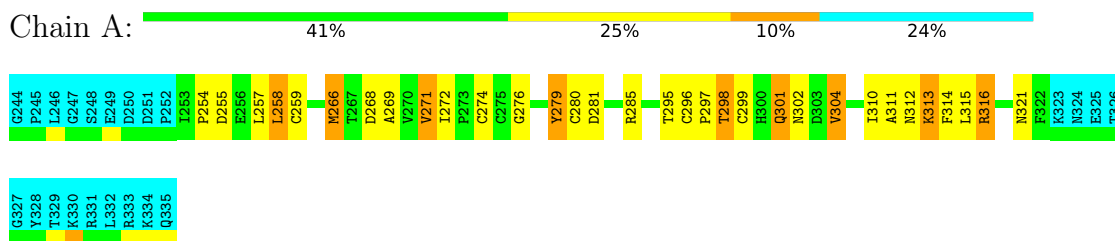
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



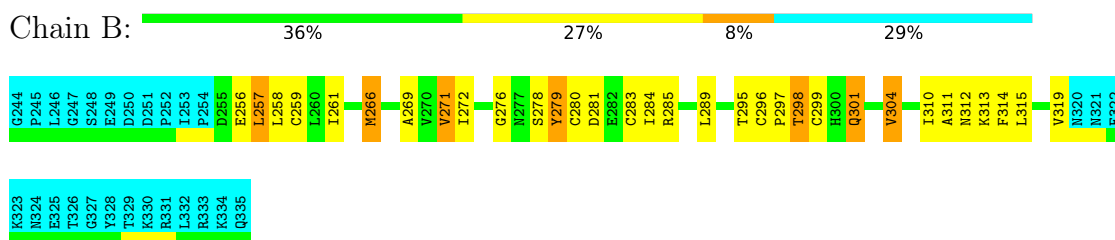


### 4.2.8 Score per residue for model 8

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

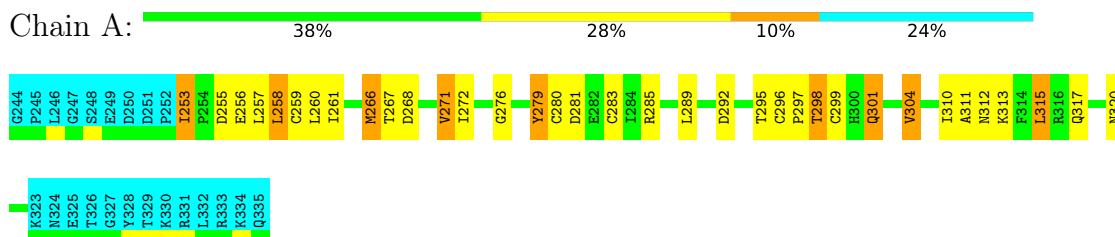


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

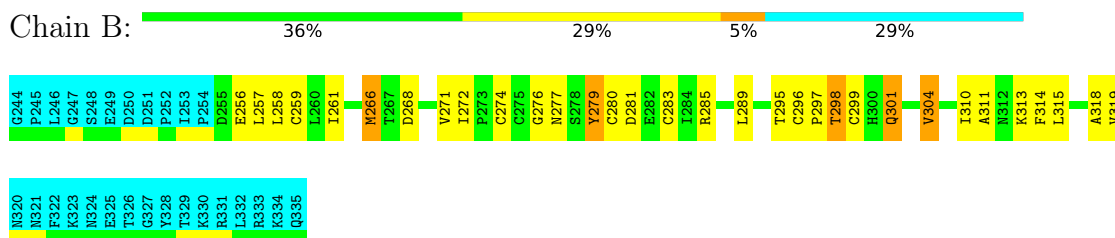


### 4.2.9 Score per residue for model 9

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

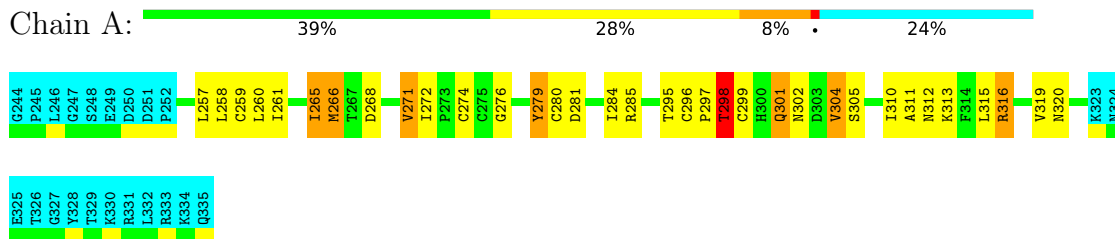


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

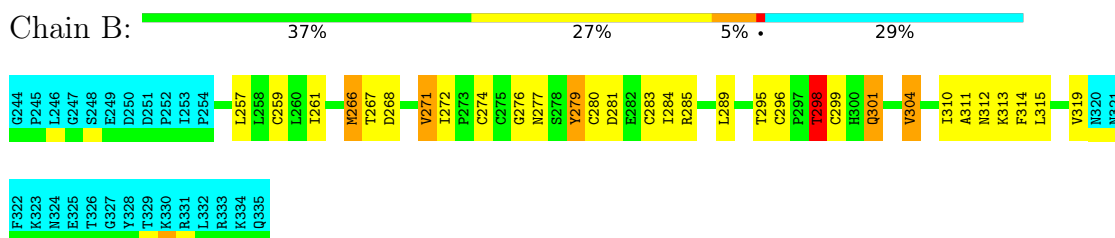


### 4.2.10 Score per residue for model 10

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

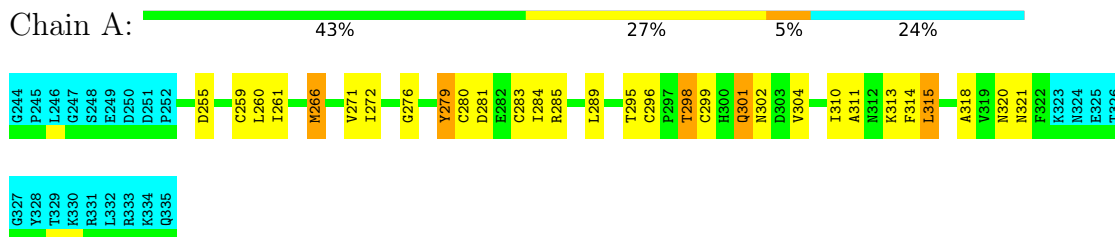


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

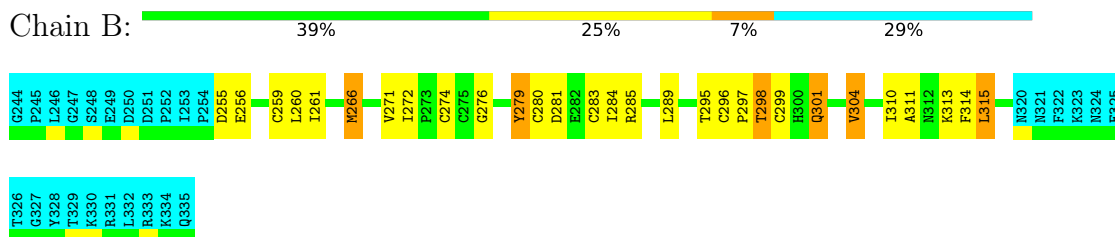


#### 4.2.11 Score per residue for model 11

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

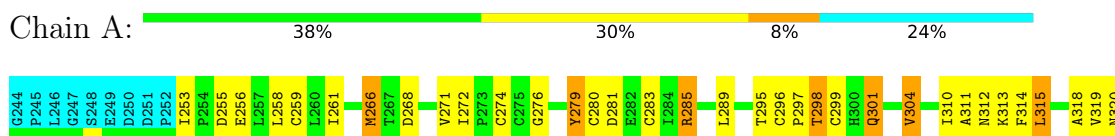


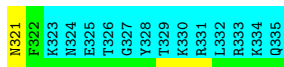
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



#### 4.2.12 Score per residue for model 12

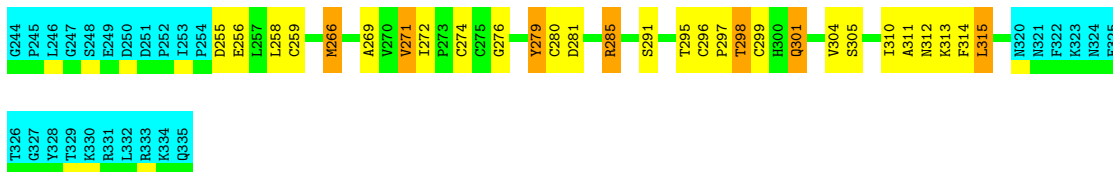
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6





• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

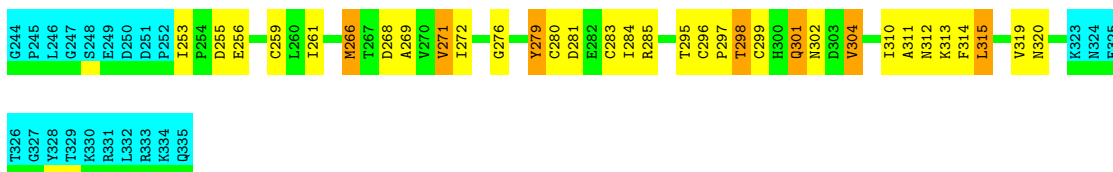
Chain B: 39% 24% 8% 29%



#### 4.2.13 Score per residue for model 13

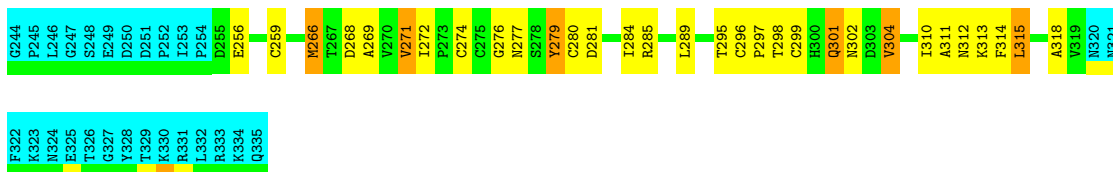
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A: 40% 28% 8% 24%



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

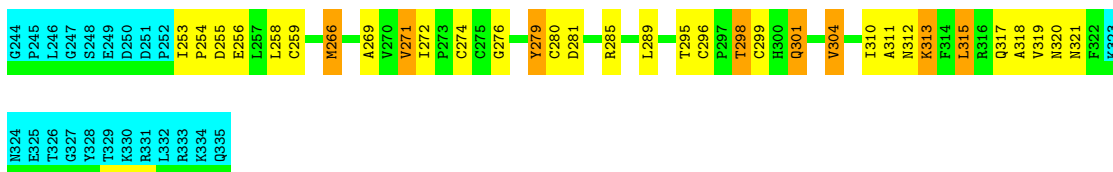
Chain B: 37% 27% 7% 29%



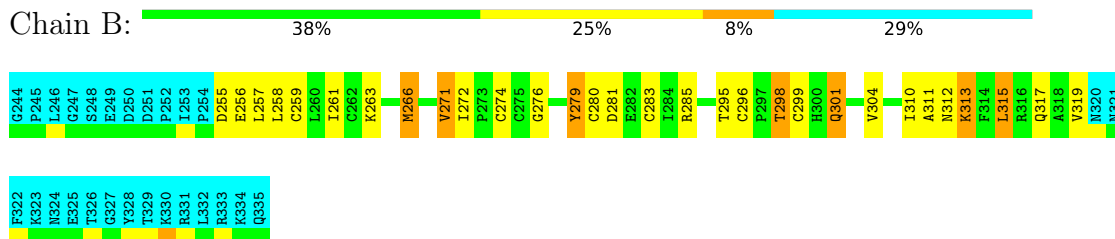
#### 4.2.14 Score per residue for model 14

• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A: 40% 27% 9% 24%

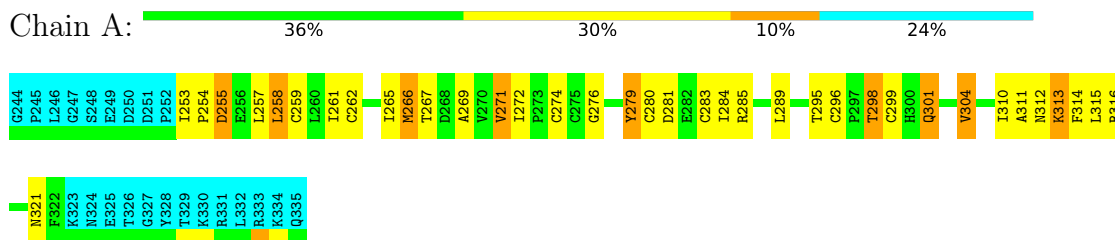


• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

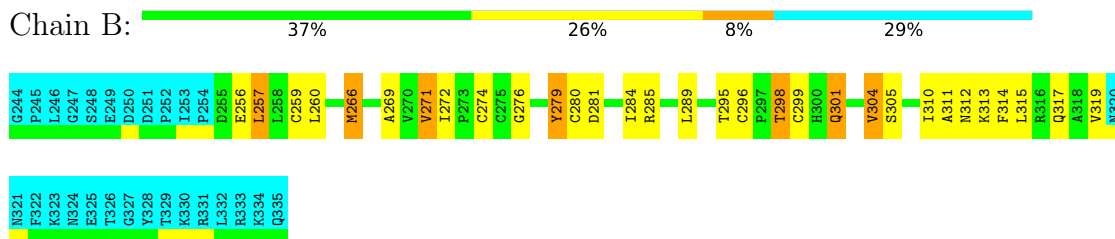


#### 4.2.15 Score per residue for model 15

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

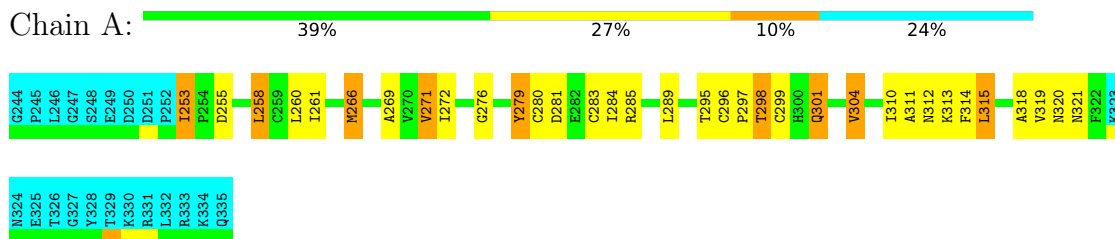


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

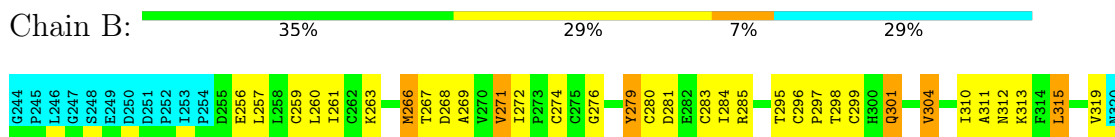


#### 4.2.16 Score per residue for model 16

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



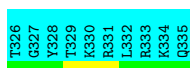
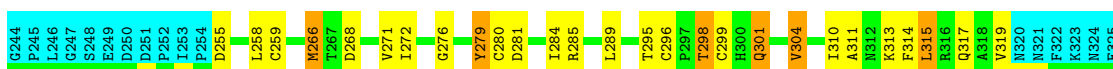


#### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

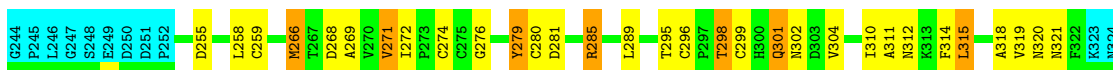


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

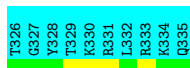
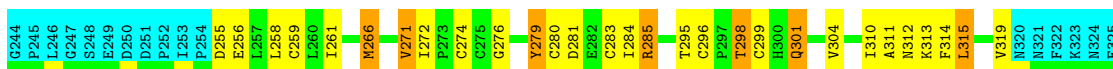
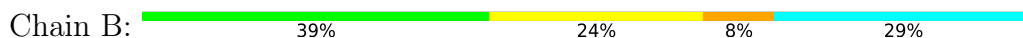


#### 4.2.18 Score per residue for model 18

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

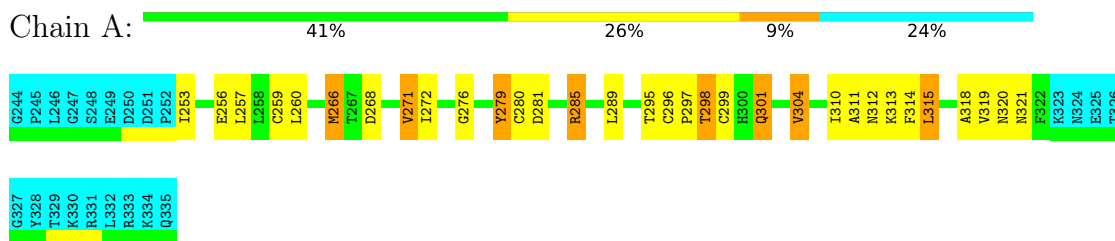


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

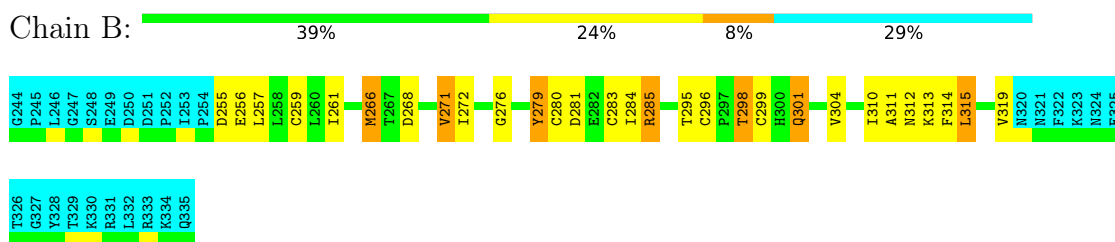


#### 4.2.19 Score per residue for model 19

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

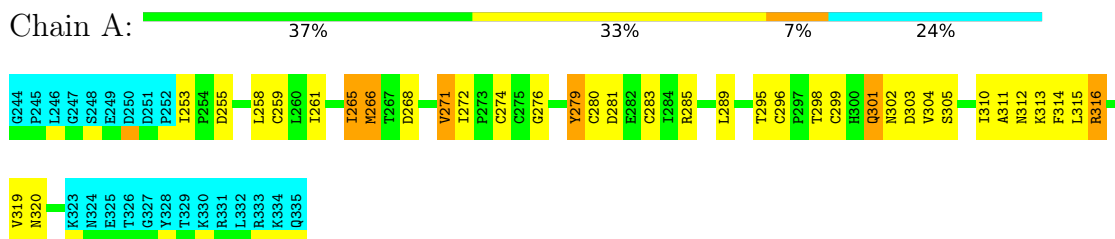


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

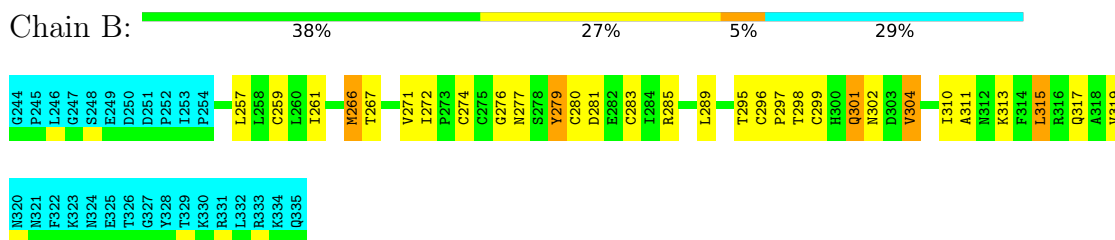


#### 4.2.20 Score per residue for model 20

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

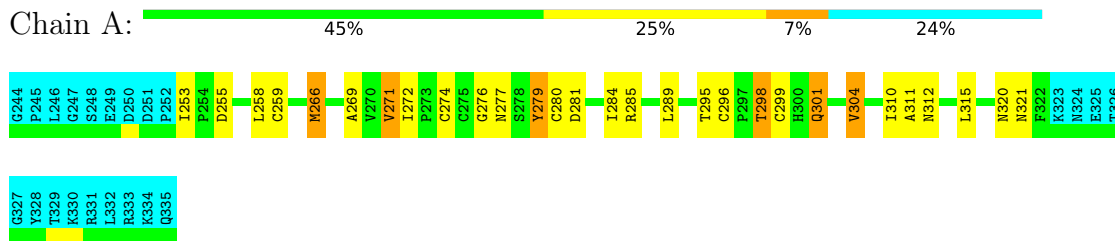


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

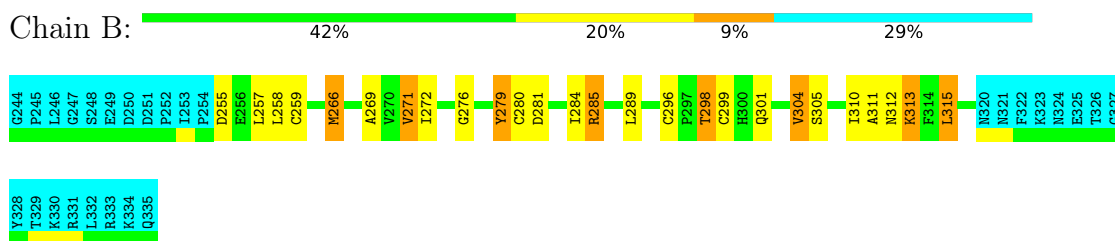


#### 4.2.21 Score per residue for model 21

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

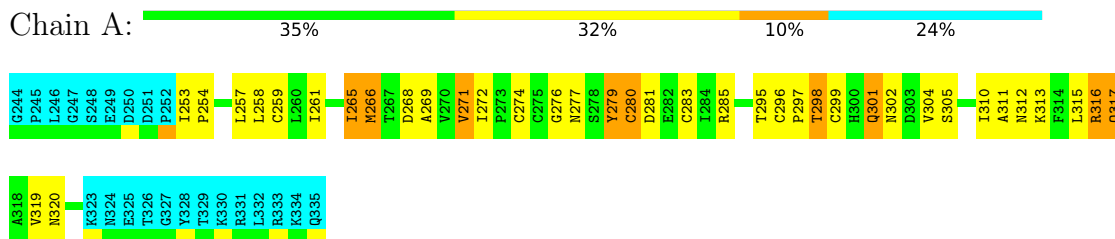


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

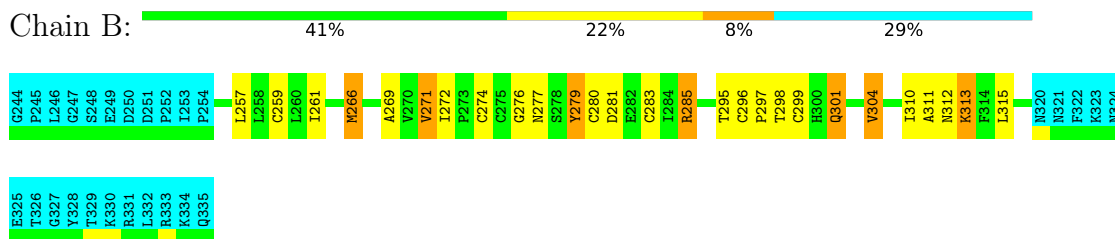


#### 4.2.22 Score per residue for model 22

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

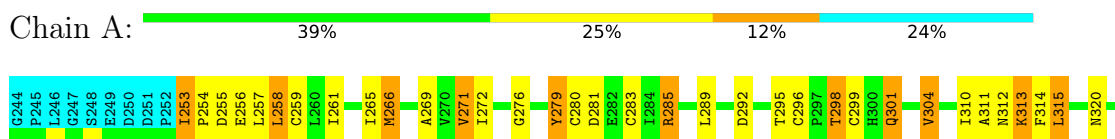


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



#### 4.2.23 Score per residue for model 23

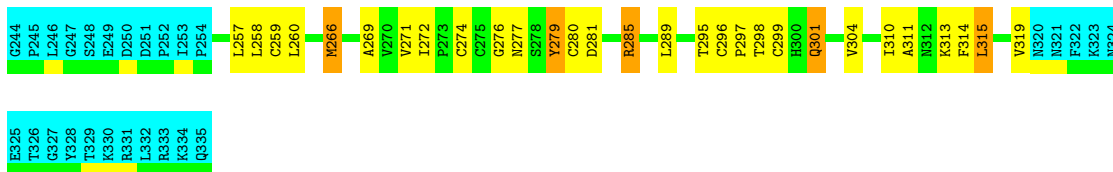
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6





- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

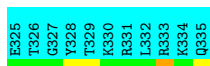
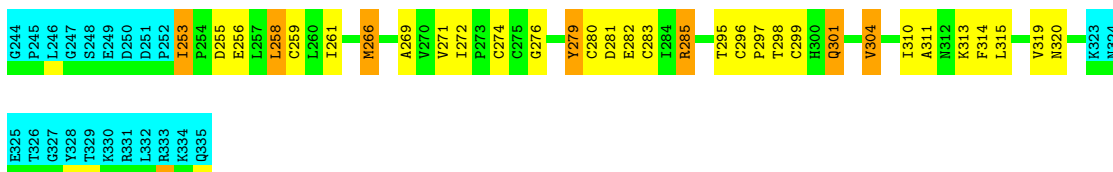
Chain B:



#### 4.2.24 Score per residue for model 24

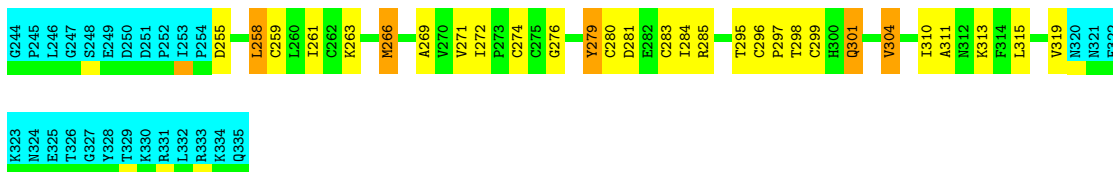
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A:



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

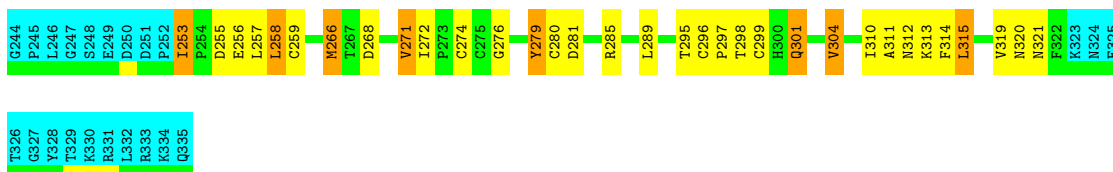
Chain B:



#### 4.2.25 Score per residue for model 25

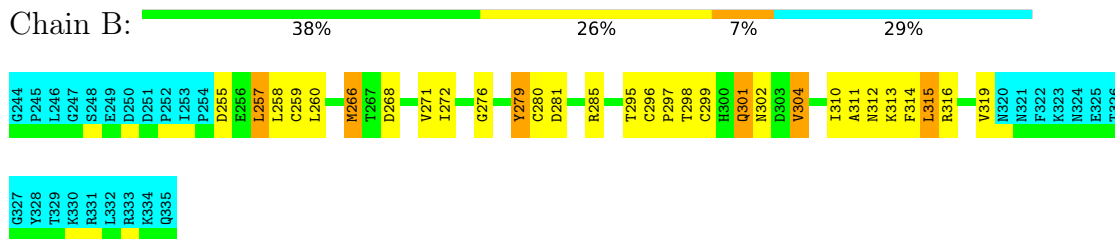
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

Chain A:



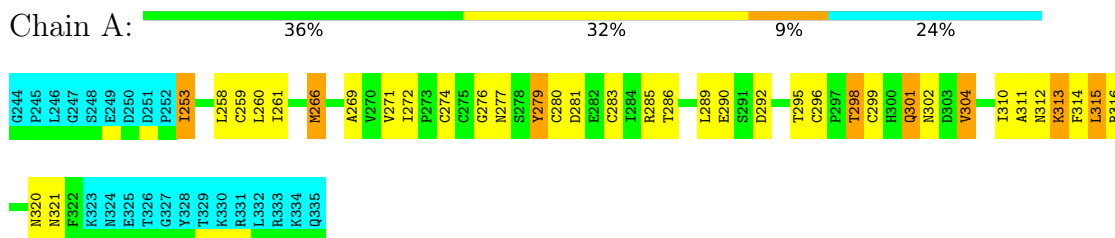
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



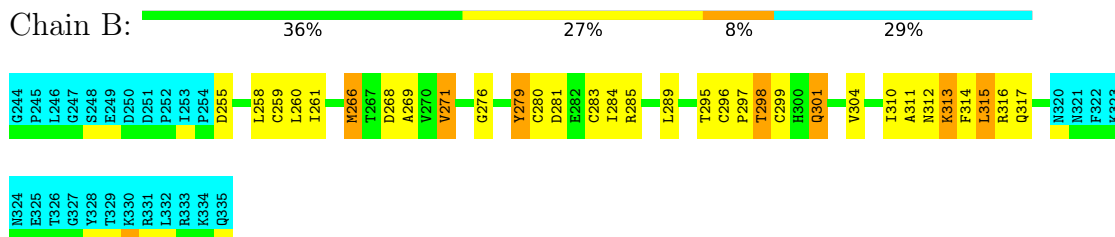


#### 4.2.26 Score per residue for model 26

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

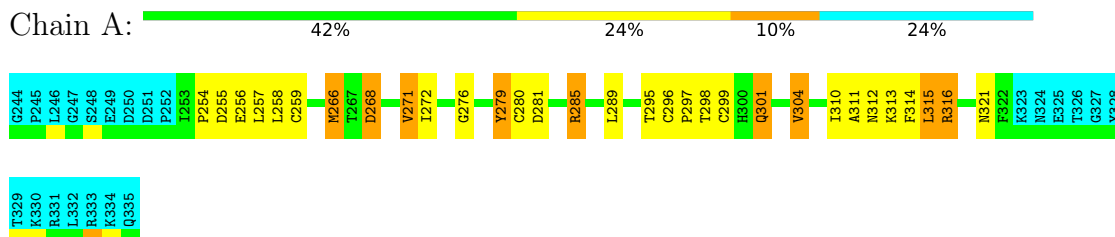


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

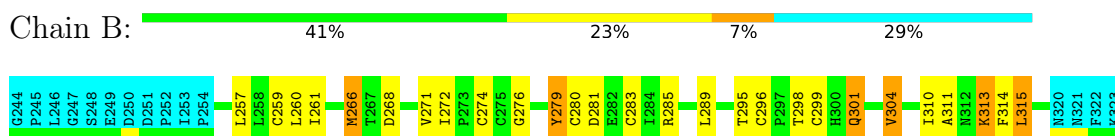


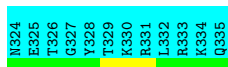
#### 4.2.27 Score per residue for model 27

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



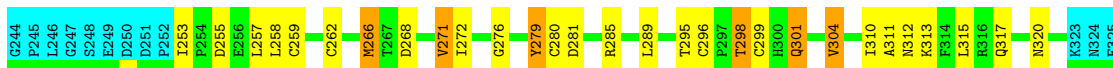
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



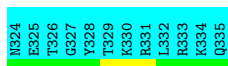


#### 4.2.28 Score per residue for model 28

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

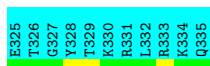


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

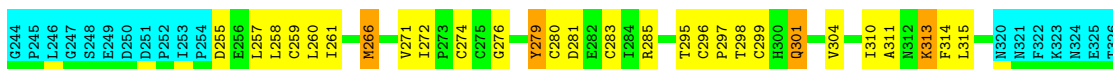


#### 4.2.29 Score per residue for model 29

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

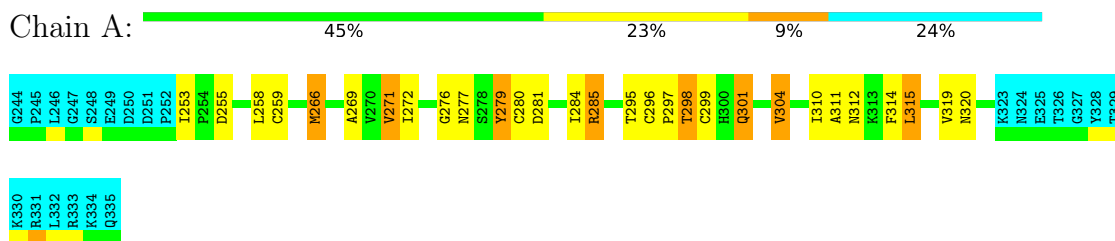


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

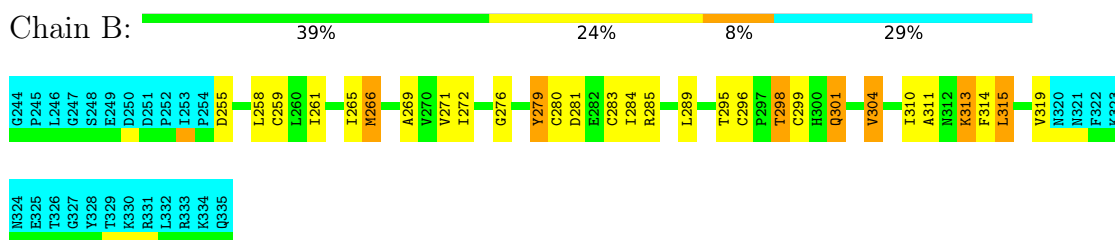


### 4.2.30 Score per residue for model 30

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

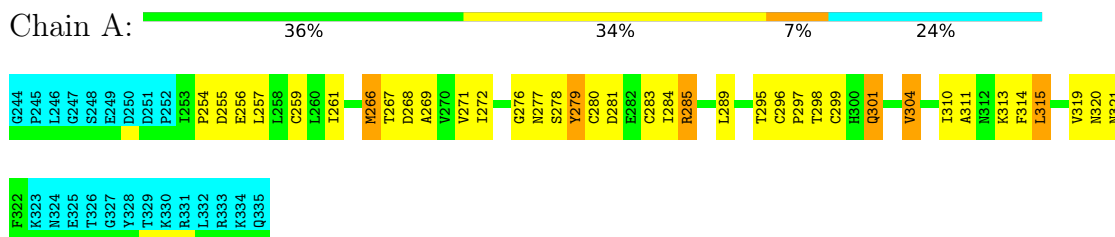


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

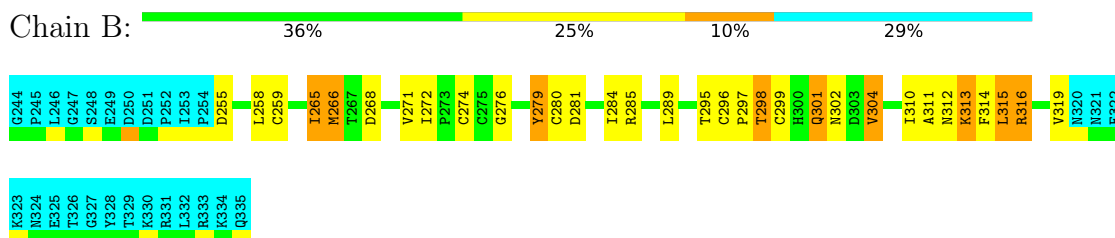


### 4.2.31 Score per residue for model 31

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

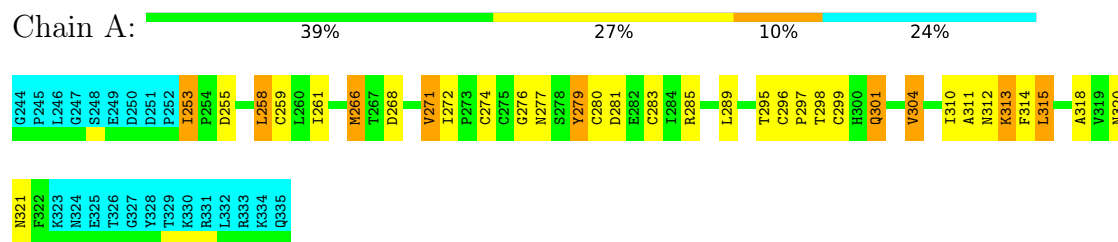


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6

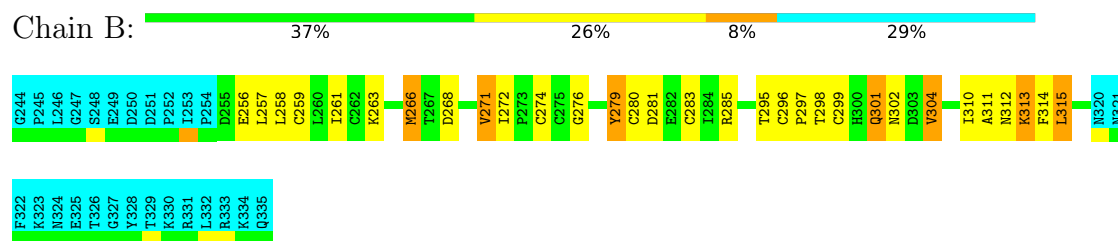


### 4.2.32 Score per residue for model 32

- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



● Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE RBBP6



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *CYANA FOLLOWED BY HADDOCK*.

Of the 400 calculated structures, 32 were deposited, based on the following criterion: *HADDOCK ENERGY, RAMACHANDRAN QUALITY*.

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

Software name	Classification	Version
CNS	refinement	2.1
CYANA	structure solution	
NMRView	structure solution	

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	1027
Number of shifts mapped to atoms	973
Number of unparsed shifts	0
Number of shifts with mapping errors	54
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

## 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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts i

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	535	454	510	20±3
1	B	493	420	471	19±2
All	All	33024	27968	31392	1118

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:266:MET:HB3	1:A:280:CYS:SG	0.80	2.15	31	32
1:B:266:MET:HB3	1:B:280:CYS:SG	0.80	2.16	20	32
1:A:271:VAL:HG22	1:A:312:ASN:HB2	0.75	1.57	28	24
1:B:296:CYS:SG	1:B:298:THR:HG22	0.75	2.21	24	32
1:A:296:CYS:SG	1:A:298:THR:HG22	0.74	2.23	3	32
1:A:253:ILE:HB	1:A:258:LEU:HD23	0.72	1.60	20	2
1:B:271:VAL:HG22	1:B:312:ASN:HB2	0.69	1.63	10	15
1:B:295:THR:HA	1:B:301:GLN:O	0.69	1.87	13	31
1:A:285:ARG:O	1:A:289:LEU:HG	0.67	1.90	23	19
1:A:261:ILE:HD12	1:A:283:CYS:HB3	0.66	1.68	22	18
1:A:295:THR:HA	1:A:301:GLN:O	0.66	1.90	2	32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:285:ARG:O	1:B:289:LEU:HG	0.65	1.91	4	18
1:B:259:CYS:SG	1:B:279:TYR:HB3	0.65	2.31	13	32
1:B:284:ILE:O	1:B:288:LEU:HD23	0.65	1.90	6	1
1:A:311:ALA:O	1:B:276:GLY:HA3	0.63	1.93	8	32
1:B:269:ALA:HB3	1:B:315:LEU:HD12	0.61	1.72	15	4
1:B:257:LEU:HA	1:B:315:LEU:HD21	0.61	1.72	5	3
1:A:260:LEU:HD12	1:A:279:TYR:CE2	0.61	2.30	10	1
1:A:276:GLY:HA3	1:B:311:ALA:O	0.61	1.96	11	32
1:B:272:ILE:HD12	1:B:284:ILE:HD11	0.61	1.73	10	18
1:A:272:ILE:HD12	1:A:284:ILE:HD11	0.60	1.72	16	13
1:B:272:ILE:HD11	1:B:304:VAL:HG11	0.60	1.70	21	14
1:A:253:ILE:HB	1:A:258:LEU:HD13	0.60	1.72	26	12
1:A:318:ALA:HA	1:B:256:GLU:OE1	0.60	1.96	11	1
1:A:259:CYS:SG	1:A:279:TYR:HB3	0.60	2.37	24	30
1:B:261:ILE:HD12	1:B:283:CYS:HB3	0.59	1.73	22	23
1:A:318:ALA:HA	1:B:256:GLU:OE2	0.59	1.98	14	8
1:A:269:ALA:HB3	1:A:315:LEU:HD12	0.58	1.75	5	3
1:A:281:ASP:O	1:A:285:ARG:HB2	0.58	1.98	9	32
1:A:313:LYS:HD3	1:B:277:ASN:OD1	0.58	1.99	9	8
1:B:281:ASP:O	1:B:285:ARG:HB2	0.57	1.99	10	32
1:A:315:LEU:HD21	1:B:314:PHE:CD2	0.57	2.34	4	19
1:A:314:PHE:CD2	1:B:315:LEU:HD21	0.56	2.35	27	17
1:A:315:LEU:HD21	1:B:314:PHE:HD2	0.55	1.59	2	8
1:B:266:MET:O	1:B:319:VAL:HG11	0.55	2.01	5	20
1:A:272:ILE:HG12	1:A:274:CYS:SG	0.54	2.43	24	19
1:A:266:MET:O	1:A:319:VAL:HG11	0.54	2.03	24	16
1:A:254:PRO:O	1:A:258:LEU:HB2	0.54	2.02	17	5
1:A:313:LYS:HA	1:A:316:ARG:CD	0.53	2.34	10	3
1:B:272:ILE:HG12	1:B:274:CYS:SG	0.52	2.45	6	22
1:A:272:ILE:HD11	1:A:304:VAL:HG11	0.51	1.81	16	13
1:A:314:PHE:HD2	1:B:315:LEU:HD21	0.50	1.66	27	5
1:A:268:ASP:HA	1:A:316:ARG:NH1	0.50	2.21	8	2
1:A:257:LEU:HA	1:A:315:LEU:HD21	0.50	1.83	5	1
1:A:277:ASN:OD1	1:B:313:LYS:HD3	0.49	2.06	30	9
1:B:266:MET:SD	1:B:315:LEU:HD11	0.49	2.47	8	2
1:A:266:MET:SD	1:A:315:LEU:HD11	0.49	2.48	8	2
1:A:298:THR:CG2	1:A:299:CYS:N	0.49	2.75	2	32
1:A:313:LYS:O	1:A:317:GLN:HG2	0.49	2.08	14	1
1:B:298:THR:CG2	1:B:299:CYS:N	0.49	2.76	25	31
1:B:296:CYS:SG	1:B:297:PRO:HD2	0.49	2.48	13	21
1:A:296:CYS:SG	1:A:297:PRO:HD2	0.49	2.47	25	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:314:PHE:CD1	1:B:314:PHE:N	0.48	2.81	25	12
1:A:253:ILE:O	1:A:258:LEU:HD12	0.48	2.07	17	1
1:A:313:LYS:HA	1:A:316:ARG:HD2	0.48	1.86	10	2
1:A:311:ALA:HB1	1:A:316:ARG:HH21	0.48	1.68	27	1
1:A:266:MET:SD	1:A:269:ALA:HB2	0.48	2.48	26	16
1:A:314:PHE:CD1	1:A:314:PHE:N	0.47	2.82	15	10
1:A:255:ASP:OD1	1:B:317:GLN:HG3	0.47	2.09	17	2
1:A:261:ILE:CD1	1:A:283:CYS:HB3	0.47	2.39	22	1
1:A:259:CYS:HB2	1:A:266:MET:CG	0.47	2.40	2	14
1:A:272:ILE:CG1	1:A:304:VAL:HG11	0.47	2.39	7	13
1:B:257:LEU:HA	1:B:315:LEU:CD2	0.47	2.39	8	1
1:B:272:ILE:CD1	1:B:304:VAL:HG11	0.47	2.40	21	1
1:A:254:PRO:HB2	1:A:256:GLU:OE1	0.46	2.09	7	5
1:A:256:GLU:OE1	1:B:318:ALA:HA	0.46	2.09	13	1
1:B:298:THR:HG23	1:B:299:CYS:N	0.46	2.26	4	15
1:B:272:ILE:CG1	1:B:304:VAL:HG11	0.46	2.40	3	16
1:B:313:LYS:HA	1:B:316:ARG:HD2	0.46	1.88	26	2
1:B:274:CYS:HB3	1:B:304:VAL:HG13	0.46	1.88	1	1
1:A:312:ASN:ND2	1:A:315:LEU:HB2	0.46	2.26	15	2
1:B:266:MET:SD	1:B:269:ALA:HB2	0.45	2.52	13	12
1:A:253:ILE:CG2	1:A:265:ILE:HD12	0.45	2.41	20	1
1:B:261:ILE:HG13	1:B:279:TYR:CD2	0.45	2.47	10	1
1:B:259:CYS:HB2	1:B:266:MET:CG	0.45	2.41	10	13
1:A:313:LYS:O	1:A:317:GLN:HB2	0.45	2.11	22	1
1:B:313:LYS:O	1:B:317:GLN:HG2	0.45	2.12	14	1
1:B:279:TYR:OH	1:B:298:THR:HG21	0.45	2.12	1	5
1:B:285:ARG:O	1:B:289:LEU:HD13	0.45	2.11	11	2
1:B:312:ASN:CG	1:B:315:LEU:HB2	0.44	2.33	25	3
1:A:312:ASN:CG	1:A:315:LEU:HB2	0.44	2.33	14	6
1:A:260:LEU:HD12	1:A:279:TYR:HE2	0.44	1.73	29	3
1:A:256:GLU:OE2	1:B:318:ALA:HA	0.44	2.12	3	1
1:A:254:PRO:O	1:A:258:LEU:HB3	0.44	2.12	6	2
1:A:313:LYS:NZ	1:A:313:LYS:HB3	0.44	2.25	8	5
1:B:280:CYS:O	1:B:284:ILE:HG22	0.44	2.13	6	5
1:A:298:THR:HG23	1:A:299:CYS:N	0.43	2.28	19	17
1:A:279:TYR:OH	1:A:298:THR:HG21	0.43	2.13	32	8
1:B:314:PHE:N	1:B:314:PHE:CD1	0.43	2.86	27	6
1:B:261:ILE:CD1	1:B:283:CYS:HB3	0.43	2.42	10	1
1:A:312:ASN:O	1:A:316:ARG:HG2	0.43	2.14	26	1
1:A:253:ILE:HD12	1:A:265:ILE:HB	0.43	1.90	15	1
1:A:253:ILE:HB	1:A:258:LEU:CD1	0.42	2.43	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:314:PHE:N	1:B:314:PHE:HD1	0.42	2.12	25	1
1:B:312:ASN:ND2	1:B:315:LEU:HB2	0.42	2.29	8	1
1:B:269:ALA:HB3	1:B:315:LEU:CD1	0.42	2.43	15	1
1:A:253:ILE:HG21	1:A:265:ILE:HB	0.42	1.91	23	1
1:A:257:LEU:HA	1:A:315:LEU:CD2	0.42	2.45	5	1
1:B:260:LEU:HD12	1:B:279:TYR:HE2	0.41	1.75	15	3
1:A:314:PHE:N	1:A:314:PHE:CD1	0.41	2.88	19	4
1:A:312:ASN:ND2	1:A:315:LEU:HD23	0.41	2.31	27	1
1:B:313:LYS:NZ	1:B:313:LYS:HB3	0.41	2.28	27	1
1:A:279:TYR:OH	1:A:298:THR:CG2	0.41	2.69	22	13
1:A:286:THR:O	1:A:290:GLU:HG3	0.41	2.15	26	1
1:B:288:LEU:N	1:B:288:LEU:CD2	0.41	2.84	6	1
1:B:257:LEU:HA	1:B:315:LEU:HD11	0.41	1.91	21	2
1:B:279:TYR:OH	1:B:298:THR:CG2	0.41	2.69	4	5
1:B:296:CYS:HB3	1:B:301:GLN:H	0.41	1.75	10	1
1:A:314:PHE:N	1:A:314:PHE:HD1	0.41	2.13	15	1
1:A:285:ARG:O	1:A:289:LEU:HD13	0.41	2.16	4	1
1:B:304:VAL:HG12	1:B:305:SER:H	0.41	1.75	21	1
1:A:259:CYS:HB2	1:A:266:MET:HG3	0.41	1.93	2	2
1:B:259:CYS:SG	1:B:261:ILE:HB	0.41	2.56	16	1
1:A:260:LEU:HD13	1:A:298:THR:OG1	0.40	2.15	10	1
1:A:261:ILE:HG13	1:A:279:TYR:CD2	0.40	2.50	10	1
1:A:253:ILE:CD1	1:A:265:ILE:HB	0.40	2.46	3	1
1:A:256:GLU:HG2	1:B:318:ALA:CA	0.40	2.47	9	1
1:A:269:ALA:HB3	1:A:315:LEU:CD1	0.40	2.46	15	1
1:A:314:PHE:CB	1:B:315:LEU:HD21	0.40	2.47	16	1
1:A:253:ILE:CB	1:A:258:LEU:HD23	0.40	2.38	20	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/92 (76%)	62±1 (88±1%)	7±1 (11±1%)	1±1 (1±1%)	18	66
1	B	65/92 (71%)	57±1 (87±1%)	8±1 (12±2%)	1±0 (1±1%)	21	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4320/5888 (73%)	3796 (88%)	482 (11%)	42 (1%)	20 68

