



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 5, 2023 – 06:22 PM JST

PDB ID : 5I8N  
BMRB ID : 30017  
Title : Solution Structure of human calcium-binding S100A9 (C3S) protein  
Authors : Chang, C.-C.; Chin, Y.  
Deposited on : 2016-02-19

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

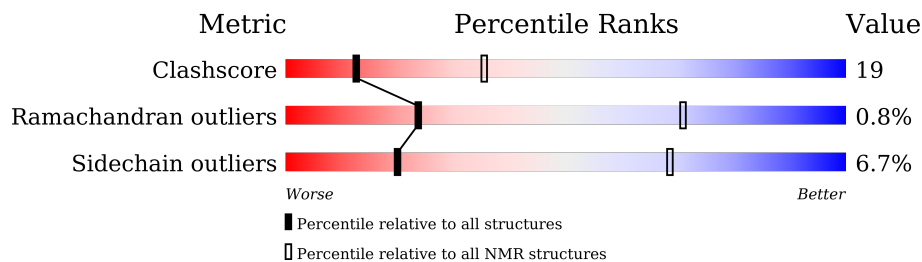
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 40%.

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	114	
1	B	114	

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:92, B:5-B:92 (176)	0.70	4

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

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

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

Cluster number	Models
1	2, 5, 7, 10
2	1, 4, 9
Single-model clusters	3; 6; 8

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3678 atoms, of which 1822 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein S100-A9.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	114	1839	579	911	163	180	6	0
1	B	114	1839	579	911	163	180	6	0

There are 2 discrepancies between the modelled and reference sequences:

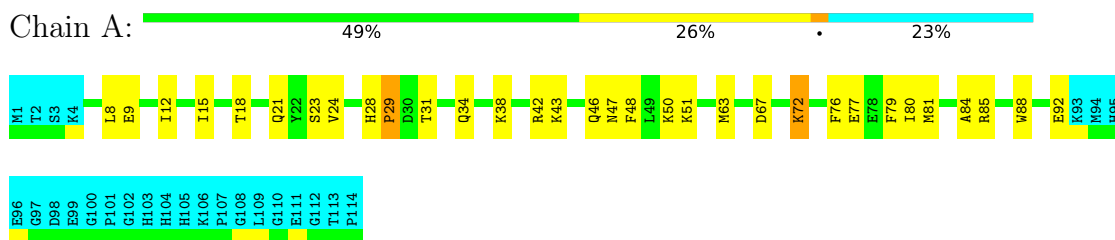
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	CYS	engineered mutation	UNP P06702
B	3	SER	CYS	engineered mutation	UNP P06702

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

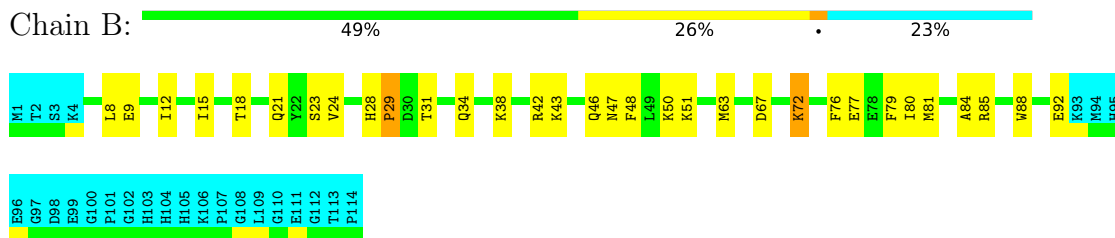
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein S100-A9



- Molecule 1: Protein S100-A9

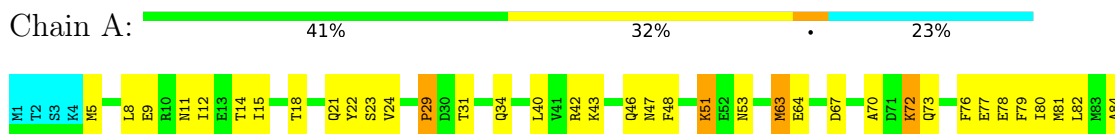


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Protein S100-A9





- Molecule 1: Protein S100-A9



#### 4.2.2 Score per residue for model 2

- Molecule 1: Protein S100-A9

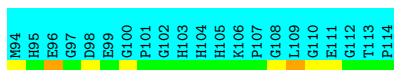
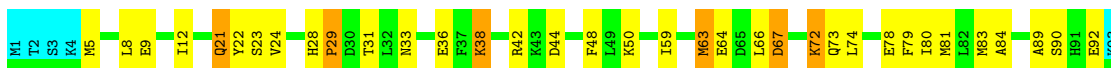