All 4 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	298	THR	21
1	B	298	THR	18
1	A	304	VAL	2
1	A	303	ASP	1

### 6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	64/83 (77%)	50±2 (78±2%)	14±2 (22±2%)	3 29
1	B	59/83 (71%)	48±1 (81±2%)	11±1 (19±2%)	4 36
All	All	3936/5312 (74%)	3122 (79%)	814 (21%)	3 32

All 59 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	266	MET	32
1	A	271	VAL	32
1	A	279	TYR	32
1	A	301	GLN	32
1	A	304	VAL	32
1	A	310	ILE	32
1	B	266	MET	32
1	B	271	VAL	32
1	B	279	TYR	32
1	B	301	GLN	32
1	B	304	VAL	32
1	B	310	ILE	32
1	B	313	LYS	32

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Mol	Chain	Res	Type	Models (Total)
1	A	315	LEU	29
1	A	255	ASP	28
1	A	320	ASN	28
1	B	315	LEU	28
1	A	258	LEU	21
1	A	253	ILE	20
1	A	313	LYS	20
1	A	268	ASP	18
1	B	255	ASP	17
1	B	257	LEU	17
1	A	321	ASN	17
1	A	257	LEU	15
1	B	268	ASP	14
1	B	258	LEU	13
1	A	302	ASN	11
1	A	285	ARG	9
1	A	316	ARG	7
1	B	285	ARG	7
1	A	256	GLU	6
1	B	267	THR	6
1	B	302	ASN	6
1	B	260	LEU	6
1	A	260	LEU	5
1	A	267	THR	4
1	B	256	GLU	4
1	A	292	ASP	4
1	A	305	SER	4
1	B	263	LYS	4
1	A	263	LYS	3
1	A	262	CYS	3
1	A	317	GLN	3
1	A	265	ILE	3
1	A	298	THR	2
1	B	305	SER	2
1	B	317	GLN	2
1	B	316	ARG	2
1	B	292	ASP	1
1	A	314	PHE	1
1	B	288	LEU	1
1	B	278	SER	1
1	B	298	THR	1
1	B	291	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	280	CYS	1
1	A	282	GLU	1
1	A	278	SER	1
1	B	265	ILE	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 i

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 43% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *rring-new.bmr.b.csh*

#### 7.1.1 Bookkeeping i

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

Total number of shifts	1027
Number of shifts mapped to atoms	973
Number of unparsed shifts	0
Number of shifts with mapping errors	54
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. All 54 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	253	ILE	HG21	0.509	0.020	1
1	A	253	ILE	HG22	0.509	0.020	1
1	A	253	ILE	HG23	0.509	0.020	1
1	A	253	ILE	HG12	0.944	0.020	.
1	A	253	ILE	HG13	1.489	0.020	.
1	A	261	ILE	HG21	0.969	0.020	1
1	A	261	ILE	HG22	0.969	0.020	1
1	A	261	ILE	HG23	0.969	0.020	1
1	A	261	ILE	HG12	1.04	0.020	.
1	A	261	ILE	HG13	1.714	0.020	.
1	A	265	ILE	HG21	0.915	0.020	1
1	A	265	ILE	HG22	0.915	0.020	1
1	A	265	ILE	HG23	0.915	0.020	1
1	A	265	ILE	HG12	1.2	0.020	.

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	265	ILE	HG13	1.545	0.020	.
1	A	270	VAL	HG11	1.022	0.020	.
1	A	270	VAL	HG12	1.022	0.020	.
1	A	270	VAL	HG13	1.022	0.020	.
1	A	270	VAL	HG21	0.986	0.020	.
1	A	270	VAL	HG22	0.986	0.020	.
1	A	270	VAL	HG23	0.986	0.020	.
1	A	271	VAL	HG11	0.884	0.020	.
1	A	271	VAL	HG12	0.884	0.020	.
1	A	271	VAL	HG13	0.884	0.020	.
1	A	271	VAL	HG21	0.873	0.020	.
1	A	271	VAL	HG22	0.873	0.020	.
1	A	271	VAL	HG23	0.873	0.020	.
1	A	272	ILE	HG21	1.732	0.020	1
1	A	272	ILE	HG22	1.732	0.020	1
1	A	272	ILE	HG23	1.732	0.020	1
1	A	272	ILE	HG12	1.519	0.020	.
1	A	272	ILE	HG13	2.422	0.020	.
1	A	284	ILE	HG21	1.048	0.020	1
1	A	284	ILE	HG22	1.048	0.020	1
1	A	284	ILE	HG23	1.048	0.020	1
1	A	284	ILE	HG12	0.865	0.020	.
1	A	284	ILE	HG13	0.957	0.020	.
1	A	304	VAL	HG11	0.837	0.020	.
1	A	304	VAL	HG12	0.837	0.020	.
1	A	304	VAL	HG13	0.837	0.020	.
1	A	304	VAL	HG21	0.965	0.020	.
1	A	304	VAL	HG22	0.965	0.020	.
1	A	304	VAL	HG23	0.965	0.020	.
1	A	310	ILE	HG21	0.97	0.020	1
1	A	310	ILE	HG22	0.97	0.020	1
1	A	310	ILE	HG23	0.97	0.020	1
1	A	310	ILE	HG12	1.169	0.020	.
1	A	310	ILE	HG13	1.669	0.020	.
1	A	319	VAL	HG11	1.14	0.020	1
1	A	319	VAL	HG12	1.14	0.020	1
1	A	319	VAL	HG13	1.14	0.020	1
1	A	319	VAL	HG21	1.14	0.020	1
1	A	319	VAL	HG22	1.14	0.020	1
1	A	319	VAL	HG23	1.14	0.020	1

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	92	$-0.41 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	88	$-0.09 \pm 0.23$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	83	$-1.00 \pm 0.22$	Should be applied

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 45%, i.e. 787 atoms were assigned a chemical shift out of a possible 1736. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	269/663 (41%)	135/265 (51%)	70/270 (26%)	64/128 (50%)
Sidechain	488/1001 (49%)	333/653 (51%)	146/320 (46%)	9/28 (32%)
Aromatic	30/72 (42%)	18/39 (46%)	12/33 (36%)	0/0 (—%)
Overall	787/1736 (45%)	486/957 (51%)	228/623 (37%)	73/156 (47%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 1026 atoms were assigned a chemical shift out of a possible 2396. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	354/904 (39%)	179/364 (49%)	92/368 (25%)	83/172 (48%)
Sidechain	636/1392 (46%)	429/898 (48%)	194/442 (44%)	13/52 (25%)
Aromatic	36/100 (36%)	22/52 (42%)	14/48 (29%)	0/0 (—%)
Overall	1026/2396 (43%)	630/1314 (48%)	300/858 (35%)	96/224 (43%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

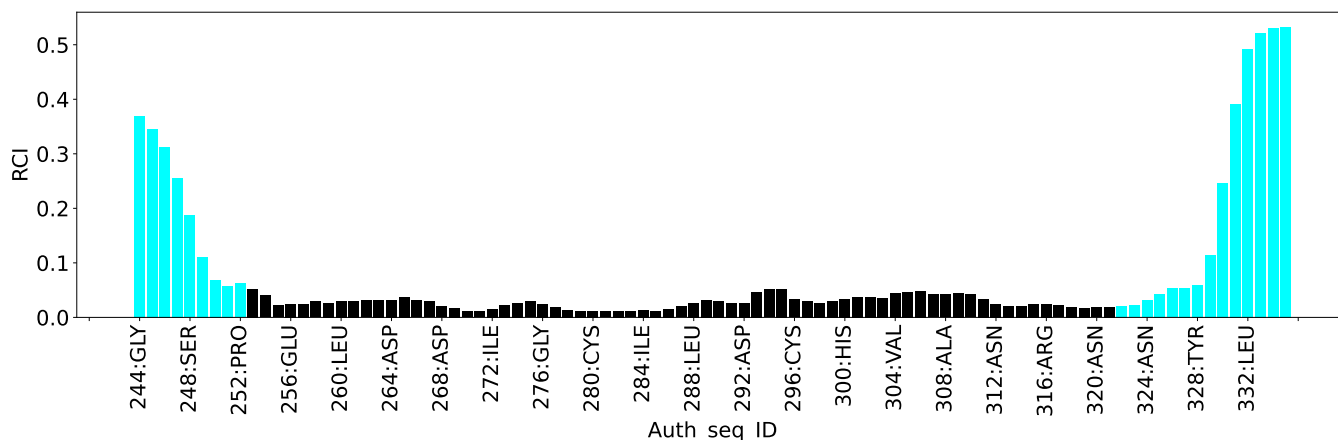
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	335	GLN	CD	21.34	173.59 – 185.85	-129.2

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

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

Random coil index (RCI) for chain A:





## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	5274
Intra-residue ( $ i-j =0$ )	1031
Sequential ( $ i-j =1$ )	1308
Medium range ( $ i-j >1$ and $ i-j <5$ )	1058
Long range ( $ i-j \geq 5$ )	1731
Inter-chain	146
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	911
Number of restraints per residue	28.7
Number of long range restraints per residue <sup>1</sup>	9.4

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

### 8.2 Residual restraint violations

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)	34.5	0.2
0.2-0.5 (Medium)	7.1	0.45
>0.5 (Large)	0.0	0.52

### 8.2.2 Average number of dihedral-angle violations per model

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis [i](#)

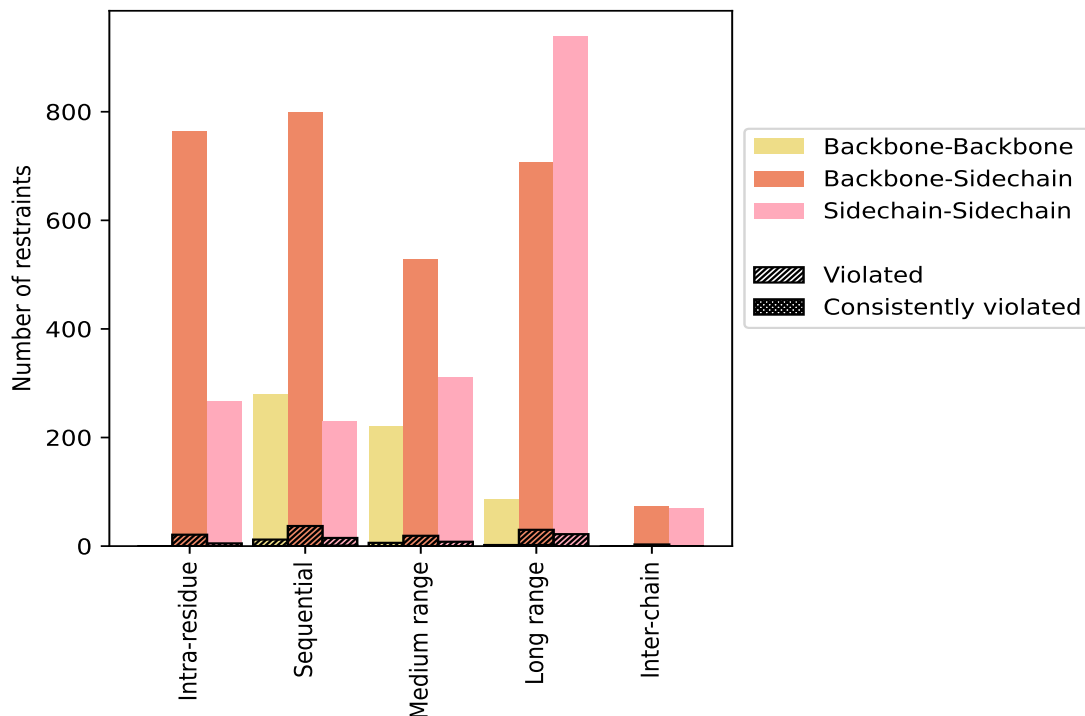
### 9.1 Summary of distance violations [i](#)

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

Restrains type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
<b>Intra-residue (<math> i-j =0</math>)</b>	<b>1031</b>	<b>19.5</b>	<b>26</b>	<b>2.5</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	2	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	763	14.5	21	2.8	0.4	0	0.0	0.0
Sidechain-Sidechain	266	5.0	5	1.9	0.1	0	0.0	0.0
<b>Sequential (<math> i-j =1</math>)</b>	<b>1308</b>	<b>24.8</b>	<b>64</b>	<b>4.9</b>	<b>1.2</b>	<b>1</b>	<b>0.1</b>	<b>0.0</b>
Backbone-Backbone	280	5.3	12	4.3	0.2	0	0.0	0.0
Backbone-Sidechain	799	15.1	37	4.6	0.7	0	0.0	0.0
Sidechain-Sidechain	229	4.3	15	6.6	0.3	1	0.4	0.0
<b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b>	<b>1058</b>	<b>20.1</b>	<b>33</b>	<b>3.1</b>	<b>0.6</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	220	4.2	6	2.7	0.1	0	0.0	0.0
Backbone-Sidechain	528	10.0	19	3.6	0.4	0	0.0	0.0
Sidechain-Sidechain	310	5.9	8	2.6	0.2	0	0.0	0.0
<b>Long range (<math> i-j \geq 5</math>)</b>	<b>1731</b>	<b>32.8</b>	<b>54</b>	<b>3.1</b>	<b>1.0</b>	<b>2</b>	<b>0.1</b>	<b>0.0</b>
Backbone-Backbone	86	1.6	2	2.3	0.0	0	0.0	0.0
Backbone-Sidechain	706	13.4	30	4.2	0.6	2	0.3	0.0
Sidechain-Sidechain	939	17.8	22	2.3	0.4	0	0.0	0.0
<b>Inter-chain</b>	<b>146</b>	<b>2.8</b>	<b>3</b>	<b>2.1</b>	<b>0.1</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	2	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	74	1.4	3	4.1	0.1	0	0.0	0.0
Sidechain-Sidechain	70	1.3	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
<b>Total</b>	<b>5274</b>	<b>100.0</b>	<b>180</b>	<b>3.4</b>	<b>3.4</b>	<b>3</b>	<b>0.1</b>	<b>0.1</b>
Backbone-Backbone	590	11.2	20	3.4	0.4	0	0.0	0.0
Backbone-Sidechain	2870	54.4	110	3.8	2.1	2	0.1	0.0
Sidechain-Sidechain	1814	34.4	50	2.8	0.9	1	0.1	0.0

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> 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 <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	7	16	7	14	0	44	0.16	0.23	0.04	0.15
2	6	14	8	11	0	39	0.16	0.42	0.05	0.15
3	7	14	7	16	1	45	0.16	0.43	0.06	0.13
4	6	11	2	14	2	35	0.18	0.44	0.06	0.18
5	7	10	8	14	0	39	0.16	0.42	0.06	0.16
6	5	17	3	11	0	36	0.17	0.43	0.07	0.15
7	7	13	4	17	1	42	0.16	0.43	0.05	0.15
8	5	15	7	16	0	43	0.18	0.52	0.09	0.15
9	4	11	3	16	0	34	0.17	0.44	0.06	0.15
10	7	20	8	16	0	51	0.17	0.45	0.07	0.15
11	7	12	4	19	0	42	0.16	0.44	0.06	0.14

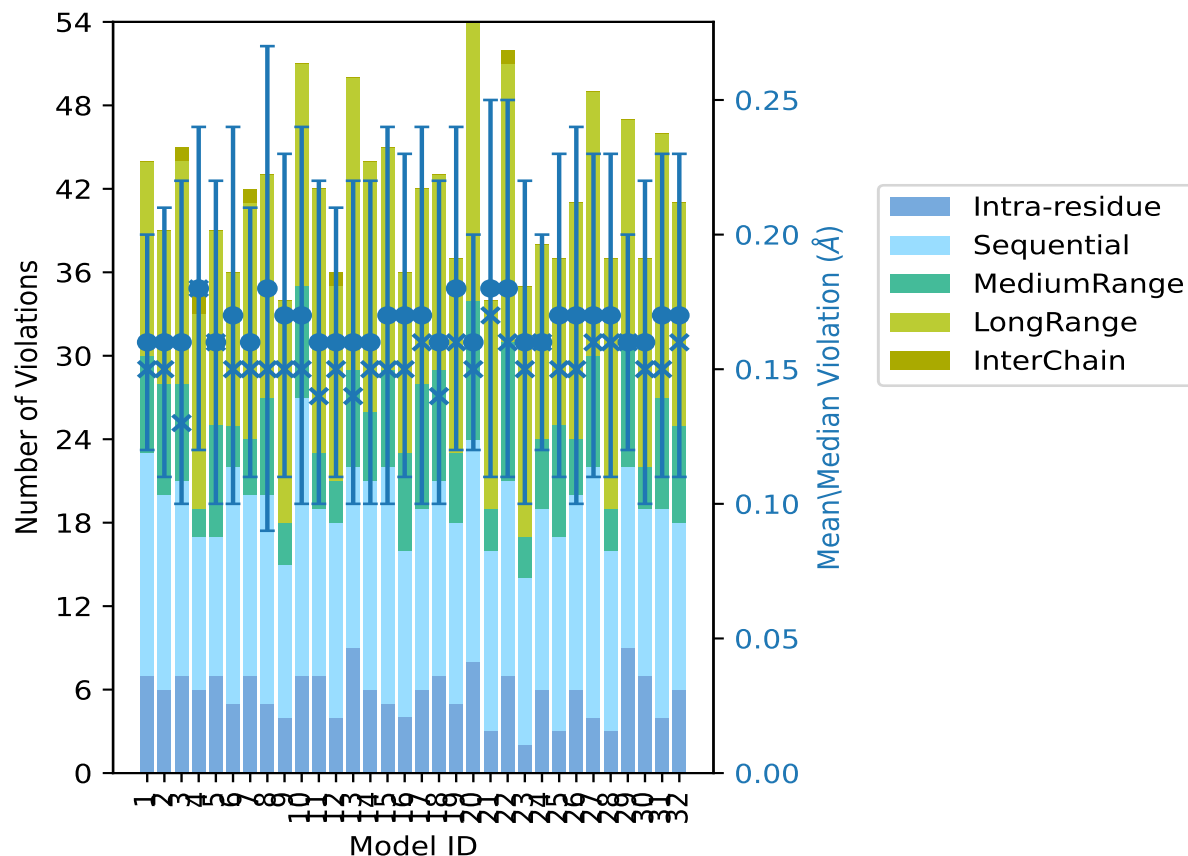
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
12	4	14	3	14	1	36	0.16	0.4	0.05	0.15
13	9	13	7	21	0	50	0.16	0.43	0.06	0.14
14	6	15	5	18	0	44	0.16	0.43	0.06	0.15
15	5	17	7	16	0	45	0.17	0.44	0.07	0.15
16	4	12	7	13	0	36	0.17	0.43	0.06	0.15
17	6	13	9	14	0	42	0.17	0.45	0.07	0.16
18	7	14	8	14	0	43	0.16	0.44	0.06	0.14
19	5	13	5	14	0	37	0.18	0.43	0.06	0.16
20	8	16	10	20	0	54	0.16	0.3	0.04	0.15
21	3	13	3	15	0	34	0.18	0.42	0.07	0.17
22	7	14	10	20	1	52	0.18	0.45	0.07	0.16
23	2	12	3	18	0	35	0.16	0.43	0.06	0.15
24	6	13	5	14	0	38	0.16	0.25	0.04	0.16
25	3	14	8	12	0	37	0.17	0.42	0.06	0.15
26	6	14	4	17	0	41	0.17	0.43	0.07	0.15
27	4	18	8	19	0	49	0.17	0.43	0.06	0.16
28	3	13	3	18	0	37	0.17	0.42	0.06	0.16
29	9	13	9	16	0	47	0.16	0.23	0.04	0.16
30	7	12	3	15	0	37	0.16	0.42	0.06	0.15
31	4	15	8	19	0	46	0.17	0.43	0.06	0.15
32	6	12	7	16	0	41	0.17	0.43	0.06	0.16

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

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



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

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 5094(IR:1005, SQ:1244, MR:1025, LR:1677, IC:143) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
7	23	10	16	2	58	1	3.1
4	9	5	9	0	27	2	6.2
0	3	2	3	0	8	3	9.4
1	5	3	3	1	13	4	12.5
2	3	4	0	0	9	5	15.6
0	0	1	2	0	3	6	18.8

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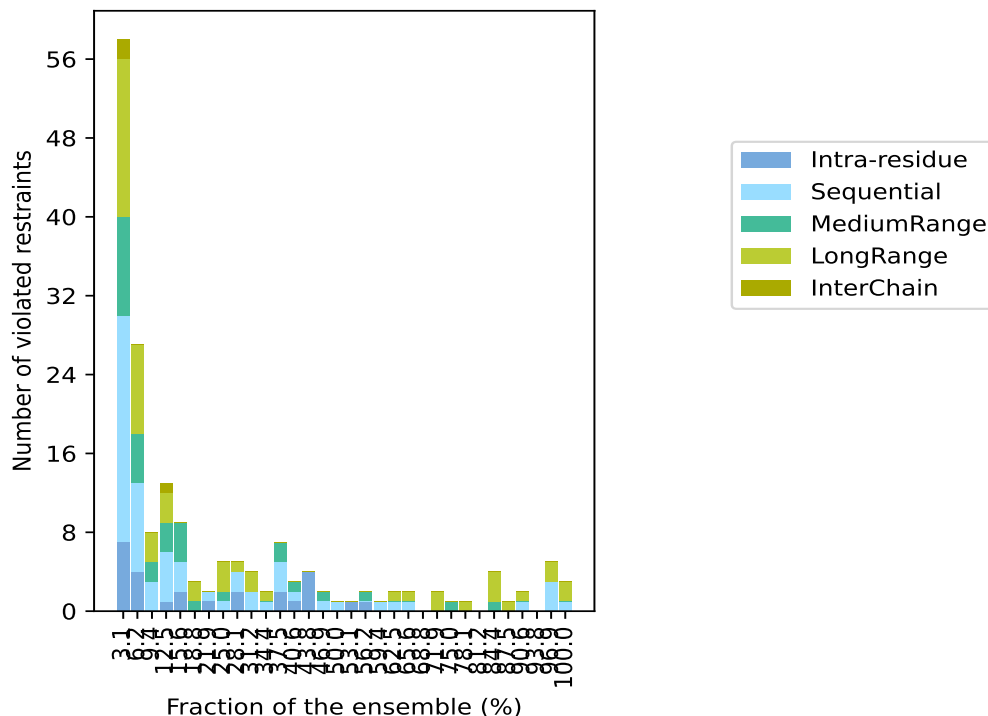
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
1	1	0	0	0	2	7	21.9
0	1	1	3	0	5	8	25.0
2	2	0	1	0	5	9	28.1
0	2	0	2	0	4	10	31.2
0	1	0	1	0	2	11	34.4
2	3	2	0	0	7	12	37.5
1	1	1	0	0	3	13	40.6
4	0	0	0	0	4	14	43.8
0	1	1	0	0	2	15	46.9
0	1	0	0	0	1	16	50.0
1	0	0	0	0	1	17	53.1
1	0	1	0	0	2	18	56.2
0	1	0	0	0	1	19	59.4
0	1	0	1	0	2	20	62.5
0	1	0	1	0	2	21	65.6
0	0	0	0	0	0	22	68.8
0	0	0	2	0	2	23	71.9
0	0	1	0	0	1	24	75.0
0	0	0	1	0	1	25	78.1
0	0	0	0	0	0	26	81.2
0	0	1	3	0	4	27	84.4
0	0	0	1	0	1	28	87.5
0	1	0	1	0	2	29	90.6
0	0	0	0	0	0	30	93.8
0	3	0	2	0	5	31	96.9
0	1	0	2	0	3	32	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

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

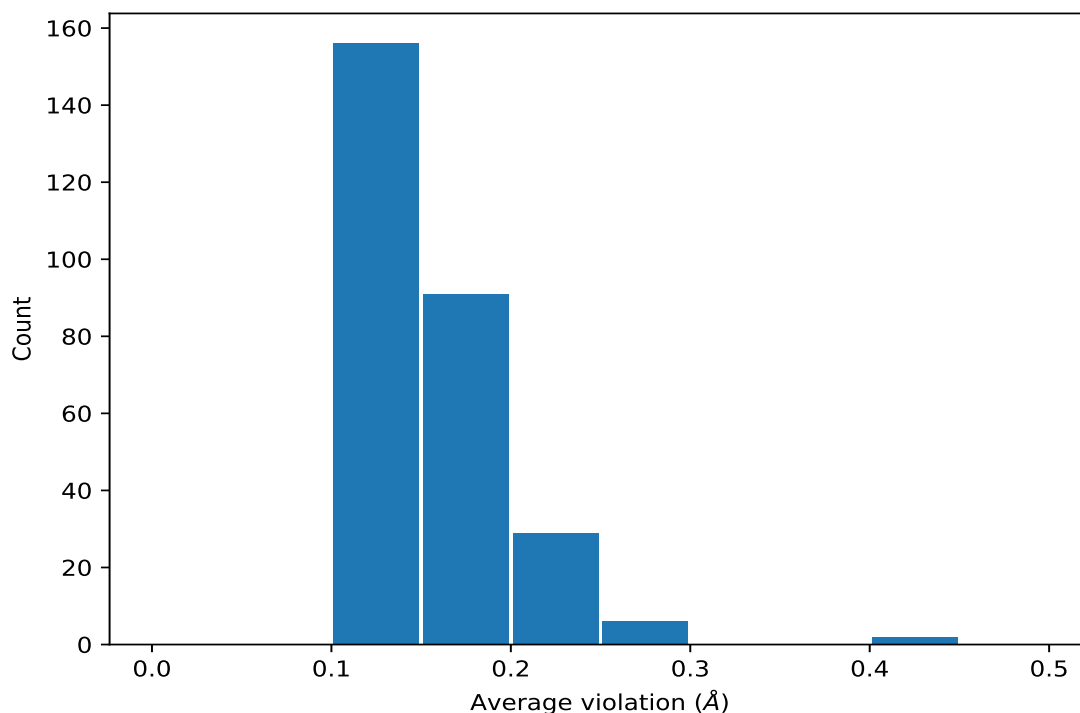


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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 <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	32	0.22	0.02	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	32	0.22	0.02	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	32	0.22	0.02	0.22
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	32	0.2	0.01	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	32	0.2	0.01	0.2
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	32	0.18	0.03	0.18
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	31	0.23	0.02	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	31	0.23	0.02	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	31	0.23	0.02	0.23
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	31	0.2	0.02	0.2
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	31	0.2	0.02	0.2
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	31	0.17	0.03	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	31	0.17	0.03	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	31	0.17	0.03	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	31	0.17	0.03	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	31	0.16	0.03	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	31	0.16	0.03	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	31	0.16	0.03	0.16
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	29	0.2	0.05	0.21
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	29	0.16	0.02	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	29	0.16	0.02	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	29	0.16	0.02	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	29	0.16	0.02	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	29	0.16	0.02	0.16
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	29	0.16	0.02	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	28	0.15	0.02	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	28	0.15	0.02	0.15
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	27	0.16	0.03	0.16
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	27	0.16	0.03	0.16
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	27	0.16	0.03	0.16
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	27	0.16	0.03	0.16
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	27	0.16	0.03	0.16
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	27	0.16	0.03	0.16
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	27	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	27	0.15	0.02	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	27	0.15	0.02	0.15
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	27	0.14	0.01	0.13
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	27	0.13	0.02	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	27	0.13	0.02	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	27	0.13	0.02	0.12
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	25	0.16	0.04	0.15
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	25	0.16	0.04	0.15
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	25	0.16	0.04	0.15
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	24	0.14	0.02	0.13
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	23	0.13	0.02	0.12
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	23	0.13	0.02	0.12
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	23	0.13	0.02	0.12
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	23	0.12	0.02	0.12
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	23	0.12	0.02	0.12
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	23	0.12	0.02	0.12
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	21	0.18	0.04	0.2
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	21	0.13	0.02	0.12
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	21	0.13	0.02	0.12
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	21	0.13	0.02	0.12
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	20	0.19	0.03	0.2
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	20	0.18	0.03	0.18
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	20	0.18	0.03	0.18
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	20	0.18	0.03	0.18
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	19	0.43	0.01	0.43
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	18	0.14	0.05	0.14
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	18	0.14	0.05	0.14
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	18	0.14	0.05	0.14
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	18	0.14	0.05	0.14
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	18	0.14	0.05	0.14
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	18	0.14	0.05	0.14
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	18	0.13	0.01	0.13
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	17	0.13	0.01	0.13
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	16	0.42	0.01	0.42
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	15	0.18	0.04	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	15	0.18	0.04	0.18
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	15	0.18	0.04	0.18
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	15	0.16	0.03	0.15
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	15	0.16	0.03	0.15
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	14	0.22	0.08	0.22
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	14	0.19	0.01	0.19
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	14	0.16	0.02	0.17
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	14	0.15	0.02	0.15
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	13	0.16	0.02	0.15
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	13	0.13	0.02	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	13	0.13	0.01	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	13	0.13	0.01	0.12
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	12	0.19	0.04	0.18
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	12	0.18	0.01	0.19
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	12	0.16	0.04	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	12	0.16	0.04	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	12	0.16	0.04	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	12	0.16	0.04	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	12	0.16	0.04	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	12	0.16	0.04	0.15
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	12	0.16	0.03	0.16
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	12	0.16	0.03	0.16
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	12	0.13	0.02	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	12	0.12	0.01	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	12	0.12	0.01	0.12
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	12	0.12	0.01	0.12
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	11	0.18	0.02	0.18
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	11	0.15	0.04	0.14
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	10	0.16	0.03	0.15
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	10	0.15	0.03	0.14
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	10	0.14	0.02	0.13
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	10	0.12	0.01	0.12
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	9	0.2	0.09	0.19
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	9	0.2	0.09	0.19
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	9	0.18	0.08	0.16
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	9	0.17	0.01	0.17
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	9	0.16	0.05	0.12
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	9	0.13	0.01	0.13
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	8	0.21	0.08	0.18
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	8	0.21	0.08	0.18
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	8	0.2	0.05	0.21
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	8	0.2	0.05	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	8	0.2	0.05	0.21
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	8	0.19	0.02	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	8	0.19	0.02	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	8	0.19	0.02	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	8	0.19	0.02	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	8	0.19	0.02	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	8	0.19	0.02	0.18
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	8	0.18	0.07	0.18
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	8	0.18	0.07	0.18
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	8	0.15	0.03	0.16
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	7	0.14	0.02	0.13
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	7	0.12	0.01	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	7	0.12	0.01	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	7	0.12	0.01	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	7	0.12	0.01	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	7	0.12	0.01	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	7	0.12	0.01	0.12
(1,4996)	1:A:328:TYR:HE1	1:A:330:LYS:H	6	0.18	0.04	0.18
(1,4996)	1:A:328:TYR:HE2	1:A:330:LYS:H	6	0.18	0.04	0.18
(1,4834)	1:A:323:LYS:HD3	1:A:329:THR:H	6	0.15	0.03	0.15
(1,1435)	1:A:266:MET:H	1:A:319:VAL:HA	6	0.12	0.0	0.12
(1,4172)	1:A:250:ASP:HB2	1:A:251:ASP:H	5	0.18	0.06	0.17
(1,4172)	1:A:250:ASP:HB3	1:A:251:ASP:H	5	0.18	0.06	0.17
(1,375)	1:A:255:ASP:HB2	1:A:258:LEU:HG	5	0.15	0.03	0.14
(1,375)	1:A:255:ASP:HB3	1:A:258:LEU:HG	5	0.15	0.03	0.14
(1,1114)	1:A:245:PRO:HB2	1:A:247:GLY:H	5	0.15	0.01	0.14
(1,3664)	1:A:301:GLN:HA	1:A:301:GLN:HE21	5	0.14	0.01	0.13
(1,5086)	1:B:331:ARG:HA	1:B:331:ARG:HE	5	0.13	0.01	0.13
(1,5176)	1:B:252:PRO:HG2	1:B:253:ILE:H	5	0.12	0.01	0.12
(1,5176)	1:B:252:PRO:HG3	1:B:253:ILE:H	5	0.12	0.01	0.12
(1,1116)	1:A:245:PRO:HD3	1:A:246:LEU:H	5	0.12	0.02	0.11
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB1	5	0.12	0.01	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB2	5	0.12	0.01	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB3	5	0.12	0.01	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB1	5	0.12	0.01	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB2	5	0.12	0.01	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB3	5	0.12	0.01	0.12
(1,4627)	1:B:320:ASN:HA	1:B:323:LYS:HD3	5	0.12	0.02	0.11
(1,5189)	1:A:333:ARG:HB2	1:A:334:LYS:H	4	0.25	0.16	0.18
(1,5189)	1:A:333:ARG:HB3	1:A:334:LYS:H	4	0.25	0.16	0.18
(1,5190)	1:A:333:ARG:HB2	1:A:335:GLN:H	4	0.21	0.06	0.22
(1,5190)	1:A:333:ARG:HB3	1:A:335:GLN:H	4	0.21	0.06	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5197)	1:A:333:ARG:HB3	1:A:334:LYS:H	4	0.18	0.04	0.19
(1,1250)	1:A:265:ILE:HD11	1:A:328:TYR:HB2	4	0.17	0.05	0.16
(1,1250)	1:A:265:ILE:HD12	1:A:328:TYR:HB2	4	0.17	0.05	0.16
(1,1250)	1:A:265:ILE:HD13	1:A:328:TYR:HB2	4	0.17	0.05	0.16
(1,665)	1:A:258:LEU:HD11	1:A:265:ILE:H	4	0.16	0.02	0.15
(1,665)	1:A:258:LEU:HD12	1:A:265:ILE:H	4	0.16	0.02	0.15
(1,665)	1:A:258:LEU:HD13	1:A:265:ILE:H	4	0.16	0.02	0.15
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG2	4	0.16	0.03	0.16
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG3	4	0.16	0.03	0.16
(1,5210)	1:B:333:ARG:HG2	1:B:335:GLN:H	4	0.14	0.02	0.14
(1,5210)	1:B:333:ARG:HG3	1:B:335:GLN:H	4	0.14	0.02	0.14
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD21	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD22	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD23	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD21	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD22	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD23	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD21	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD22	4	0.14	0.02	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD23	4	0.14	0.02	0.13
(1,4786)	1:A:251:ASP:H	1:A:252:PRO:HD2	4	0.14	0.02	0.14
(1,4175)	1:B:250:ASP:HB2	1:B:251:ASP:HA	4	0.13	0.01	0.14
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB1	4	0.13	0.02	0.12
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB2	4	0.13	0.02	0.12
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB3	4	0.13	0.02	0.12
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB1	4	0.13	0.02	0.12
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB2	4	0.13	0.02	0.12
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB3	4	0.13	0.02	0.12
(1,12)	1:A:305:SER:H	1:A:305:SER:HB3	4	0.12	0.02	0.11
(1,4218)	1:A:313:LYS:HG3	1:B:278:SER:H	4	0.12	0.01	0.12
(1,5180)	1:A:333:ARG:HA	1:A:334:LYS:H	3	0.21	0.01	0.21
(1,4169)	1:A:250:ASP:HA	1:A:251:ASP:H	3	0.18	0.03	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB1	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB2	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB3	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB1	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB2	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB3	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB1	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB2	3	0.17	0.0	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB3	3	0.17	0.0	0.17
(1,2202)	1:A:274:CYS:HB2	1:A:304:VAL:H	3	0.13	0.02	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2633)	1:B:247:GLY:H	1:B:250:ASP:HB2	3	0.12	0.01	0.12
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD1	3	0.12	0.01	0.11
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD2	3	0.12	0.01	0.11
(1,4989)	1:B:328:TYR:HD1	1:B:329:THR:HB	3	0.12	0.0	0.12
(1,4989)	1:B:328:TYR:HD2	1:B:329:THR:HB	3	0.12	0.0	0.12
(1,4239)	1:B:313:LYS:HG2	1:B:316:ARG:HE	3	0.11	0.0	0.11
(1,4229)	1:A:313:LYS:HG2	1:A:313:LYS:HE3	2	0.3	0.01	0.3
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG21	2	0.26	0.04	0.26
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG22	2	0.26	0.04	0.26
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG23	2	0.26	0.04	0.26
(1,693)	1:A:258:LEU:H	1:A:258:LEU:HG	2	0.22	0.02	0.22
(1,1565)	1:B:269:ALA:HB1	1:B:316:ARG:HB2	2	0.21	0.01	0.21
(1,1565)	1:B:269:ALA:HB1	1:B:316:ARG:HB3	2	0.21	0.01	0.21
(1,1565)	1:B:269:ALA:HB2	1:B:316:ARG:HB2	2	0.21	0.01	0.21
(1,1565)	1:B:269:ALA:HB2	1:B:316:ARG:HB3	2	0.21	0.01	0.21
(1,1565)	1:B:269:ALA:HB3	1:B:316:ARG:HB2	2	0.21	0.01	0.21
(1,1565)	1:B:269:ALA:HB3	1:B:316:ARG:HB3	2	0.21	0.01	0.21
(1,4170)	1:B:250:ASP:HA	1:B:251:ASP:H	2	0.16	0.03	0.16
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD21	2	0.16	0.01	0.16
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD22	2	0.16	0.01	0.16
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD23	2	0.16	0.01	0.16
(1,1230)	1:A:265:ILE:HD11	1:A:266:MET:HA	2	0.16	0.01	0.16
(1,1230)	1:A:265:ILE:HD12	1:A:266:MET:HA	2	0.16	0.01	0.16
(1,1230)	1:A:265:ILE:HD13	1:A:266:MET:HA	2	0.16	0.01	0.16
(1,5000)	1:B:328:TYR:HE1	1:B:330:LYS:H	2	0.16	0.02	0.16
(1,5000)	1:B:328:TYR:HE2	1:B:330:LYS:H	2	0.16	0.02	0.16
(1,547)	1:B:257:LEU:HD21	1:B:258:LEU:H	2	0.14	0.03	0.14
(1,547)	1:B:257:LEU:HD22	1:B:258:LEU:H	2	0.14	0.03	0.14
(1,547)	1:B:257:LEU:HD23	1:B:258:LEU:H	2	0.14	0.03	0.14
(1,2621)	1:B:247:GLY:HA3	1:B:249:GLU:H	2	0.14	0.03	0.14
(1,3343)	1:A:248:SER:HA	1:A:250:ASP:H	2	0.14	0.02	0.14
(1,5177)	1:A:333:ARG:HA	1:A:333:ARG:HD2	2	0.14	0.01	0.14
(1,5177)	1:A:333:ARG:HA	1:A:333:ARG:HD3	2	0.14	0.01	0.14
(1,1117)	1:B:245:PRO:HD3	1:B:246:LEU:H	2	0.13	0.01	0.13
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD11	2	0.12	0.02	0.12
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD12	2	0.12	0.02	0.12
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD13	2	0.12	0.02	0.12
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD21	2	0.12	0.02	0.12
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD22	2	0.12	0.02	0.12
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD23	2	0.12	0.02	0.12
(1,2215)	1:B:274:CYS:HB2	1:B:304:VAL:H	2	0.12	0.0	0.12
(1,2268)	1:B:275:CYS:HB2	1:B:299:CYS:HA	2	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,2629)	1:B:247:GLY:H	1:B:248:SER:HA	2	0.12	0.01	0.12
(1,5080)	1:A:331:ARG:HA	1:A:331:ARG:HD2	2	0.12	0.01	0.12
(1,5080)	1:A:331:ARG:HA	1:A:331:ARG:HD3	2	0.12	0.01	0.12
(1,1447)	1:B:266:MET:H	1:B:319:VAL:HA	2	0.12	0.0	0.12
(1,4984)	1:A:328:TYR:HD1	1:A:329:THR:HB	2	0.12	0.0	0.12
(1,4984)	1:A:328:TYR:HD2	1:A:329:THR:HB	2	0.12	0.0	0.12
(1,5052)	1:B:330:LYS:HD2	1:B:331:ARG:H	2	0.12	0.0	0.12
(1,101)	1:A:253:ILE:HD11	1:A:264:ASP:HB2	2	0.11	0.0	0.11
(1,101)	1:A:253:ILE:HD12	1:A:264:ASP:HB2	2	0.11	0.0	0.11
(1,101)	1:A:253:ILE:HD13	1:A:264:ASP:HB2	2	0.11	0.0	0.11
(1,1698)	1:A:271:VAL:HB	1:A:312:ASN:HA	2	0.11	0.0	0.11
(1,3432)	1:A:294:HIS:HE1	1:A:306:PRO:HD3	2	0.11	0.0	0.11
(1,3436)	1:B:294:HIS:HE1	1:B:306:PRO:HD3	2	0.11	0.0	0.11
(1,3799)	1:A:303:ASP:H	1:A:304:VAL:HB	2	0.11	0.0	0.11
(1,5208)	1:A:333:ARG:HG2	1:A:335:GLN:H	2	0.11	0.0	0.11
(1,5208)	1:A:333:ARG:HG3	1:A:335:GLN:H	2	0.11	0.0	0.11

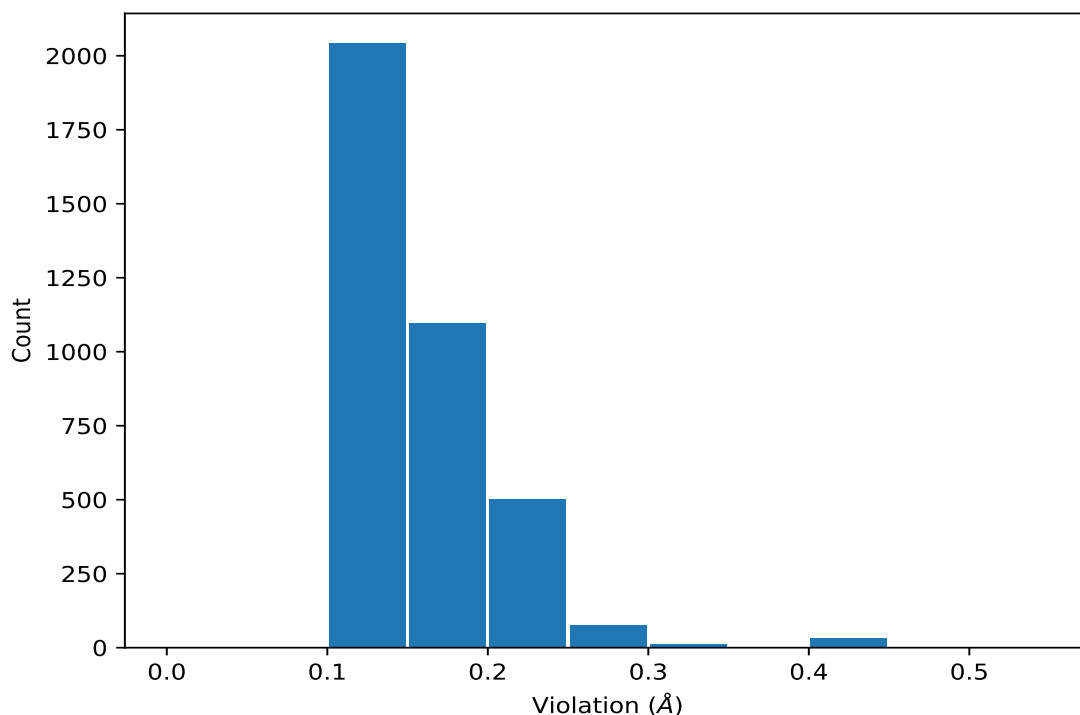
<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

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

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





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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5189)	1:A:333:ARG:HB2	1:A:334:LYS:H	8	0.52
(1,5189)	1:A:333:ARG:HB3	1:A:334:LYS:H	8	0.52
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	10	0.45
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	17	0.45
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	22	0.45
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	4	0.44
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	9	0.44
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	8	0.44
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	11	0.44
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	15	0.44
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	18	0.44
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	3	0.43
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	6	0.43
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	8	0.43
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	13	0.43
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	23	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	7	0.43
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	14	0.43
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	16	0.43
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	19	0.43
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	26	0.43
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	27	0.43
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	31	0.43
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	32	0.43
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	2	0.42
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	5	0.42
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	15	0.42
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	17	0.42
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	28	0.42
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	30	0.42
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	6	0.42
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	21	0.42
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	25	0.42
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	10	0.41
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	21	0.4
(1,4976)	1:B:328:TYR:HA	1:B:329:THR:H	27	0.4
(1,4973)	1:A:328:TYR:HA	1:A:329:THR:H	12	0.4
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	26	0.4
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	13	0.39
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	13	0.39
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	14	0.34
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	31	0.33
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	31	0.33
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	11	0.33
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	10	0.32
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	10	0.32
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	9	0.31
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	26	0.31
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	26	0.31
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	26	0.31
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	26	0.31
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	26	0.31
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	26	0.31
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG21	22	0.3
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG22	22	0.3
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG23	22	0.3
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	20	0.3
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	22	0.3
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	22	0.3
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	19	0.3
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	32	0.3
(1,4229)	1:A:313:LYS:HG2	1:A:313:LYS:HE3	18	0.3
(1,716)	1:B:259:CYS:HA	1:B:260:LEU:HG	25	0.29
(1,4229)	1:A:313:LYS:HG2	1:A:313:LYS:HE3	6	0.29
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	22	0.29
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	16	0.28
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	10	0.28
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	10	0.28
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	10	0.28
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	22	0.28
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	22	0.28
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	22	0.28
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	22	0.28
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	22	0.28
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	22	0.28
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	22	0.27
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	22	0.27
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	22	0.27
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	22	0.27
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	22	0.27
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	22	0.27
(1,5190)	1:A:333:ARG:HB2	1:A:335:GLN:H	15	0.27
(1,5190)	1:A:333:ARG:HB3	1:A:335:GLN:H	15	0.27
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	12	0.27
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	8	0.27
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	23	0.27
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	4	0.27
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	4	0.27
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	4	0.27
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	19	0.27
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	19	0.27
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	19	0.27
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	10	0.27
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	10	0.27
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	10	0.27
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	3	0.27
(1,5190)	1:A:333:ARG:HB2	1:A:335:GLN:H	27	0.26
(1,5190)	1:A:333:ARG:HB3	1:A:335:GLN:H	27	0.26
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	16	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	16	0.26
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	16	0.26
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	16	0.26
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	16	0.26
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	16	0.26
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	15	0.26
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	15	0.26
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	3	0.26
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	13	0.26
(1,4172)	1:A:250:ASP:HB2	1:A:251:ASP:H	27	0.26
(1,4172)	1:A:250:ASP:HB3	1:A:251:ASP:H	27	0.26
(1,896)	1:B:260:LEU:HG	1:B:298:THR:HG21	10	0.25
(1,896)	1:B:260:LEU:HG	1:B:298:THR:HG22	10	0.25
(1,896)	1:B:260:LEU:HG	1:B:298:THR:HG23	10	0.25
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	8	0.25
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	8	0.25
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	7	0.25
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	15	0.25
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	24	0.25
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	24	0.25
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	24	0.25
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	31	0.25
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	31	0.25
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	31	0.25
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	21	0.25
(1,1250)	1:A:265:ILE:HD11	1:A:328:TYR:HB2	20	0.25
(1,1250)	1:A:265:ILE:HD12	1:A:328:TYR:HB2	20	0.25
(1,1250)	1:A:265:ILE:HD13	1:A:328:TYR:HB2	20	0.25
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	8	0.24
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	8	0.24
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	8	0.24
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	32	0.24
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	32	0.24
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	32	0.24
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	17	0.24
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	4	0.24
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	28	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	6	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	6	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	6	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	7	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	7	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	12	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	12	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	12	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	17	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	17	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	17	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	23	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	23	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	23	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	28	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	28	0.24
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	28	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	3	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	3	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	3	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	11	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	11	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	11	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	20	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	20	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	20	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	26	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	26	0.24
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	26	0.24
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	10	0.24
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	10	0.24
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	10	0.24
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	2	0.24
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	6	0.24
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	21	0.24
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	20	0.24
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	20	0.24
(1,693)	1:A:258:LEU:H	1:A:258:LEU:HG	22	0.23
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	28	0.23
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	28	0.23
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	28	0.23
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	18	0.23
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	29	0.23
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	4	0.23
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	16	0.23
(1,5197)	1:A:333:ARG:HB3	1:A:334:LYS:H	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	28	0.23
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	28	0.23
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	5	0.23
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	5	0.23
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	5	0.23
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	5	0.23
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	5	0.23
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	5	0.23
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	22	0.23
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	11	0.23
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	25	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	1	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	1	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	1	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	3	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	3	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	3	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	9	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	9	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	9	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	18	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	18	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	18	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	20	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	20	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	20	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	21	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	21	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	21	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	25	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	25	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	25	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	26	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	26	0.23
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	26	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	2	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	2	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	2	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	12	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	12	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	12	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	14	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	14	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	16	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	16	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	16	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	18	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	18	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	18	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	21	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	21	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	21	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	28	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	28	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	28	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	29	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	29	0.23
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	29	0.23
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	1	0.23
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	1	0.23
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	27	0.23
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	27	0.23
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	30	0.22
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	30	0.22
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	30	0.22
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	30	0.22
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	30	0.22
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	30	0.22
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	30	0.22
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	30	0.22
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	30	0.22
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	30	0.22
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	30	0.22
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	30	0.22
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	30	0.22
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	30	0.22
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	30	0.22
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	30	0.22
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	30	0.22
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	30	0.22
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	32	0.22
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	32	0.22
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	32	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	9	0.22
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	9	0.22
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	9	0.22
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	21	0.22
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	21	0.22
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	25	0.22
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	28	0.22
(1,5180)	1:A:333:ARG:HA	1:A:334:LYS:H	15	0.22
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	31	0.22
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	20	0.22
(1,4996)	1:A:328:TYR:HE1	1:A:330:LYS:H	8	0.22
(1,4996)	1:A:328:TYR:HE2	1:A:330:LYS:H	8	0.22
(1,4996)	1:A:328:TYR:HE1	1:A:330:LYS:H	17	0.22
(1,4996)	1:A:328:TYR:HE2	1:A:330:LYS:H	17	0.22
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	27	0.22
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	27	0.22
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	28	0.22
(1,4290)	1:A:314:PHE:HE1	1:B:259:CYS:H	22	0.22
(1,4290)	1:A:314:PHE:HE2	1:B:259:CYS:H	22	0.22
(1,4172)	1:A:250:ASP:HB2	1:A:251:ASP:H	13	0.22
(1,4172)	1:A:250:ASP:HB3	1:A:251:ASP:H	13	0.22
(1,4169)	1:A:250:ASP:HA	1:A:251:ASP:H	10	0.22
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	26	0.22
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	30	0.22
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	16	0.22
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	16	0.22
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	16	0.22
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	19	0.22
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	19	0.22
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	19	0.22
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	13	0.22
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	13	0.22
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	13	0.22
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	31	0.22
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	31	0.22
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	31	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	8	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	8	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	8	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	13	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	13	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	14	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	14	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	14	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	22	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	22	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	22	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	27	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	27	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	27	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	29	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	29	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	29	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	32	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	32	0.22
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	32	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	8	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	8	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	8	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	17	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	17	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	17	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	23	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	23	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	23	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	24	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	24	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	24	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	25	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	25	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	25	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	32	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	32	0.22
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	32	0.22
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	23	0.22
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	23	0.22
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	23	0.22
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	5	0.22
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	11	0.22
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	4	0.22
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	4	0.22
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	8	0.22
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	13	0.22
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	13	0.22
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	22	0.22
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	22	0.22
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	4	0.22
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	4	0.22
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	8	0.22
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	8	0.22
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	9	0.22
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	9	0.22
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	16	0.22
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	16	0.22
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	27	0.22
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	27	0.22
(1,1565)	1:B:269:ALA:HB1	1:B:316:ARG:HB2	15	0.22
(1,1565)	1:B:269:ALA:HB1	1:B:316:ARG:HB3	15	0.22
(1,1565)	1:B:269:ALA:HB2	1:B:316:ARG:HB2	15	0.22
(1,1565)	1:B:269:ALA:HB2	1:B:316:ARG:HB3	15	0.22
(1,1565)	1:B:269:ALA:HB3	1:B:316:ARG:HB2	15	0.22
(1,1565)	1:B:269:ALA:HB3	1:B:316:ARG:HB3	15	0.22
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG21	10	0.21
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG22	10	0.21
(1,891)	1:A:260:LEU:HG	1:A:298:THR:HG23	10	0.21
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	4	0.21
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	4	0.21
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	4	0.21
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	11	0.21
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	11	0.21
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	11	0.21
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	1	0.21
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	12	0.21
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	14	0.21
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	24	0.21
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	26	0.21
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	1	0.21
(1,5180)	1:A:333:ARG:HA	1:A:334:LYS:H	17	0.21
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	25	0.21
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	19	0.21
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	19	0.21
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	19	0.21
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	19	0.21
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	19	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	19	0.21
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	11	0.21
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	16	0.21
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	20	0.21
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	27	0.21
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	31	0.21
(1,375)	1:A:255:ASP:HB2	1:A:258:LEU:HG	27	0.21
(1,375)	1:A:255:ASP:HB3	1:A:258:LEU:HG	27	0.21
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	5	0.21
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	5	0.21
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	5	0.21
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	29	0.21
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	29	0.21
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	29	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	5	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	5	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	5	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	15	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	15	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	15	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	16	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	16	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	16	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	19	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	19	0.21
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	19	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	1	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	1	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	1	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	4	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	4	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	4	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	5	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	5	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	5	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	7	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	7	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	7	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	13	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	13	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	13	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	15	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	15	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	15	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	27	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	27	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	27	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	30	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	30	0.21
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	30	0.21
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	29	0.21
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	26	0.21
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	31	0.21
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	5	0.21
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	5	0.21
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	9	0.21
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	9	0.21
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	16	0.21
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	16	0.21
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	26	0.21
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	26	0.21
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	1	0.21
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	1	0.21
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	6	0.21
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	6	0.21
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	11	0.21
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	11	0.21
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	13	0.21
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	13	0.21
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	20	0.21
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	20	0.21
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	23	0.21
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	23	0.21
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	31	0.21
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	31	0.21
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	4	0.21
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	19	0.2
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	19	0.2
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	19	0.2
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	19	0.2
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	19	0.2
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	19	0.2
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	6	0.2
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	6	0.2
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	6	0.2
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	6	0.2
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	6	0.2
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	6	0.2
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	6	0.2
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	6	0.2
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	6	0.2
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	6	0.2
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	6	0.2
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	6	0.2
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	6	0.2
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	6	0.2
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	6	0.2
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	6	0.2
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	6	0.2
(1,693)	1:A:258:LEU:H	1:A:258:LEU:HG	20	0.2
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	11	0.2
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	11	0.2
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	11	0.2
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	26	0.2
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	26	0.2
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	26	0.2
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	3	0.2
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	30	0.2
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	3	0.2
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	9	0.2
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	14	0.2
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	30	0.2
(1,5197)	1:A:333:ARG:HB3	1:A:334:LYS:H	15	0.2
(1,5180)	1:A:333:ARG:HA	1:A:334:LYS:H	27	0.2
(1,5175)	1:A:252:PRO:HG2	1:A:253:ILE:H	2	0.2
(1,5175)	1:A:252:PRO:HG3	1:A:253:ILE:H	2	0.2
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	20	0.2
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	11	0.2
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	14	0.2
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	14	0.2
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	14	0.2
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	14	0.2
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	14	0.2
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	14	0.2
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	25	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	25	0.2
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	24	0.2
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	24	0.2
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	24	0.2
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	24	0.2
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	24	0.2
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	24	0.2
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	29	0.2
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	29	0.2
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	29	0.2
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	29	0.2
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	29	0.2
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	29	0.2
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	20	0.2
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	20	0.2
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	22	0.2
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	22	0.2
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	29	0.2
(1,4834)	1:A:323:LYS:HD3	1:A:329:THR:H	4	0.2
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG2	1	0.2
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG3	1	0.2
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	4	0.2
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	9	0.2
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	7	0.2
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	14	0.2
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	18	0.2
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	24	0.2
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	29	0.2
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	5	0.2
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	24	0.2
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	19	0.2
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	32	0.2
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	5	0.2
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	5	0.2
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	5	0.2
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	11	0.2
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	11	0.2
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	11	0.2
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	30	0.2
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	30	0.2
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	30	0.2
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	19	0.2
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	19	0.2
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	31	0.2
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	31	0.2
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	31	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	20	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	20	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	20	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	24	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	24	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	24	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	32	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	32	0.2
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	32	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	10	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	10	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	10	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	25	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	25	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	25	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	29	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	29	0.2
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	29	0.2
(1,3346)	1:B:248:SER:HA	1:B:250:ASP:H	29	0.2
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	10	0.2
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	4	0.2
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	24	0.2
(1,3051)	1:B:287:ALA:H	1:B:288:LEU:HG	6	0.2
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	1	0.2
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	1	0.2
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	11	0.2
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	11	0.2
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	15	0.2
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	15	0.2
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	18	0.2
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	18	0.2
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	19	0.2
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	19	0.2
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	32	0.2
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	32	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	2	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	15	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	15	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	17	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	17	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	18	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	18	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	19	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	19	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	22	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	22	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	24	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	24	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	25	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	25	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	26	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	26	0.2
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	32	0.2
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	32	0.2
(1,1565)	1:B:269:ALA:HB1	1:B:316:ARG:HB2	8	0.2
(1,1565)	1:B:269:ALA:HB1	1:B:316:ARG:HB3	8	0.2
(1,1565)	1:B:269:ALA:HB2	1:B:316:ARG:HB2	8	0.2
(1,1565)	1:B:269:ALA:HB2	1:B:316:ARG:HB3	8	0.2
(1,1565)	1:B:269:ALA:HB3	1:B:316:ARG:HB2	8	0.2
(1,1565)	1:B:269:ALA:HB3	1:B:316:ARG:HB3	8	0.2
(1,1272)	1:B:265:ILE:HD11	1:B:328:TYR:HB2	31	0.2
(1,1272)	1:B:265:ILE:HD12	1:B:328:TYR:HB2	31	0.2
(1,1272)	1:B:265:ILE:HD13	1:B:328:TYR:HB2	31	0.2
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	10	0.19
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	10	0.19
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	10	0.19
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	13	0.19
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	13	0.19
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	13	0.19
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	13	0.19
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	13	0.19
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	13	0.19
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	15	0.19
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	15	0.19
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	15	0.19
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	15	0.19
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	15	0.19
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	21	0.19
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	21	0.19
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	21	0.19
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	21	0.19
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	21	0.19
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	21	0.19
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	32	0.19
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	32	0.19
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	32	0.19
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	32	0.19
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	32	0.19
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	32	0.19
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	2	0.19
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	2	0.19
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	2	0.19
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	2	0.19
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	2	0.19
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	2	0.19
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	8	0.19
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	8	0.19
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	8	0.19
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	8	0.19
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	8	0.19
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	8	0.19
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	15	0.19
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	15	0.19
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	15	0.19
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	26	0.19
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	26	0.19
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	26	0.19
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	7	0.19
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	7	0.19
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	7	0.19
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	21	0.19
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	21	0.19
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	21	0.19
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	25	0.19
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	25	0.19
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	25	0.19
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	28	0.19
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	28	0.19
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	28	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	31	0.19
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	31	0.19
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	31	0.19
(1,665)	1:A:258:LEU:HD11	1:A:265:ILE:H	10	0.19
(1,665)	1:A:258:LEU:HD12	1:A:265:ILE:H	10	0.19
(1,665)	1:A:258:LEU:HD13	1:A:265:ILE:H	10	0.19
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	6	0.19
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	6	0.19
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	7	0.19
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	12	0.19
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	18	0.19
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	24	0.19
(1,5190)	1:A:333:ARG:HB2	1:A:335:GLN:H	8	0.19
(1,5190)	1:A:333:ARG:HB3	1:A:335:GLN:H	8	0.19
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	5	0.19
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	27	0.19
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	27	0.19
(1,4996)	1:A:328:TYR:HE1	1:A:330:LYS:H	27	0.19
(1,4996)	1:A:328:TYR:HE2	1:A:330:LYS:H	27	0.19
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	31	0.19
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	31	0.19
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	32	0.19
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	32	0.19
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	25	0.19
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	25	0.19
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	18	0.19
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	20	0.19
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	5	0.19
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	5	0.19
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	2	0.19
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	1	0.19
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	11	0.19
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	16	0.19
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	19	0.19
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	22	0.19
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	18	0.19
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	29	0.19
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	1	0.19
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	2	0.19
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	3	0.19
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	4	0.19
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	13	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	29	0.19
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	30	0.19
(1,4170)	1:B:250:ASP:HA	1:B:251:ASP:H	31	0.19
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	8	0.19
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	8	0.19
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	8	0.19
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	20	0.19
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	20	0.19
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	20	0.19
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	25	0.19
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	25	0.19
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	25	0.19
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	22	0.19
(1,3347)	1:A:248:SER:HB2	1:A:249:GLU:HG2	15	0.19
(1,3347)	1:A:248:SER:HB2	1:A:249:GLU:HG3	15	0.19
(1,3347)	1:A:248:SER:HB3	1:A:249:GLU:HG2	15	0.19
(1,3347)	1:A:248:SER:HB3	1:A:249:GLU:HG3	15	0.19
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	2	0.19
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	3	0.19
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	11	0.19
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	13	0.19
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	19	0.19
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	28	0.19
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	19	0.19
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	28	0.19
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	29	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	6	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	6	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	12	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	12	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	21	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	21	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	23	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	23	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	24	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	24	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	28	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	28	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	29	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	29	0.19
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	30	0.19
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	30	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	7	0.19
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	7	0.19
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	12	0.19
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	12	0.19
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	14	0.19
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	14	0.19
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	28	0.19
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	28	0.19
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	29	0.19
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	29	0.19
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	30	0.19
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	30	0.19
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	1	0.19
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	22	0.18
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	22	0.18
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	22	0.18
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	14	0.18
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	14	0.18
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	14	0.18
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	14	0.18
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	14	0.18
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	14	0.18
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	14	0.18
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	14	0.18
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	14	0.18
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	14	0.18
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	14	0.18
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	14	0.18
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	14	0.18
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	14	0.18
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	14	0.18
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	14	0.18
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	14	0.18
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	14	0.18
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	26	0.18
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	26	0.18
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	26	0.18
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	26	0.18
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	26	0.18
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	26	0.18
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	26	0.18
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	26	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	26	0.18
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	26	0.18
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	26	0.18
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	26	0.18
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	26	0.18
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	26	0.18
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	26	0.18
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	26	0.18
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	26	0.18
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	26	0.18
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	4	0.18
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	4	0.18
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	4	0.18
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	4	0.18
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	4	0.18
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	4	0.18
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	5	0.18
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	5	0.18
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	5	0.18
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	5	0.18
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	5	0.18
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	5	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	9	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	9	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	9	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	9	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	9	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	9	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	9	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	9	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	9	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	9	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	9	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	9	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	9	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	9	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	9	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	9	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	9	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	9	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	11	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	11	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	11	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	11	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	11	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	11	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	11	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	11	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	11	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	11	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	11	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	11	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	11	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	11	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	11	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	11	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	11	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	11	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	30	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	30	0.18
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	30	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	30	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	30	0.18
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	30	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	30	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	30	0.18
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	30	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	30	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	30	0.18
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	30	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	30	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	30	0.18
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	30	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	30	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	30	0.18
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	30	0.18
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	4	0.18
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	4	0.18
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	4	0.18
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	4	0.18
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	4	0.18
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	4	0.18
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	15	0.18
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	15	0.18
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	15	0.18
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	15	0.18
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	15	0.18
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	27	0.18
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	27	0.18
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	27	0.18
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	27	0.18
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	27	0.18
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	27	0.18
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	31	0.18
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	31	0.18
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	31	0.18
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	31	0.18
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	31	0.18
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	31	0.18
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	5	0.18
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	5	0.18
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	5	0.18
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	4	0.18
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	4	0.18
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	4	0.18
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	12	0.18
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	12	0.18
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	12	0.18
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	23	0.18
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	23	0.18
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	23	0.18
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	7	0.18
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	23	0.18
(1,5197)	1:A:333:ARG:HB3	1:A:334:LYS:H	27	0.18
(1,5189)	1:A:333:ARG:HB2	1:A:334:LYS:H	27	0.18
(1,5189)	1:A:333:ARG:HB3	1:A:334:LYS:H	27	0.18
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	21	0.18
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	31	0.18
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	10	0.18
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	21	0.18
(1,5000)	1:B:328:TYR:HE1	1:B:330:LYS:H	25	0.18
(1,5000)	1:B:328:TYR:HE2	1:B:330:LYS:H	25	0.18
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	2	0.18
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	2	0.18
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	14	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	2	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	2	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	2	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	2	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	2	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	2	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	4	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	4	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	4	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	4	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	4	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	4	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	30	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	30	0.18
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	30	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	30	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	30	0.18
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	30	0.18
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	17	0.18
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	17	0.18
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	31	0.18
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	31	0.18
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	32	0.18
(1,4834)	1:A:323:LYS:HD3	1:A:329:THR:H	3	0.18
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	30	0.18
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	18	0.18
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	12	0.18
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	20	0.18
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	32	0.18
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	24	0.18
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	5	0.18
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	18	0.18
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	10	0.18
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	22	0.18
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	22	0.18
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	22	0.18
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	22	0.18
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	22	0.18
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	22	0.18
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	15	0.18
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	15	0.18
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	32	0.18
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	32	0.18
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	32	0.18
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG21	4	0.18
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG22	4	0.18
(1,3562)	1:B:297:PRO:HB3	1:B:298:THR:HG23	4	0.18
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	6	0.18
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	6	0.18
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	6	0.18
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG21	9	0.18
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG22	9	0.18
(1,3560)	1:A:297:PRO:HB3	1:A:298:THR:HG23	9	0.18
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	1	0.18
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	1	0.18
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	1	0.18
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	29	0.18
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	29	0.18
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	29	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	3	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	3	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	3	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	4	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	4	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	4	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	11	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	11	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	11	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	24	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	24	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	24	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	32	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	32	0.18
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	32	0.18
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	1	0.18
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	22	0.18
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	22	0.18
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	2	0.18
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	7	0.18
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	27	0.18
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	10	0.18
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	27	0.18
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	32	0.18
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	3	0.18
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	3	0.18
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	7	0.18
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	7	0.18
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	17	0.18
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	17	0.18
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	31	0.18
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	31	0.18
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	3	0.18
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	3	0.18
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	5	0.18
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	5	0.18
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	21	0.18
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	21	0.18
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	19	0.18
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	20	0.17
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	20	0.17
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	20	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	1	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	1	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	1	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	1	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	1	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	1	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	1	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	1	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	1	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	1	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	1	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	1	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	1	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	1	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	1	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	1	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	1	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	1	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	4	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	4	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	4	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	4	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	4	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	4	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	4	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	4	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	4	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	4	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	4	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	4	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	4	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	4	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	4	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	4	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	4	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	6	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	6	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	6	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	6	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	6	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	6	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	6	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	6	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	6	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	6	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	6	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	6	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	6	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	6	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	6	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	6	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	6	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	6	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	9	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	9	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	9	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	9	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	9	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	9	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	9	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	9	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	9	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	9	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	9	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	9	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	9	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	9	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	9	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	9	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	9	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	17	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	17	0.17
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	17	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	17	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	17	0.17
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	17	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	17	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	17	0.17
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	17	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	17	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	17	0.17
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	17	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	17	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	17	0.17
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	17	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	17	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	17	0.17
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	17	0.17
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	27	0.17
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	27	0.17
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	27	0.17
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	27	0.17
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	27	0.17
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	27	0.17
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	28	0.17
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	28	0.17
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	28	0.17
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	28	0.17
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	28	0.17
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	28	0.17
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	31	0.17
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	31	0.17
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	31	0.17
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	31	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	31	0.17
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	31	0.17
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	1	0.17
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	1	0.17
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	1	0.17
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	1	0.17
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	1	0.17
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	1	0.17
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	1	0.17
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	1	0.17
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	1	0.17
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	1	0.17
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	1	0.17
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	1	0.17
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	1	0.17
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	1	0.17
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	1	0.17
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	1	0.17
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	1	0.17
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	1	0.17
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	17	0.17
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	17	0.17
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	17	0.17
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	17	0.17
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	17	0.17
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	17	0.17
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	17	0.17
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	17	0.17
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	17	0.17
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	17	0.17
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	17	0.17
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	17	0.17
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	17	0.17
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	17	0.17
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	17	0.17
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	17	0.17
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	17	0.17
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	17	0.17
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	10	0.17
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	10	0.17
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	10	0.17
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	10	0.17
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	10	0.17
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	19	0.17
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	19	0.17
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	19	0.17
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	19	0.17
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	19	0.17
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	19	0.17
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	21	0.17
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	21	0.17
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	21	0.17
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	21	0.17
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	21	0.17
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	21	0.17
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	28	0.17
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	28	0.17
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	28	0.17
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	28	0.17
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	28	0.17
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	28	0.17
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	29	0.17
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	29	0.17
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	29	0.17
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	29	0.17
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	29	0.17
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	29	0.17
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	32	0.17
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	32	0.17
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	32	0.17
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	32	0.17
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	32	0.17
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	32	0.17
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	23	0.17
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	23	0.17
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	23	0.17
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	5	0.17
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	5	0.17
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	5	0.17
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	2	0.17
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	29	0.17
(1,547)	1:B:257:LEU:HD21	1:B:258:LEU:H	31	0.17
(1,547)	1:B:257:LEU:HD22	1:B:258:LEU:H	31	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:B:257:LEU:HD23	1:B:258:LEU:H	31	0.17
(1,5189)	1:A:333:ARG:HB2	1:A:334:LYS:H	15	0.17
(1,5189)	1:A:333:ARG:HB3	1:A:334:LYS:H	15	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB1	10	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB2	10	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB3	10	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB1	10	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB2	10	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB3	10	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB1	10	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB2	10	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB3	10	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB1	20	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB2	20	0.17
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB3	20	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB1	20	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB2	20	0.17
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB3	20	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB1	20	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB2	20	0.17
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB3	20	0.17
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	12	0.17
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	21	0.17
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	21	0.17
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	30	0.17
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	30	0.17
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	20	0.17
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	20	0.17
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	20	0.17
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	20	0.17
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	20	0.17
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	20	0.17
(1,4996)	1:A:328:TYR:HE1	1:A:330:LYS:H	15	0.17
(1,4996)	1:A:328:TYR:HE2	1:A:330:LYS:H	15	0.17
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	11	0.17
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	11	0.17
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	16	0.17
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	16	0.17
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	13	0.17
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	13	0.17
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	13	0.17
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	13	0.17
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	13	0.17
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	23	0.17
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	23	0.17
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	1	0.17
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	7	0.17
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG2	19	0.17
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG3	19	0.17
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	21	0.17
(1,4456)	1:B:317:GLN:HG2	1:B:317:GLN:HE22	26	0.17
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	7	0.17
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	14	0.17
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	19	0.17
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	20	0.17
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	22	0.17
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	23	0.17
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	1	0.17
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	2	0.17
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	3	0.17
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	13	0.17
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	24	0.17
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	30	0.17
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	5	0.17
(1,4172)	1:A:250:ASP:HB2	1:A:251:ASP:H	8	0.17
(1,4172)	1:A:250:ASP:HB3	1:A:251:ASP:H	8	0.17
(1,4169)	1:A:250:ASP:HA	1:A:251:ASP:H	22	0.17
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	3	0.17
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	14	0.17
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	17	0.17
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	29	0.17
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	27	0.17
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	29	0.17
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	2	0.17
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	2	0.17
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	2	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	6	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	6	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	6	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	12	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	12	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	12	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	22	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	22	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	22	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	28	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	28	0.17
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	28	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	12	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	12	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	12	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	18	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	18	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	18	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	20	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	20	0.17
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	20	0.17
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	7	0.17
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	26	0.17
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	27	0.17
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	26	0.17
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	1	0.17
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	29	0.17
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	9	0.17
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	22	0.17
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	7	0.17
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	15	0.17
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	20	0.17
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	22	0.17
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	30	0.17
(1,3049)	1:B:287:ALA:H	1:B:288:LEU:HD11	6	0.17
(1,3049)	1:B:287:ALA:H	1:B:288:LEU:HD12	6	0.17
(1,3049)	1:B:287:ALA:H	1:B:288:LEU:HD13	6	0.17
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	27	0.17
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	27	0.17
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	27	0.17
(1,2621)	1:B:247:GLY:HA3	1:B:249:GLU:H	29	0.17
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	14	0.17
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	14	0.17
(1,1114)	1:A:245:PRO:HB2	1:A:247:GLY:H	21	0.17
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	16	0.16
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	16	0.16
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	16	0.16
(1,885)	1:B:260:LEU:HD21	1:B:261:ILE:H	10	0.16
(1,885)	1:B:260:LEU:HD22	1:B:261:ILE:H	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,885)	1:B:260:LEU:HD23	1:B:261:ILE:H	10	0.16
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	19	0.16
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	19	0.16
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	19	0.16
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	19	0.16
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	19	0.16
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	19	0.16
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	19	0.16
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	19	0.16
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	19	0.16
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	19	0.16
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	19	0.16
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	19	0.16
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	19	0.16
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	19	0.16
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	19	0.16
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	19	0.16
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	19	0.16
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	19	0.16
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	28	0.16
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	28	0.16
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	28	0.16
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	28	0.16
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	28	0.16
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	28	0.16
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	28	0.16
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	28	0.16
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	28	0.16
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	28	0.16
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	28	0.16
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	28	0.16
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	28	0.16
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	28	0.16
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	28	0.16
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	28	0.16
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	28	0.16
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	28	0.16
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	12	0.16
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	12	0.16
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	12	0.16
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	12	0.16
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	12	0.16
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	14	0.16
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	14	0.16
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	14	0.16
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	14	0.16
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	14	0.16
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	14	0.16
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	29	0.16
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	29	0.16
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	29	0.16
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	29	0.16
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	29	0.16
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	29	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	5	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	5	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	5	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	5	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	5	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	5	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	5	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	5	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	5	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	5	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	5	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	5	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	5	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	5	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	5	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	5	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	5	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	5	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	7	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	7	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	7	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	7	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	7	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	7	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	7	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	7	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	7	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	7	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	7	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	7	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	7	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	7	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	7	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	7	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	7	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	20	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	20	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	20	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	20	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	20	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	20	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	20	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	20	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	20	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	20	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	20	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	20	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	20	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	20	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	20	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	20	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	20	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	20	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	23	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	23	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	23	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	23	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	23	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	23	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	23	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	23	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	23	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	23	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	23	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	23	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	23	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	23	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	23	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	23	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	23	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	23	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	32	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	32	0.16
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	32	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	32	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	32	0.16
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	32	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	32	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	32	0.16
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	32	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	32	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	32	0.16
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	32	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	32	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	32	0.16
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	32	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	32	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	32	0.16
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	32	0.16
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	5	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	5	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	5	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	5	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	5	0.16
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	5	0.16
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	7	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	7	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	7	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	7	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	7	0.16
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	7	0.16
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	12	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	12	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	12	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	12	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	12	0.16
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	12	0.16
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	14	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	14	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	14	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	14	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	14	0.16
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	17	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	17	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	17	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	17	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	17	0.16
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	17	0.16
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	24	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	24	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	24	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	24	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	24	0.16
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	24	0.16
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	25	0.16
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	25	0.16
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	25	0.16
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	25	0.16
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	25	0.16
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	25	0.16
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	9	0.16
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	9	0.16
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	9	0.16
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	24	0.16
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	24	0.16
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	24	0.16
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	27	0.16
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	27	0.16
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	27	0.16
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	19	0.16
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	19	0.16
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	19	0.16
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	29	0.16
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	29	0.16
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	29	0.16
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	32	0.16
(1,5210)	1:B:333:ARG:HG2	1:B:335:GLN:H	16	0.16
(1,5210)	1:B:333:ARG:HG3	1:B:335:GLN:H	16	0.16
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB1	22	0.16
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB2	22	0.16
(1,512)	1:A:257:LEU:HD11	1:A:318:ALA:HB3	22	0.16
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB1	22	0.16
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB2	22	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,512)	1:A:257:LEU:HD12	1:A:318:ALA:HB3	22	0.16
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB1	22	0.16
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB2	22	0.16
(1,512)	1:A:257:LEU:HD13	1:A:318:ALA:HB3	22	0.16
(1,5088)	1:B:331:ARG:HA	1:B:332:LEU:H	26	0.16
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	28	0.16
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	16	0.16
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	2	0.16
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	5	0.16
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	5	0.16
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	6	0.16
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	6	0.16
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	29	0.16
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	29	0.16
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	29	0.16
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	29	0.16
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	29	0.16
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	29	0.16
(1,4996)	1:A:328:TYR:HE1	1:A:330:LYS:H	20	0.16
(1,4996)	1:A:328:TYR:HE2	1:A:330:LYS:H	20	0.16
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	14	0.16
(1,4834)	1:A:323:LYS:HD3	1:A:329:THR:H	2	0.16
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	17	0.16
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	10	0.16
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	10	0.16
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	1	0.16
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	11	0.16
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	16	0.16
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	9	0.16
(1,4454)	1:A:317:GLN:HG2	1:A:317:GLN:HE22	28	0.16
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	4	0.16
(1,4453)	1:A:317:GLN:HG2	1:A:317:GLN:HE21	29	0.16
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB1	22	0.16
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB2	22	0.16
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB3	22	0.16
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB1	22	0.16
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB2	22	0.16
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB3	22	0.16
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	13	0.16
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	22	0.16
(1,4174)	1:B:250:ASP:HB3	1:B:251:ASP:H	29	0.16
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	31	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	1	0.16
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	7	0.16
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	28	0.16
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	29	0.16
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	32	0.16
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	17	0.16
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	8	0.16
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	8	0.16
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	8	0.16
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	8	0.16
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	8	0.16
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	8	0.16
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	23	0.16
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	23	0.16
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	23	0.16
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	23	0.16
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	23	0.16
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	23	0.16
(1,382)	1:B:255:ASP:HB2	1:B:258:LEU:HG	25	0.16
(1,382)	1:B:255:ASP:HB3	1:B:258:LEU:HG	25	0.16
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	13	0.16
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	13	0.16
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	13	0.16
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	22	0.16
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	22	0.16
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	22	0.16
(1,3664)	1:A:301:GLN:HA	1:A:301:GLN:HE21	11	0.16
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD21	22	0.16
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD22	22	0.16
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD23	22	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	3	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	3	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	3	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	4	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	4	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	4	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	9	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	9	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	9	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	14	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	14	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	16	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	16	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	16	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	17	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	17	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	17	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	18	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	18	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	18	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	27	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	27	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	27	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	31	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	31	0.16
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	31	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	2	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	2	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	2	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	14	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	14	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	14	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	23	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	23	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	23	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	31	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	31	0.16
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	31	0.16
(1,3343)	1:A:248:SER:HA	1:A:250:ASP:H	3	0.16
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	14	0.16
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	19	0.16
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	24	0.16
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	10	0.16
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	17	0.16
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	24	0.16
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	12	0.16
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	17	0.16
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	24	0.16
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	26	0.16
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	30	0.16
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	32	0.16
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	3	0.16
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	13	0.16
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	23	0.16
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	18	0.16
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	18	0.16
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	18	0.16
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	7	0.16
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	7	0.16
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	7	0.16
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	18	0.16
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	18	0.16
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	18	0.16
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	8	0.16
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	8	0.16
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	25	0.16
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	25	0.16
(1,2202)	1:A:274:CYS:HB2	1:A:304:VAL:H	27	0.16
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD21	9	0.16
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD22	9	0.16
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD23	9	0.16
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD21	9	0.16
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD22	9	0.16
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD23	9	0.16
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD21	9	0.16
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD22	9	0.16
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD23	9	0.16
(1,1250)	1:A:265:ILE:HD11	1:A:328:TYR:HB2	10	0.16
(1,1250)	1:A:265:ILE:HD12	1:A:328:TYR:HB2	10	0.16
(1,1250)	1:A:265:ILE:HD13	1:A:328:TYR:HB2	10	0.16
(1,1230)	1:A:265:ILE:HD11	1:A:266:MET:HA	20	0.16
(1,1230)	1:A:265:ILE:HD12	1:A:266:MET:HA	20	0.16
(1,1230)	1:A:265:ILE:HD13	1:A:266:MET:HA	20	0.16
(1,1114)	1:A:245:PRO:HB2	1:A:247:GLY:H	14	0.16
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	2	0.15
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	2	0.15
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	2	0.15
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	9	0.15
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	9	0.15
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	9	0.15
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	16	0.15
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	16	0.15
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	16	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	5	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	5	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	5	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	5	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	5	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	5	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	5	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	5	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	5	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	5	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	5	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	5	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	5	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	5	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	5	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	5	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	5	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	7	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	7	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	7	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	7	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	7	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	7	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	7	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	7	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	7	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	7	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	7	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	7	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	7	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	7	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	7	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	7	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	7	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	7	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	11	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	11	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	11	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	11	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	11	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	11	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	11	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	11	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	11	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	11	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	11	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	11	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	11	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	11	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	11	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	11	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	11	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	12	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	12	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	12	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	12	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	12	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	12	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	12	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	12	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	12	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	12	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	12	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	12	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	12	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	12	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	12	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	12	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	12	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	12	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	18	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	18	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	18	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	18	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	18	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	18	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	18	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	18	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	18	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	18	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	18	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	18	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	18	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	18	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	18	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	18	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	18	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	21	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	21	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	21	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	21	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	21	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	21	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	21	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	21	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	21	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	21	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	21	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	21	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	21	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	21	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	21	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	21	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	21	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	21	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	27	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	27	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	27	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	27	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	27	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	27	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	27	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	27	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	27	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	27	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	27	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	27	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	27	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	27	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	27	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	27	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	27	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	27	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	29	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	29	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	29	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	29	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	29	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	29	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	29	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	29	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	29	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	29	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	29	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	29	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	29	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	29	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	29	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	29	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	29	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	29	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	32	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	32	0.15
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	32	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	32	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	32	0.15
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	32	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	32	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	32	0.15
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	32	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	32	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	32	0.15
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	32	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	32	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	32	0.15
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	32	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	32	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	32	0.15
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	32	0.15
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	3	0.15
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	3	0.15
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	3	0.15
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	3	0.15
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	3	0.15
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	3	0.15
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	8	0.15
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	8	0.15
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	8	0.15
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	8	0.15
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	8	0.15
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	17	0.15
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	17	0.15
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	17	0.15
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	17	0.15
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	17	0.15
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	17	0.15
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	24	0.15
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	24	0.15
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	24	0.15
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	24	0.15
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	24	0.15
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	24	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	4	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	4	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	4	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	4	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	4	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	4	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	4	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	4	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	4	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	4	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	4	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	4	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	4	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	4	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	4	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	4	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	4	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	4	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	12	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	12	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	12	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	12	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	12	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	12	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	12	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	12	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	12	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	12	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	12	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	12	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	12	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	12	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	12	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	12	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	12	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	14	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	14	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	14	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	14	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	14	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	14	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	14	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	14	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	14	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	14	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	14	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	14	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	14	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	14	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	14	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	14	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	14	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	14	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	19	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	19	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	19	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	19	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	19	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	19	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	19	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	19	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	19	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	19	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	19	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	19	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	19	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	19	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	19	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	19	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	19	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	27	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	27	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	27	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	27	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	27	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	27	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	27	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	27	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	27	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	27	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	27	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	27	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	27	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	27	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	27	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	27	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	27	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	27	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	28	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	28	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	28	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	28	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	28	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	28	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	28	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	28	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	28	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	28	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	28	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	28	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	28	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	28	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	28	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	28	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	28	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	28	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	31	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	31	0.15
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	31	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	31	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	31	0.15
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	31	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	31	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	31	0.15
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	31	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	31	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	31	0.15
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	31	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	31	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	31	0.15
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	31	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	31	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	31	0.15
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	31	0.15
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	7	0.15
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	7	0.15
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	7	0.15
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	13	0.15
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	13	0.15
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	13	0.15
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	2	0.15
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	2	0.15
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	2	0.15
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	24	0.15
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	24	0.15
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	24	0.15
(1,665)	1:A:258:LEU:HD11	1:A:265:ILE:H	8	0.15
(1,665)	1:A:258:LEU:HD12	1:A:265:ILE:H	8	0.15
(1,665)	1:A:258:LEU:HD13	1:A:265:ILE:H	8	0.15
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	32	0.15
(1,5210)	1:B:333:ARG:HG2	1:B:335:GLN:H	20	0.15
(1,5210)	1:B:333:ARG:HG3	1:B:335:GLN:H	20	0.15
(1,5177)	1:A:333:ARG:HA	1:A:333:ARG:HD2	27	0.15
(1,5177)	1:A:333:ARG:HA	1:A:333:ARG:HD3	27	0.15
(1,5086)	1:B:331:ARG:HA	1:B:331:ARG:HE	6	0.15
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	25	0.15
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	7	0.15
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	14	0.15
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	22	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	9	0.15
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	9	0.15
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	10	0.15
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	10	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	7	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	7	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	7	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	7	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	7	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	7	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	24	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	24	0.15
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	24	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	24	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	24	0.15
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	24	0.15
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	6	0.15
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	6	0.15
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	12	0.15
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	12	0.15
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG21	1	0.15
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG22	1	0.15
(1,4994)	1:A:328:TYR:HE1	1:A:329:THR:HG23	1	0.15
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG21	1	0.15
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG22	1	0.15
(1,4994)	1:A:328:TYR:HE2	1:A:329:THR:HG23	1	0.15
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	12	0.15
(1,4836)	1:B:323:LYS:HD3	1:B:329:THR:H	19	0.15
(1,4786)	1:A:251:ASP:H	1:A:252:PRO:HD2	2	0.15
(1,4786)	1:A:251:ASP:H	1:A:252:PRO:HD2	10	0.15
(1,4627)	1:B:320:ASN:HA	1:B:323:LYS:HD3	7	0.15
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	17	0.15
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	17	0.15
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	12	0.15
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	32	0.15
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	10	0.15
(1,4175)	1:B:250:ASP:HB2	1:B:251:ASP:HA	26	0.15
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	29	0.15
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	2	0.15
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	3	0.15
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	9	0.15
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	17	0.15
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	20	0.15
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	10	0.15
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	32	0.15
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	9	0.15
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	9	0.15
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	9	0.15
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	9	0.15
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	9	0.15
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	9	0.15
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	27	0.15
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	27	0.15
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	27	0.15
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	27	0.15
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	27	0.15
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	27	0.15
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	32	0.15
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	32	0.15
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	32	0.15
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	32	0.15
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	32	0.15
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	32	0.15
(1,375)	1:A:255:ASP:HB2	1:A:258:LEU:HG	10	0.15
(1,375)	1:A:255:ASP:HB3	1:A:258:LEU:HG	10	0.15
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	23	0.15
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	23	0.15
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	23	0.15
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	27	0.15
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	27	0.15
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	27	0.15
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD21	20	0.15
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD22	20	0.15
(1,359)	1:A:255:ASP:HA	1:A:258:LEU:HD23	20	0.15
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	26	0.15
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	26	0.15
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	26	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	5	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	5	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	5	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	7	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	7	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	8	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	8	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	8	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	13	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	13	0.15
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	13	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	1	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	1	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	1	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	13	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	13	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	13	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	15	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	15	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	15	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	16	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	16	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	16	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	19	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	19	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	19	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	26	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	26	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	26	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	28	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	28	0.15
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	28	0.15
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	7	0.15
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	18	0.15
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	25	0.15
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	32	0.15
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	1	0.15
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	5	0.15
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	8	0.15
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	13	0.15
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	30	0.15
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	4	0.15
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	8	0.15
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	15	0.15
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	16	0.15
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	20	0.15
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	23	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	31	0.15
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	16	0.15
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	17	0.15
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	17	0.15
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	17	0.15
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	21	0.15
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	21	0.15
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	21	0.15
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	14	0.15
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	14	0.15
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	14	0.15
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	16	0.15
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	16	0.15
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	16	0.15
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	20	0.15
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	20	0.15
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	20	0.15
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	26	0.15
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	26	0.15
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	26	0.15
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	7	0.15
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	15	0.15
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	17	0.15
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	14	0.15
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	32	0.15
(1,2439)	1:B:279:TYR:HE1	1:B:299:CYS:H	10	0.15
(1,2439)	1:B:279:TYR:HE2	1:B:299:CYS:H	10	0.15
(1,2424)	1:A:279:TYR:HE1	1:A:299:CYS:H	10	0.15
(1,2424)	1:A:279:TYR:HE2	1:A:299:CYS:H	10	0.15
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	29	0.15
(1,1252)	1:B:265:ILE:HD11	1:B:266:MET:HA	31	0.15
(1,1252)	1:B:265:ILE:HD12	1:B:266:MET:HA	31	0.15
(1,1252)	1:B:265:ILE:HD13	1:B:266:MET:HA	31	0.15
(1,1250)	1:A:265:ILE:HD11	1:A:328:TYR:HB2	22	0.15
(1,1250)	1:A:265:ILE:HD12	1:A:328:TYR:HB2	22	0.15
(1,1250)	1:A:265:ILE:HD13	1:A:328:TYR:HB2	22	0.15
(1,1230)	1:A:265:ILE:HD11	1:A:266:MET:HA	10	0.15
(1,1230)	1:A:265:ILE:HD12	1:A:266:MET:HA	10	0.15
(1,1230)	1:A:265:ILE:HD13	1:A:266:MET:HA	10	0.15
(1,12)	1:A:305:SER:H	1:A:305:SER:HB3	30	0.15
(1,1116)	1:A:245:PRO:HD3	1:A:246:LEU:H	4	0.15
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	7	0.14
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	7	0.14
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	9	0.14
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	9	0.14
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	9	0.14
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	22	0.14
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	22	0.14
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	22	0.14
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	24	0.14
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	24	0.14
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	24	0.14
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	26	0.14
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	26	0.14
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	26	0.14
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	8	0.14
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	8	0.14
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	8	0.14
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	8	0.14
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	8	0.14
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	8	0.14
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	8	0.14
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	8	0.14
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	8	0.14
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	8	0.14
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	8	0.14
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	8	0.14
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	8	0.14
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	8	0.14
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	8	0.14
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	8	0.14
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	8	0.14
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	8	0.14
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	31	0.14
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	31	0.14
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	31	0.14
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	31	0.14
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	31	0.14
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	31	0.14
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	31	0.14
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	31	0.14
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	31	0.14
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	31	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	31	0.14
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	31	0.14
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	31	0.14
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	31	0.14
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	31	0.14
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	31	0.14
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	31	0.14
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	31	0.14
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	6	0.14
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	6	0.14
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	6	0.14
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	6	0.14
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	6	0.14
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	6	0.14
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	18	0.14
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	18	0.14
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	18	0.14
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	18	0.14
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	18	0.14
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	18	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	15	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	15	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	15	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	15	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	15	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	15	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	15	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	15	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	15	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	15	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	15	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	15	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	15	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	15	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	15	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	15	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	15	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	15	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	16	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	16	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	16	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	16	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	16	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	16	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	16	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	16	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	16	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	16	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	16	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	16	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	16	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	16	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	16	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	16	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	16	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	18	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	18	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	18	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	18	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	18	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	18	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	18	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	18	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	18	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	18	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	18	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	18	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	18	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	18	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	18	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	18	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	18	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	18	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	24	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	24	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	24	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	24	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	24	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	24	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	24	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	24	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	24	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	24	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	24	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	24	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	24	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	24	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	24	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	24	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	24	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	24	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	25	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	25	0.14
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	25	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	25	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	25	0.14
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	25	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	25	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	25	0.14
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	25	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	25	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	25	0.14
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	25	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	25	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	25	0.14
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	25	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	25	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	25	0.14
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	25	0.14
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	13	0.14
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	13	0.14
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	13	0.14
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	13	0.14
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	13	0.14
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	13	0.14
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	18	0.14
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	18	0.14
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	18	0.14
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	18	0.14
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	18	0.14
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	18	0.14
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	30	0.14
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	30	0.14
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	30	0.14
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	30	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	30	0.14
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	30	0.14
(1,80)	1:A:253:ILE:HB	1:A:258:LEU:H	8	0.14
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	27	0.14
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	27	0.14
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	27	0.14
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	27	0.14
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	27	0.14
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	27	0.14
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	3	0.14
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	3	0.14
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	3	0.14
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	12	0.14
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	12	0.14
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	12	0.14
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	16	0.14
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	16	0.14
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	16	0.14
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	20	0.14
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	20	0.14
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	20	0.14
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	22	0.14
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	22	0.14
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	22	0.14
(1,665)	1:A:258:LEU:HD11	1:A:265:ILE:H	15	0.14
(1,665)	1:A:258:LEU:HD12	1:A:265:ILE:H	15	0.14
(1,665)	1:A:258:LEU:HD13	1:A:265:ILE:H	15	0.14
(1,665)	1:A:258:LEU:HD11	1:A:265:ILE:H	27	0.14
(1,665)	1:A:258:LEU:HD12	1:A:265:ILE:H	27	0.14
(1,665)	1:A:258:LEU:HD13	1:A:265:ILE:H	27	0.14
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	9	0.14
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	28	0.14
(1,525)	1:B:257:LEU:HD11	1:B:318:ALA:HB1	31	0.14
(1,525)	1:B:257:LEU:HD11	1:B:318:ALA:HB2	31	0.14
(1,525)	1:B:257:LEU:HD11	1:B:318:ALA:HB3	31	0.14
(1,525)	1:B:257:LEU:HD12	1:B:318:ALA:HB1	31	0.14
(1,525)	1:B:257:LEU:HD12	1:B:318:ALA:HB2	31	0.14
(1,525)	1:B:257:LEU:HD12	1:B:318:ALA:HB3	31	0.14
(1,525)	1:B:257:LEU:HD13	1:B:318:ALA:HB1	31	0.14
(1,525)	1:B:257:LEU:HD13	1:B:318:ALA:HB2	31	0.14
(1,525)	1:B:257:LEU:HD13	1:B:318:ALA:HB3	31	0.14
(1,5189)	1:A:333:ARG:HB2	1:A:334:LYS:H	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5189)	1:A:333:ARG:HB3	1:A:334:LYS:H	17	0.14
(1,5176)	1:B:252:PRO:HG2	1:B:253:ILE:H	16	0.14
(1,5176)	1:B:252:PRO:HG3	1:B:253:ILE:H	16	0.14
(1,5176)	1:B:252:PRO:HG2	1:B:253:ILE:H	19	0.14
(1,5176)	1:B:252:PRO:HG3	1:B:253:ILE:H	19	0.14
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	27	0.14
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	14	0.14
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	18	0.14
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	25	0.14
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	13	0.14
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	13	0.14
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	11	0.14
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	11	0.14
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	11	0.14
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	11	0.14
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	11	0.14
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	11	0.14
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	12	0.14
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	12	0.14
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	12	0.14
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	12	0.14
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	12	0.14
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	12	0.14
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	18	0.14
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	18	0.14
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	8	0.14
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	8	0.14
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	15	0.14
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	15	0.14
(1,4860)	1:B:323:LYS:HG2	1:B:328:TYR:HD1	31	0.14
(1,4860)	1:B:323:LYS:HG2	1:B:328:TYR:HD2	31	0.14
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG2	12	0.14
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG3	12	0.14
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	10	0.14
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	6	0.14
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	31	0.14
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	1	0.14
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	1	0.14
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	17	0.14
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	17	0.14
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	20	0.14
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	15	0.14
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	15	0.14
(1,4237)	1:B:313:LYS:HG2	1:B:316:ARG:HD3	26	0.14
(1,4218)	1:A:313:LYS:HG3	1:B:278:SER:H	7	0.14
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	20	0.14
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	21	0.14
(1,4175)	1:B:250:ASP:HB2	1:B:251:ASP:HA	14	0.14
(1,4169)	1:A:250:ASP:HA	1:A:251:ASP:H	20	0.14
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	9	0.14
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	25	0.14
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	13	0.14
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	13	0.14
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	21	0.14
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	23	0.14
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	11	0.14
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	24	0.14
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	31	0.14
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	15	0.14
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	15	0.14
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	15	0.14
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	15	0.14
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	15	0.14
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	15	0.14
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	31	0.14
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	31	0.14
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	31	0.14
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	31	0.14
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	31	0.14
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	31	0.14
(1,375)	1:A:255:ASP:HB2	1:A:258:LEU:HG	15	0.14
(1,375)	1:A:255:ASP:HB3	1:A:258:LEU:HG	15	0.14
(1,375)	1:A:255:ASP:HB2	1:A:258:LEU:HG	17	0.14
(1,375)	1:A:255:ASP:HB3	1:A:258:LEU:HG	17	0.14
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	2	0.14
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	2	0.14
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	2	0.14
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	11	0.14
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	11	0.14
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	11	0.14
(1,3664)	1:A:301:GLN:HA	1:A:301:GLN:HE21	2	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	11	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	11	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	19	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	19	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	19	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	26	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	26	0.14
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	26	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	8	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	8	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	8	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	17	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	17	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	17	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	27	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	27	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	27	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	30	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	30	0.14
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	30	0.14
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	8	0.14
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	13	0.14
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	18	0.14
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	27	0.14
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	16	0.14
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	20	0.14
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	20	0.14
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	4	0.14
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD11	13	0.14
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD12	13	0.14
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD13	13	0.14
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD21	13	0.14
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD22	13	0.14
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD23	13	0.14
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	5	0.14
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	25	0.14
(1,3168)	1:B:288:LEU:HD11	1:B:309:LEU:H	6	0.14
(1,3168)	1:B:288:LEU:HD12	1:B:309:LEU:H	6	0.14
(1,3168)	1:B:288:LEU:HD13	1:B:309:LEU:H	6	0.14
(1,3168)	1:B:288:LEU:HD21	1:B:309:LEU:H	6	0.14
(1,3168)	1:B:288:LEU:HD22	1:B:309:LEU:H	6	0.14
(1,3168)	1:B:288:LEU:HD23	1:B:309:LEU:H	6	0.14
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	3	0.14
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	3	0.14
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	15	0.14
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	15	0.14
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	15	0.14
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	19	0.14
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	19	0.14
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	19	0.14
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	25	0.14
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	25	0.14
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	25	0.14
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	26	0.14
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	26	0.14
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	26	0.14
(1,3028)	1:B:287:ALA:HB1	1:B:288:LEU:HG	6	0.14
(1,3028)	1:B:287:ALA:HB2	1:B:288:LEU:HG	6	0.14
(1,3028)	1:B:287:ALA:HB3	1:B:288:LEU:HG	6	0.14
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	17	0.14
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	17	0.14
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	17	0.14
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	21	0.14
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	21	0.14
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	21	0.14
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	25	0.14
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	25	0.14
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	25	0.14
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	32	0.14
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	32	0.14
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	32	0.14
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	1	0.14
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	4	0.14
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	29	0.14
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	32	0.14
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	5	0.14
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	7	0.14
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	20	0.14
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	26	0.14
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	7	0.14
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	8	0.14
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	14	0.14
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	13	0.14
(1,1117)	1:B:245:PRO:HD3	1:B:246:LEU:H	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1114)	1:A:245:PRO:HB2	1:A:247:GLY:H	25	0.14
(1,1114)	1:A:245:PRO:HB2	1:A:247:GLY:H	32	0.14
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	1	0.13
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	1	0.13
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	1	0.13
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	14	0.13
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	14	0.13
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	14	0.13
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	25	0.13
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	25	0.13
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	25	0.13
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	1	0.13
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	1	0.13
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	1	0.13
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	6	0.13
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	6	0.13
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	6	0.13
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	19	0.13
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	19	0.13
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	19	0.13
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	24	0.13
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	24	0.13
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	24	0.13
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	28	0.13
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	28	0.13
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	28	0.13
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	32	0.13
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	32	0.13
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	32	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	13	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	13	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	13	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	13	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	13	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	13	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	13	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	13	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	13	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	13	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	13	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	13	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	13	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	13	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	13	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	13	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	13	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	15	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	15	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	15	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	15	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	15	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	15	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	15	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	15	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	15	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	15	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	15	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	15	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	15	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	15	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	15	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	15	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	15	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	15	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	24	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	24	0.13
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	24	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	24	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	24	0.13
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	24	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	24	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	24	0.13
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	24	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	24	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	24	0.13
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	24	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	24	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	24	0.13
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	24	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	24	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	24	0.13
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	24	0.13
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	7	0.13
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	7	0.13
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	7	0.13
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	7	0.13
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	7	0.13
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	9	0.13
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	9	0.13
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	9	0.13
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	9	0.13
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	9	0.13
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	9	0.13
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	20	0.13
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	20	0.13
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	20	0.13
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	20	0.13
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	20	0.13
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	20	0.13
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	23	0.13
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	23	0.13
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	23	0.13
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	23	0.13
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	23	0.13
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	23	0.13
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	26	0.13
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	26	0.13
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	26	0.13
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	26	0.13
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	26	0.13
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	26	0.13
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	21	0.13
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	21	0.13
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	21	0.13
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	21	0.13
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	21	0.13
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	21	0.13
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	21	0.13
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	21	0.13
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	21	0.13
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	21	0.13
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	21	0.13
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	21	0.13
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	21	0.13
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	21	0.13
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	21	0.13
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	21	0.13
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	21	0.13
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	26	0.13
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	26	0.13
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	26	0.13
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	26	0.13
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	26	0.13
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	26	0.13
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	26	0.13
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	26	0.13
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	26	0.13
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	26	0.13
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	26	0.13
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	26	0.13
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	26	0.13
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	26	0.13
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	26	0.13
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	26	0.13
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	26	0.13
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	26	0.13
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	1	0.13
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	1	0.13
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	1	0.13
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	1	0.13
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	1	0.13
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	1	0.13
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	3	0.13
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	3	0.13
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	3	0.13
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	3	0.13
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	3	0.13
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	3	0.13
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	23	0.13
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	23	0.13
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	23	0.13
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	23	0.13
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	23	0.13
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	23	0.13
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	26	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	26	0.13
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	26	0.13
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	26	0.13
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	26	0.13
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	26	0.13
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	19	0.13
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	19	0.13
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	19	0.13
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	19	0.13
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	19	0.13
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	19	0.13
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	2	0.13
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	2	0.13
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	2	0.13
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	14	0.13
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	14	0.13
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	14	0.13
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	14	0.13
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	14	0.13
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	14	0.13
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	15	0.13
(1,5197)	1:A:333:ARG:HB3	1:A:334:LYS:H	8	0.13
(1,5190)	1:A:333:ARG:HB2	1:A:335:GLN:H	17	0.13
(1,5190)	1:A:333:ARG:HB3	1:A:335:GLN:H	17	0.13
(1,5177)	1:A:333:ARG:HA	1:A:333:ARG:HD2	15	0.13
(1,5177)	1:A:333:ARG:HA	1:A:333:ARG:HD3	15	0.13
(1,5133)	1:A:332:LEU:HB2	1:A:333:ARG:H	27	0.13
(1,5086)	1:B:331:ARG:HA	1:B:331:ARG:HE	13	0.13
(1,5086)	1:B:331:ARG:HA	1:B:331:ARG:HE	15	0.13
(1,5080)	1:A:331:ARG:HA	1:A:331:ARG:HD2	18	0.13
(1,5080)	1:A:331:ARG:HA	1:A:331:ARG:HD3	18	0.13
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	2	0.13
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	19	0.13
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	26	0.13
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	30	0.13
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	26	0.13
(1,5000)	1:B:328:TYR:HE1	1:B:330:LYS:H	31	0.13
(1,5000)	1:B:328:TYR:HE2	1:B:330:LYS:H	31	0.13
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	8	0.13
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	8	0.13
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	17	0.13
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	23	0.13
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	23	0.13
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	18	0.13
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	18	0.13
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	18	0.13
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	18	0.13
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	18	0.13
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	18	0.13
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	26	0.13
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	26	0.13
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD1	22	0.13
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD2	22	0.13
(1,4834)	1:A:323:LYS:HD3	1:A:329:THR:H	13	0.13
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	1	0.13
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	1	0.13
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	2	0.13
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	2	0.13
(1,4786)	1:A:251:ASP:H	1:A:252:PRO:HD2	17	0.13
(1,4778)	1:A:251:ASP:HB2	1:A:252:PRO:HD2	22	0.13
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	5	0.13
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	26	0.13
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	27	0.13
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	29	0.13
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	29	0.13
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	2	0.13
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	2	0.13
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	13	0.13
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	13	0.13
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	30	0.13
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	30	0.13
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	18	0.13
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	24	0.13
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB1	10	0.13
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB2	10	0.13
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB3	10	0.13
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB1	10	0.13
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB2	10	0.13
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB3	10	0.13
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB1	5	0.13
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB2	5	0.13
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB3	5	0.13
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB1	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB2	5	0.13
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB3	5	0.13
(1,4175)	1:B:250:ASP:HB2	1:B:251:ASP:HA	32	0.13
(1,4172)	1:A:250:ASP:HB2	1:A:251:ASP:H	15	0.13
(1,4172)	1:A:250:ASP:HB3	1:A:251:ASP:H	15	0.13
(1,4170)	1:B:250:ASP:HA	1:B:251:ASP:H	25	0.13
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	11	0.13
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	28	0.13
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	2	0.13
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	12	0.13
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	24	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	1	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	7	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	14	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	16	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	18	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	19	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	24	0.13
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	27	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	1	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	3	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	7	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	12	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	14	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	16	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	18	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	19	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	20	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	22	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	25	0.13
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	26	0.13
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	10	0.13
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	10	0.13
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	10	0.13
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	10	0.13
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	10	0.13
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	10	0.13
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	19	0.13
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	19	0.13
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	19	0.13
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	19	0.13
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	19	0.13
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD11	10	0.13
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD12	10	0.13
(1,367)	1:B:255:ASP:HA	1:B:258:LEU:HD13	10	0.13
(1,3664)	1:A:301:GLN:HA	1:A:301:GLN:HE21	3	0.13
(1,3664)	1:A:301:GLN:HA	1:A:301:GLN:HE21	13	0.13
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	15	0.13
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	15	0.13
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	15	0.13
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	21	0.13
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	21	0.13
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	21	0.13
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	5	0.13
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	5	0.13
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	5	0.13
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	21	0.13
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	21	0.13
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	21	0.13
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	3	0.13
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	7	0.13
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	13	0.13
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	10	0.13
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	23	0.13
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	28	0.13
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	29	0.13
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	31	0.13
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	12	0.13
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	16	0.13
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	23	0.13
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	12	0.13
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	16	0.13
(1,3202)	1:A:288:LEU:H	1:A:289:LEU:HD11	18	0.13
(1,3202)	1:A:288:LEU:H	1:A:289:LEU:HD12	18	0.13
(1,3202)	1:A:288:LEU:H	1:A:289:LEU:HD13	18	0.13
(1,3202)	1:A:288:LEU:H	1:A:289:LEU:HD21	18	0.13
(1,3202)	1:A:288:LEU:H	1:A:289:LEU:HD22	18	0.13
(1,3202)	1:A:288:LEU:H	1:A:289:LEU:HD23	18	0.13
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	14	0.13
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	25	0.13
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	9	0.13
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	14	0.13
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	30	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	30	0.13
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	30	0.13
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	32	0.13
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	32	0.13
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	32	0.13
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	10	0.13
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	14	0.13
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	20	0.13
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	25	0.13
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	26	0.13
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	6	0.13
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	15	0.13
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	29	0.13
(1,29)	1:B:305:SER:H	1:B:305:SER:HB3	3	0.13
(1,2633)	1:B:247:GLY:H	1:B:250:ASP:HB2	22	0.13
(1,2629)	1:B:247:GLY:H	1:B:248:SER:HA	22	0.13
(1,2268)	1:B:275:CYS:HB2	1:B:299:CYS:HA	24	0.13
(1,1563)	1:B:269:ALA:HB1	1:B:315:LEU:HD21	9	0.13
(1,1563)	1:B:269:ALA:HB1	1:B:315:LEU:HD22	9	0.13
(1,1563)	1:B:269:ALA:HB1	1:B:315:LEU:HD23	9	0.13
(1,1563)	1:B:269:ALA:HB2	1:B:315:LEU:HD21	9	0.13
(1,1563)	1:B:269:ALA:HB2	1:B:315:LEU:HD22	9	0.13
(1,1563)	1:B:269:ALA:HB2	1:B:315:LEU:HD23	9	0.13
(1,1563)	1:B:269:ALA:HB3	1:B:315:LEU:HD21	9	0.13
(1,1563)	1:B:269:ALA:HB3	1:B:315:LEU:HD22	9	0.13
(1,1563)	1:B:269:ALA:HB3	1:B:315:LEU:HD23	9	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD21	13	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD22	13	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD23	13	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD21	13	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD22	13	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD23	13	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD21	13	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD22	13	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD23	13	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD21	23	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD22	23	0.13
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD23	23	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD21	23	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD22	23	0.13
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD23	23	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD21	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD22	23	0.13
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD23	23	0.13
(1,1121)	1:B:245:PRO:HG2	1:B:246:LEU:H	20	0.13
(1,1121)	1:B:245:PRO:HG3	1:B:246:LEU:H	20	0.13
(1,1114)	1:A:245:PRO:HB2	1:A:247:GLY:H	16	0.13
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	3	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	3	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	3	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	6	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	6	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	6	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	11	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	11	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	11	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	13	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	13	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	13	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	19	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	19	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	19	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	21	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	21	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	21	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	28	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	28	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	28	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	29	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	29	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	29	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	32	0.12
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	32	0.12
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	32	0.12
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	2	0.12
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	2	0.12
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	2	0.12
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	7	0.12
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	7	0.12
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	7	0.12
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	12	0.12
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	12	0.12
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	12	0.12
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	14	0.12
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	14	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	3	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	3	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	3	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	3	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	3	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	3	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	3	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	3	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	3	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	3	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	3	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	3	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	3	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	3	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	3	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	3	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	3	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	3	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	20	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	20	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	20	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	20	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	20	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	20	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	20	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	20	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	20	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	20	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	20	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	20	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	20	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	20	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	20	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	20	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	20	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	20	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG21	23	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG22	23	0.12
(1,868)	1:B:260:LEU:HD11	1:B:298:THR:HG23	23	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG21	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG22	23	0.12
(1,868)	1:B:260:LEU:HD12	1:B:298:THR:HG23	23	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG21	23	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG22	23	0.12
(1,868)	1:B:260:LEU:HD13	1:B:298:THR:HG23	23	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG21	23	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG22	23	0.12
(1,868)	1:B:260:LEU:HD21	1:B:298:THR:HG23	23	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG21	23	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG22	23	0.12
(1,868)	1:B:260:LEU:HD22	1:B:298:THR:HG23	23	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG21	23	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG22	23	0.12
(1,868)	1:B:260:LEU:HD23	1:B:298:THR:HG23	23	0.12
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	1	0.12
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	1	0.12
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	1	0.12
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	1	0.12
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	1	0.12
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	1	0.12
(1,862)	1:B:260:LEU:HD11	1:B:279:TYR:HB3	30	0.12
(1,862)	1:B:260:LEU:HD12	1:B:279:TYR:HB3	30	0.12
(1,862)	1:B:260:LEU:HD13	1:B:279:TYR:HB3	30	0.12
(1,862)	1:B:260:LEU:HD21	1:B:279:TYR:HB3	30	0.12
(1,862)	1:B:260:LEU:HD22	1:B:279:TYR:HB3	30	0.12
(1,862)	1:B:260:LEU:HD23	1:B:279:TYR:HB3	30	0.12
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	11	0.12
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	11	0.12
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	11	0.12
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	11	0.12
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	11	0.12
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	11	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	8	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	8	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	8	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	8	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	8	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	8	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	15	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	15	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	15	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	15	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	15	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	17	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	17	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	17	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	17	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	17	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	17	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	31	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	31	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	31	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	31	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	31	0.12
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	31	0.12
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	10	0.12
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	10	0.12
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	10	0.12
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	19	0.12
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	19	0.12
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	19	0.12
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	30	0.12
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	30	0.12
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	30	0.12
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	16	0.12
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	16	0.12
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	16	0.12
(1,677)	1:A:258:LEU:HD21	1:A:265:ILE:H	30	0.12
(1,677)	1:A:258:LEU:HD22	1:A:265:ILE:H	30	0.12
(1,677)	1:A:258:LEU:HD23	1:A:265:ILE:H	30	0.12
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	8	0.12
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	20	0.12
(1,5222)	1:B:333:ARG:H	1:B:335:GLN:H	31	0.12
(1,5210)	1:B:333:ARG:HG2	1:B:335:GLN:H	24	0.12
(1,5210)	1:B:333:ARG:HG3	1:B:335:GLN:H	24	0.12
(1,5210)	1:B:333:ARG:HG2	1:B:335:GLN:H	32	0.12
(1,5210)	1:B:333:ARG:HG3	1:B:335:GLN:H	32	0.12
(1,5176)	1:B:252:PRO:HG2	1:B:253:ILE:H	12	0.12
(1,5176)	1:B:252:PRO:HG3	1:B:253:ILE:H	12	0.12
(1,5086)	1:B:331:ARG:HA	1:B:331:ARG:HE	8	0.12
(1,5086)	1:B:331:ARG:HA	1:B:331:ARG:HE	9	0.12
(1,5083)	1:A:331:ARG:HA	1:A:332:LEU:H	28	0.12
(1,5052)	1:B:330:LYS:HD2	1:B:331:ARG:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	8	0.12
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	9	0.12
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	30	0.12
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	11	0.12
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	3	0.12
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	6	0.12
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	3	0.12
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	3	0.12
(1,4999)	1:B:328:TYR:HE1	1:B:329:THR:H	15	0.12
(1,4999)	1:B:328:TYR:HE2	1:B:329:THR:H	15	0.12
(1,4996)	1:A:328:TYR:HE1	1:A:330:LYS:H	22	0.12
(1,4996)	1:A:328:TYR:HE2	1:A:330:LYS:H	22	0.12
(1,4989)	1:B:328:TYR:HD1	1:B:329:THR:HB	1	0.12
(1,4989)	1:B:328:TYR:HD2	1:B:329:THR:HB	1	0.12
(1,4989)	1:B:328:TYR:HD1	1:B:329:THR:HB	18	0.12
(1,4989)	1:B:328:TYR:HD2	1:B:329:THR:HB	18	0.12
(1,4984)	1:A:328:TYR:HD1	1:A:329:THR:HB	23	0.12
(1,4984)	1:A:328:TYR:HD2	1:A:329:THR:HB	23	0.12
(1,4834)	1:A:323:LYS:HD3	1:A:329:THR:H	1	0.12
(1,4834)	1:A:323:LYS:HD3	1:A:329:THR:H	29	0.12
(1,4674)	1:B:321:ASN:H	1:B:321:ASN:HD22	23	0.12
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	21	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	6	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	6	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	11	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	11	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	18	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	18	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	24	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	24	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	25	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	25	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	31	0.12
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	31	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	5	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	5	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	6	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	6	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	29	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	29	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	31	0.12
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	31	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	5	0.12
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	9	0.12
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	14	0.12
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	15	0.12
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	17	0.12
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	27	0.12
(1,4371)	1:A:316:ARG:HA	1:A:319:VAL:HA	14	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB1	2	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB2	2	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB3	2	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB1	2	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB2	2	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB3	2	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB1	22	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB2	22	0.12
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB3	22	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB1	22	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB2	22	0.12
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB3	22	0.12
(1,4218)	1:A:313:LYS:HG3	1:B:278:SER:H	3	0.12
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	7	0.12
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	19	0.12
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	23	0.12
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	27	0.12
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	11	0.12
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	12	0.12
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	22	0.12
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	30	0.12
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	31	0.12
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	4	0.12
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	8	0.12
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	5	0.12
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	5	0.12
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	5	0.12
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	5	0.12
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	5	0.12
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	5	0.12
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	28	0.12
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	28	0.12
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	28	0.12
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	28	0.12
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	28	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	28	0.12
(1,375)	1:A:255:ASP:HB2	1:A:258:LEU:HG	8	0.12
(1,375)	1:A:255:ASP:HB3	1:A:258:LEU:HG	8	0.12
(1,3672)	1:B:301:GLN:HA	1:B:301:GLN:HE21	13	0.12
(1,3664)	1:A:301:GLN:HA	1:A:301:GLN:HE21	20	0.12
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	3	0.12
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	8	0.12
(1,3462)	1:A:295:THR:HG21	1:A:300:HIS:H	15	0.12
(1,3462)	1:A:295:THR:HG22	1:A:300:HIS:H	15	0.12
(1,3462)	1:A:295:THR:HG23	1:A:300:HIS:H	15	0.12
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	13	0.12
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	27	0.12
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	27	0.12
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	28	0.12
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	29	0.12
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	30	0.12
(1,3343)	1:A:248:SER:HA	1:A:250:ASP:H	13	0.12
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	11	0.12
(1,3252)	1:A:289:LEU:H	1:A:289:LEU:HG	3	0.12
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	8	0.12
(1,3190)	1:A:288:LEU:HG	1:A:305:SER:HA	18	0.12
(1,3082)	1:B:288:LEU:HB3	1:B:294:HIS:H	6	0.12
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	7	0.12
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	7	0.12
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	7	0.12
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	8	0.12
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	8	0.12
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	8	0.12
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	11	0.12
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	11	0.12
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	11	0.12
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	14	0.12
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	14	0.12
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	14	0.12
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	29	0.12
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	29	0.12
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	29	0.12
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	13	0.12
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	13	0.12
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	13	0.12
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	23	0.12
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	23	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	23	0.12
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	27	0.12
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	27	0.12
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	27	0.12
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	6	0.12
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	30	0.12
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	2	0.12
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	4	0.12
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	10	0.12
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	25	0.12
(1,2633)	1:B:247:GLY:H	1:B:250:ASP:HB2	1	0.12
(1,2491)	1:A:280:CYS:HB2	1:A:285:ARG:H	8	0.12
(1,2215)	1:B:274:CYS:HB2	1:B:304:VAL:H	3	0.12
(1,2215)	1:B:274:CYS:HB2	1:B:304:VAL:H	21	0.12
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	1	0.12
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	18	0.12
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	21	0.12
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	24	0.12
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	2	0.12
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	5	0.12
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	24	0.12
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	29	0.12
(1,2059)	1:A:246:LEU:HD11	1:A:247:GLY:HA3	15	0.12
(1,2059)	1:A:246:LEU:HD12	1:A:247:GLY:HA3	15	0.12
(1,2059)	1:A:246:LEU:HD13	1:A:247:GLY:HA3	15	0.12
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD21	22	0.12
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD22	22	0.12
(1,1544)	1:A:269:ALA:HB1	1:A:315:LEU:HD23	22	0.12
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD21	22	0.12
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD22	22	0.12
(1,1544)	1:A:269:ALA:HB2	1:A:315:LEU:HD23	22	0.12
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD21	22	0.12
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD22	22	0.12
(1,1544)	1:A:269:ALA:HB3	1:A:315:LEU:HD23	22	0.12
(1,1447)	1:B:266:MET:H	1:B:319:VAL:HA	16	0.12
(1,1435)	1:A:266:MET:H	1:A:319:VAL:HA	21	0.12
(1,1435)	1:A:266:MET:H	1:A:319:VAL:HA	22	0.12
(1,1435)	1:A:266:MET:H	1:A:319:VAL:HA	27	0.12
(1,1250)	1:A:265:ILE:HD11	1:A:328:TYR:HB2	30	0.12
(1,1250)	1:A:265:ILE:HD12	1:A:328:TYR:HB2	30	0.12
(1,1250)	1:A:265:ILE:HD13	1:A:328:TYR:HB2	30	0.12
(1,1117)	1:B:245:PRO:HD3	1:B:246:LEU:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1116)	1:A:245:PRO:HD3	1:A:246:LEU:H	12	0.12
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	5	0.11
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	5	0.11
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	5	0.11
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	12	0.11
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	12	0.11
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	12	0.11
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	18	0.11
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	18	0.11
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	18	0.11
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	27	0.11
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	27	0.11
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	27	0.11
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	30	0.11
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	30	0.11
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	30	0.11
(1,978)	1:B:261:ILE:HD11	1:B:280:CYS:HB3	31	0.11
(1,978)	1:B:261:ILE:HD12	1:B:280:CYS:HB3	31	0.11
(1,978)	1:B:261:ILE:HD13	1:B:280:CYS:HB3	31	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	4	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	4	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	4	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	5	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	5	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	5	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	10	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	10	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	10	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	11	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	11	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	11	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	13	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	13	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	13	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	21	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	21	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	21	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	23	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	23	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	23	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	26	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	26	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	26	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	29	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	29	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	29	0.11
(1,951)	1:A:261:ILE:HD11	1:A:280:CYS:HB3	31	0.11
(1,951)	1:A:261:ILE:HD12	1:A:280:CYS:HB3	31	0.11
(1,951)	1:A:261:ILE:HD13	1:A:280:CYS:HB3	31	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	3	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	3	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	3	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	3	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	3	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	3	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	3	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	3	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	3	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	3	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	3	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	3	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	3	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	3	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	3	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	3	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	3	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	3	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	13	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	13	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	13	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	13	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	13	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	13	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	13	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	13	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	13	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	13	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	13	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	13	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	13	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	13	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	13	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	13	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	13	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG21	29	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG22	29	0.11
(1,848)	1:A:260:LEU:HD11	1:A:298:THR:HG23	29	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG21	29	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG22	29	0.11
(1,848)	1:A:260:LEU:HD12	1:A:298:THR:HG23	29	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG21	29	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG22	29	0.11
(1,848)	1:A:260:LEU:HD13	1:A:298:THR:HG23	29	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG21	29	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG22	29	0.11
(1,848)	1:A:260:LEU:HD21	1:A:298:THR:HG23	29	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG21	29	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG22	29	0.11
(1,848)	1:A:260:LEU:HD22	1:A:298:THR:HG23	29	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG21	29	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG22	29	0.11
(1,848)	1:A:260:LEU:HD23	1:A:298:THR:HG23	29	0.11
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	9	0.11
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	9	0.11
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	9	0.11
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	9	0.11
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	9	0.11
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	9	0.11
(1,842)	1:A:260:LEU:HD11	1:A:279:TYR:HB3	20	0.11
(1,842)	1:A:260:LEU:HD12	1:A:279:TYR:HB3	20	0.11
(1,842)	1:A:260:LEU:HD13	1:A:279:TYR:HB3	20	0.11
(1,842)	1:A:260:LEU:HD21	1:A:279:TYR:HB3	20	0.11
(1,842)	1:A:260:LEU:HD22	1:A:279:TYR:HB3	20	0.11
(1,842)	1:A:260:LEU:HD23	1:A:279:TYR:HB3	20	0.11
(1,702)	1:B:258:LEU:H	1:B:258:LEU:HG	31	0.11
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD11	10	0.11
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD12	10	0.11
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD13	10	0.11
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD21	10	0.11
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD22	10	0.11
(1,690)	1:A:258:LEU:H	1:A:258:LEU:HD23	10	0.11
(1,683)	1:B:258:LEU:HD21	1:B:265:ILE:H	17	0.11
(1,683)	1:B:258:LEU:HD22	1:B:265:ILE:H	17	0.11
(1,683)	1:B:258:LEU:HD23	1:B:265:ILE:H	17	0.11
(1,675)	1:A:258:LEU:HD21	1:A:264:ASP:HA	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,675)	1:A:258:LEU:HD22	1:A:264:ASP:HA	13	0.11
(1,675)	1:A:258:LEU:HD23	1:A:264:ASP:HA	13	0.11
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	10	0.11
(1,592)	1:B:257:LEU:H	1:B:258:LEU:HG	22	0.11
(1,577)	1:A:257:LEU:H	1:A:258:LEU:HG	26	0.11
(1,547)	1:B:257:LEU:HD21	1:B:258:LEU:H	32	0.11
(1,547)	1:B:257:LEU:HD22	1:B:258:LEU:H	32	0.11
(1,547)	1:B:257:LEU:HD23	1:B:258:LEU:H	32	0.11
(1,5240)	1:B:334:LYS:HG2	1:B:335:GLN:H	20	0.11
(1,5240)	1:B:334:LYS:HG3	1:B:335:GLN:H	20	0.11
(1,5216)	1:A:333:ARG:H	1:A:335:GLN:H	20	0.11
(1,5208)	1:A:333:ARG:HG2	1:A:335:GLN:H	2	0.11
(1,5208)	1:A:333:ARG:HG3	1:A:335:GLN:H	2	0.11
(1,5208)	1:A:333:ARG:HG2	1:A:335:GLN:H	17	0.11
(1,5208)	1:A:333:ARG:HG3	1:A:335:GLN:H	17	0.11
(1,5182)	1:B:333:ARG:HA	1:B:333:ARG:HD2	7	0.11
(1,5182)	1:B:333:ARG:HA	1:B:333:ARG:HD3	7	0.11
(1,5176)	1:B:252:PRO:HG2	1:B:253:ILE:H	1	0.11
(1,5176)	1:B:252:PRO:HG3	1:B:253:ILE:H	1	0.11
(1,5176)	1:B:252:PRO:HG2	1:B:253:ILE:H	24	0.11
(1,5176)	1:B:252:PRO:HG3	1:B:253:ILE:H	24	0.11
(1,5081)	1:A:331:ARG:HA	1:A:331:ARG:HE	11	0.11
(1,5080)	1:A:331:ARG:HA	1:A:331:ARG:HD2	31	0.11
(1,5080)	1:A:331:ARG:HA	1:A:331:ARG:HD3	31	0.11
(1,5052)	1:B:330:LYS:HD2	1:B:331:ARG:H	10	0.11
(1,5029)	1:B:329:THR:H	1:B:330:LYS:HA	15	0.11
(1,5025)	1:A:329:THR:H	1:A:330:LYS:HA	6	0.11
(1,5021)	1:B:329:THR:HG21	1:B:330:LYS:HE2	4	0.11
(1,5021)	1:B:329:THR:HG21	1:B:330:LYS:HE3	4	0.11
(1,5021)	1:B:329:THR:HG22	1:B:330:LYS:HE2	4	0.11
(1,5021)	1:B:329:THR:HG22	1:B:330:LYS:HE3	4	0.11
(1,5021)	1:B:329:THR:HG23	1:B:330:LYS:HE2	4	0.11
(1,5021)	1:B:329:THR:HG23	1:B:330:LYS:HE3	4	0.11
(1,5017)	1:B:329:THR:HB	1:B:330:LYS:HB3	31	0.11
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	10	0.11
(1,5015)	1:A:329:THR:HB	1:A:330:LYS:HB3	31	0.11
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	1	0.11
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	1	0.11
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	1	0.11
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	1	0.11
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	1	0.11
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG21	22	0.11
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG22	22	0.11
(1,4998)	1:B:328:TYR:HE1	1:B:329:THR:HG23	22	0.11
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG21	22	0.11
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG22	22	0.11
(1,4998)	1:B:328:TYR:HE2	1:B:329:THR:HG23	22	0.11
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	19	0.11
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	19	0.11
(1,4995)	1:A:328:TYR:HE1	1:A:329:THR:H	27	0.11
(1,4995)	1:A:328:TYR:HE2	1:A:329:THR:H	27	0.11
(1,4989)	1:B:328:TYR:HD1	1:B:329:THR:HB	7	0.11
(1,4989)	1:B:328:TYR:HD2	1:B:329:THR:HB	7	0.11
(1,4984)	1:A:328:TYR:HD1	1:A:329:THR:HB	3	0.11
(1,4984)	1:A:328:TYR:HD2	1:A:329:THR:HB	3	0.11
(1,4977)	1:A:328:TYR:HB3	1:A:329:THR:HG21	23	0.11
(1,4977)	1:A:328:TYR:HB3	1:A:329:THR:HG22	23	0.11
(1,4977)	1:A:328:TYR:HB3	1:A:329:THR:HG23	23	0.11
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	1	0.11
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	1	0.11
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	4	0.11
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	4	0.11
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD1	17	0.11
(1,4882)	1:B:323:LYS:H	1:B:328:TYR:HD2	17	0.11
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD1	13	0.11
(1,4871)	1:A:323:LYS:H	1:A:328:TYR:HD2	13	0.11
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD1	10	0.11
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD2	10	0.11
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD1	20	0.11
(1,4855)	1:A:323:LYS:HG2	1:A:328:TYR:HD2	20	0.11
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG2	20	0.11
(1,4794)	1:B:251:ASP:H	1:B:252:PRO:HG3	20	0.11
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	10	0.11
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	10	0.11
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG2	30	0.11
(1,4787)	1:A:251:ASP:H	1:A:252:PRO:HG3	30	0.11
(1,4786)	1:A:251:ASP:H	1:A:252:PRO:HD2	6	0.11
(1,4669)	1:A:321:ASN:H	1:A:321:ASN:HD22	17	0.11
(1,4638)	1:A:320:ASN:H	1:A:320:ASN:HD22	29	0.11
(1,4627)	1:B:320:ASN:HA	1:B:323:LYS:HD3	1	0.11
(1,4627)	1:B:320:ASN:HA	1:B:323:LYS:HD3	12	0.11
(1,4627)	1:B:320:ASN:HA	1:B:323:LYS:HD3	18	0.11
(1,4627)	1:B:320:ASN:HA	1:B:323:LYS:HD3	29	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4620)	1:A:320:ASN:HA	1:A:323:LYS:HD3	3	0.11
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	7	0.11
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	7	0.11
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE1	16	0.11
(1,4549)	1:B:319:VAL:HA	1:B:322:PHE:HE2	16	0.11
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	1	0.11
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	1	0.11
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	3	0.11
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	3	0.11
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE1	18	0.11
(1,4534)	1:A:319:VAL:HA	1:A:322:PHE:HE2	18	0.11
(1,4489)	1:B:318:ALA:HA	1:B:321:ASN:HD22	32	0.11
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	2	0.11
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	20	0.11
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	22	0.11
(1,4485)	1:B:318:ALA:HA	1:B:320:ASN:HD22	30	0.11
(1,4455)	1:B:317:GLN:HG2	1:B:317:GLN:HE21	26	0.11
(1,4443)	1:B:317:GLN:HB2	1:B:320:ASN:HD22	25	0.11
(1,4443)	1:B:317:GLN:HB3	1:B:320:ASN:HD22	25	0.11
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB1	5	0.11
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB2	5	0.11
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB3	5	0.11
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB1	5	0.11
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB2	5	0.11
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB3	5	0.11
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB1	18	0.11
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB2	18	0.11
(1,4287)	1:B:314:PHE:HD1	1:B:318:ALA:HB3	18	0.11
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB1	18	0.11
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB2	18	0.11
(1,4287)	1:B:314:PHE:HD2	1:B:318:ALA:HB3	18	0.11
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB1	10	0.11
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB2	10	0.11
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB3	10	0.11
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB1	10	0.11
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB2	10	0.11
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB3	10	0.11
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB1	20	0.11
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB2	20	0.11
(1,4283)	1:A:314:PHE:HD1	1:A:318:ALA:HB3	20	0.11
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB1	20	0.11
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB2	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4283)	1:A:314:PHE:HD2	1:A:318:ALA:HB3	20	0.11
(1,4239)	1:B:313:LYS:HG2	1:B:316:ARG:HE	1	0.11
(1,4239)	1:B:313:LYS:HG2	1:B:316:ARG:HE	5	0.11
(1,4239)	1:B:313:LYS:HG2	1:B:316:ARG:HE	8	0.11
(1,4218)	1:A:313:LYS:HG3	1:B:278:SER:H	4	0.11
(1,4218)	1:A:313:LYS:HG3	1:B:278:SER:H	12	0.11
(1,4193)	1:B:313:LYS:HA	1:B:313:LYS:HD3	30	0.11
(1,4175)	1:B:250:ASP:HB2	1:B:251:ASP:HA	22	0.11
(1,4172)	1:A:250:ASP:HB2	1:A:251:ASP:H	3	0.11
(1,4172)	1:A:250:ASP:HB3	1:A:251:ASP:H	3	0.11
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	14	0.11
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	22	0.11
(1,4167)	1:B:312:ASN:H	1:B:313:LYS:HG2	26	0.11
(1,4164)	1:A:312:ASN:H	1:A:313:LYS:HG2	21	0.11
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	6	0.11
(1,4156)	1:B:312:ASN:HD21	1:B:316:ARG:H	25	0.11
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	13	0.11
(1,4149)	1:A:312:ASN:HD21	1:A:316:ARG:H	21	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	3	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	3	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	3	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	3	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	3	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	3	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	13	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	13	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	13	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	13	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	13	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	13	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	16	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	16	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	16	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	16	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	16	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	16	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	18	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	18	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	18	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	18	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	18	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE2	25	0.11
(1,4097)	1:B:311:ALA:HB1	1:B:313:LYS:HE3	25	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE2	25	0.11
(1,4097)	1:B:311:ALA:HB2	1:B:313:LYS:HE3	25	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE2	25	0.11
(1,4097)	1:B:311:ALA:HB3	1:B:313:LYS:HE3	25	0.11
(1,404)	1:A:256:GLU:HG2	1:A:257:LEU:H	23	0.11
(1,3799)	1:A:303:ASP:H	1:A:304:VAL:HB	3	0.11
(1,3799)	1:A:303:ASP:H	1:A:304:VAL:HB	27	0.11
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD11	3	0.11
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD12	3	0.11
(1,358)	1:A:255:ASP:HA	1:A:258:LEU:HD13	3	0.11
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG21	2	0.11
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG22	2	0.11
(1,3557)	1:B:297:PRO:HA	1:B:298:THR:HG23	2	0.11
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	7	0.11
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	7	0.11
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	7	0.11
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG21	9	0.11
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG22	9	0.11
(1,3554)	1:A:297:PRO:HA	1:A:298:THR:HG23	9	0.11
(1,3551)	1:B:296:CYS:H	1:B:301:GLN:HE21	20	0.11
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	2	0.11
(1,3541)	1:A:296:CYS:H	1:A:301:GLN:HE21	11	0.11
(1,3436)	1:B:294:HIS:HE1	1:B:306:PRO:HD3	14	0.11
(1,3436)	1:B:294:HIS:HE1	1:B:306:PRO:HD3	26	0.11
(1,3434)	1:B:294:HIS:HE1	1:B:303:ASP:HA	11	0.11
(1,3432)	1:A:294:HIS:HE1	1:A:306:PRO:HD3	11	0.11
(1,3432)	1:A:294:HIS:HE1	1:A:306:PRO:HD3	14	0.11
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	13	0.11
(1,3430)	1:A:294:HIS:HE1	1:A:303:ASP:HA	14	0.11
(1,3330)	1:B:292:ASP:HB2	1:B:293:GLU:HG2	10	0.11
(1,3330)	1:B:292:ASP:HB2	1:B:293:GLU:HG3	10	0.11
(1,3330)	1:B:292:ASP:HB3	1:B:293:GLU:HG2	10	0.11
(1,3330)	1:B:292:ASP:HB3	1:B:293:GLU:HG3	10	0.11
(1,3258)	1:B:289:LEU:H	1:B:289:LEU:HG	29	0.11
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD11	10	0.11
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD12	10	0.11
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD13	10	0.11
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD21	10	0.11
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD22	10	0.11
(1,3211)	1:B:288:LEU:H	1:B:289:LEU:HD23	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3194)	1:B:288:LEU:HG	1:B:305:SER:H	3	0.11
(1,3193)	1:B:288:LEU:HG	1:B:305:SER:HA	18	0.11
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	4	0.11
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	4	0.11
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	4	0.11
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	5	0.11
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	5	0.11
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	5	0.11
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	9	0.11
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	9	0.11
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	9	0.11
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	13	0.11
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	13	0.11
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	13	0.11
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	23	0.11
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	23	0.11
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	23	0.11
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	24	0.11
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	24	0.11
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	24	0.11
(1,3040)	1:B:287:ALA:HB1	1:B:298:THR:H	28	0.11
(1,3040)	1:B:287:ALA:HB2	1:B:298:THR:H	28	0.11
(1,3040)	1:B:287:ALA:HB3	1:B:298:THR:H	28	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	2	0.11
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	2	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	2	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	6	0.11
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	6	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	6	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	9	0.11
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	9	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	9	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	11	0.11
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	11	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	11	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	15	0.11
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	15	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	15	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	22	0.11
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	22	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	22	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	30	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	30	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	30	0.11
(1,3023)	1:A:287:ALA:HB1	1:A:298:THR:H	31	0.11
(1,3023)	1:A:287:ALA:HB2	1:A:298:THR:H	31	0.11
(1,3023)	1:A:287:ALA:HB3	1:A:298:THR:H	31	0.11
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	5	0.11
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	9	0.11
(1,2920)	1:B:285:ARG:H	1:B:285:ARG:HD3	27	0.11
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	11	0.11
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	17	0.11
(1,2907)	1:A:285:ARG:H	1:A:285:ARG:HD3	22	0.11
(1,269)	1:B:254:PRO:HB3	1:B:255:ASP:HB2	24	0.11
(1,269)	1:B:254:PRO:HB3	1:B:255:ASP:HB3	24	0.11
(1,2633)	1:B:247:GLY:H	1:B:250:ASP:HB2	29	0.11
(1,2629)	1:B:247:GLY:H	1:B:248:SER:HA	1	0.11
(1,2621)	1:B:247:GLY:HA3	1:B:249:GLU:H	28	0.11
(1,242)	1:A:253:ILE:H	1:A:258:LEU:HD21	17	0.11
(1,242)	1:A:253:ILE:H	1:A:258:LEU:HD22	17	0.11
(1,242)	1:A:253:ILE:H	1:A:258:LEU:HD23	17	0.11
(1,2368)	1:A:278:SER:H	1:B:313:LYS:HG3	4	0.11
(1,2268)	1:B:275:CYS:HB2	1:B:299:CYS:HA	15	0.11
(1,2202)	1:A:274:CYS:HB2	1:A:304:VAL:H	11	0.11
(1,2202)	1:A:274:CYS:HB2	1:A:304:VAL:H	25	0.11
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	13	0.11
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	20	0.11
(1,2080)	1:B:246:LEU:H	1:B:247:GLY:HA2	32	0.11
(1,2074)	1:A:246:LEU:H	1:A:247:GLY:HA2	16	0.11
(1,1708)	1:B:271:VAL:HB	1:B:312:ASN:HA	20	0.11
(1,1698)	1:A:271:VAL:HB	1:A:312:ASN:HA	18	0.11
(1,1698)	1:A:271:VAL:HB	1:A:312:ASN:HA	28	0.11
(1,1447)	1:B:266:MET:H	1:B:319:VAL:HA	23	0.11
(1,1435)	1:A:266:MET:H	1:A:319:VAL:HA	5	0.11
(1,1435)	1:A:266:MET:H	1:A:319:VAL:HA	11	0.11
(1,1435)	1:A:266:MET:H	1:A:319:VAL:HA	28	0.11
(1,1344)	1:B:266:MET:HA	1:B:267:THR:HG21	10	0.11
(1,1344)	1:B:266:MET:HA	1:B:267:THR:HG22	10	0.11
(1,1344)	1:B:266:MET:HA	1:B:267:THR:HG23	10	0.11
(1,13)	1:A:305:SER:H	1:A:305:SER:HB2	10	0.11
(1,126)	1:B:253:ILE:HD11	1:B:264:ASP:HB2	31	0.11
(1,126)	1:B:253:ILE:HD12	1:B:264:ASP:HB2	31	0.11
(1,126)	1:B:253:ILE:HD13	1:B:264:ASP:HB2	31	0.11
(1,1224)	1:A:265:ILE:HB	1:A:328:TYR:HE1	22	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1224)	1:A:265:ILE:HB	1:A:328:TYR:HE2	22	0.11
(1,12)	1:A:305:SER:H	1:A:305:SER:HB3	3	0.11
(1,12)	1:A:305:SER:H	1:A:305:SER:HB3	13	0.11
(1,12)	1:A:305:SER:H	1:A:305:SER:HB3	28	0.11
(1,1116)	1:A:245:PRO:HD3	1:A:246:LEU:H	6	0.11
(1,1116)	1:A:245:PRO:HD3	1:A:246:LEU:H	11	0.11
(1,1116)	1:A:245:PRO:HD3	1:A:246:LEU:H	28	0.11
(1,1060)	1:A:261:ILE:H	1:A:263:LYS:HE2	2	0.11
(1,1060)	1:A:261:ILE:H	1:A:263:LYS:HE3	2	0.11
(1,101)	1:A:253:ILE:HD11	1:A:264:ASP:HB2	28	0.11
(1,101)	1:A:253:ILE:HD12	1:A:264:ASP:HB2	28	0.11
(1,101)	1:A:253:ILE:HD13	1:A:264:ASP:HB2	28	0.11
(1,101)	1:A:253:ILE:HD11	1:A:264:ASP:HB2	32	0.11
(1,101)	1:A:253:ILE:HD12	1:A:264:ASP:HB2	32	0.11
(1,101)	1:A:253:ILE:HD13	1:A:264:ASP:HB2	32	0.11

## 10 Dihedral-angle violation analysis

No dihedral-angle restraints found