- Molecule 1: Protein S100-A9

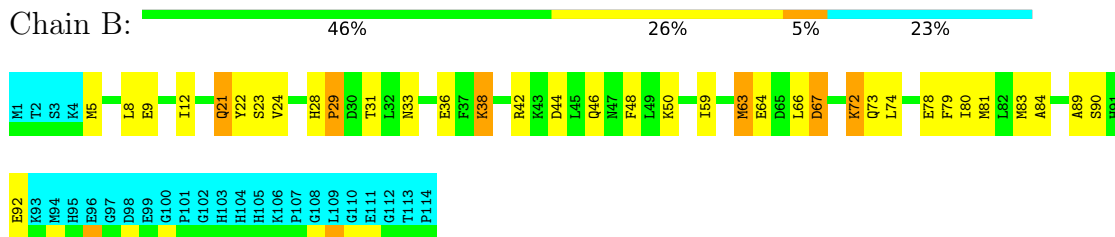


#### 4.2.3 Score per residue for model 3

- Molecule 1: Protein S100-A9

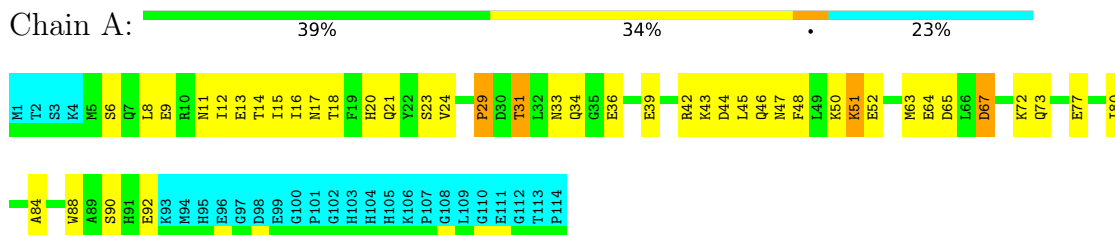


- Molecule 1: Protein S100-A9

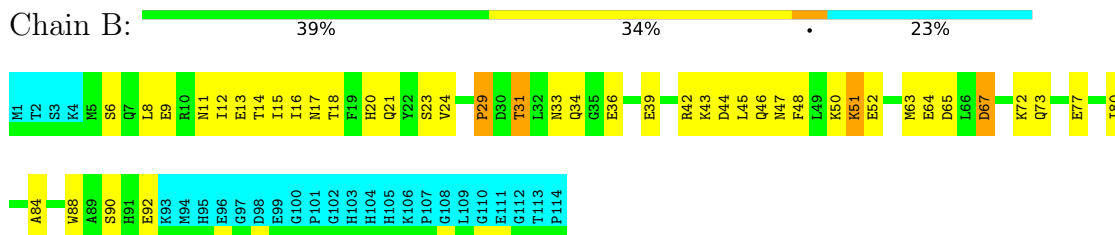


#### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Protein S100-A9

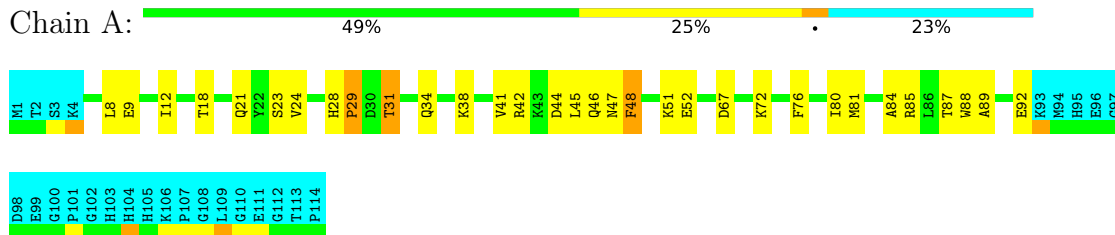


- Molecule 1: Protein S100-A9

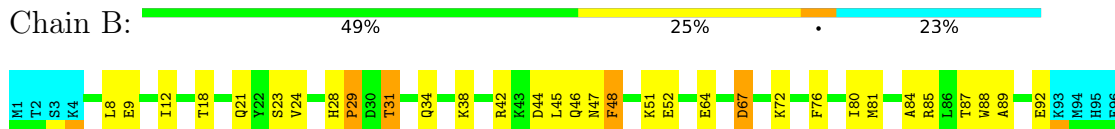


#### 4.2.5 Score per residue for model 5

- Molecule 1: Protein S100-A9



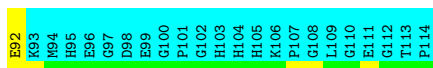
- Molecule 1: Protein S100-A9



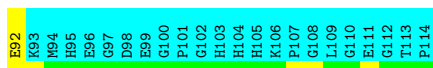


#### 4.2.6 Score per residue for model 6

- Molecule 1: Protein S100-A9

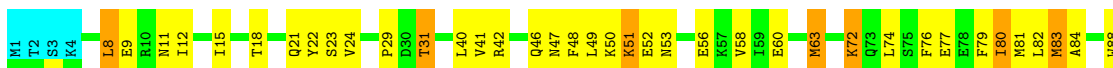


- Molecule 1: Protein S100-A9

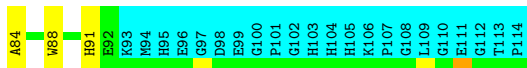
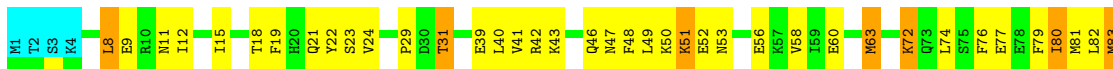


#### 4.2.7 Score per residue for model 7

- Molecule 1: Protein S100-A9



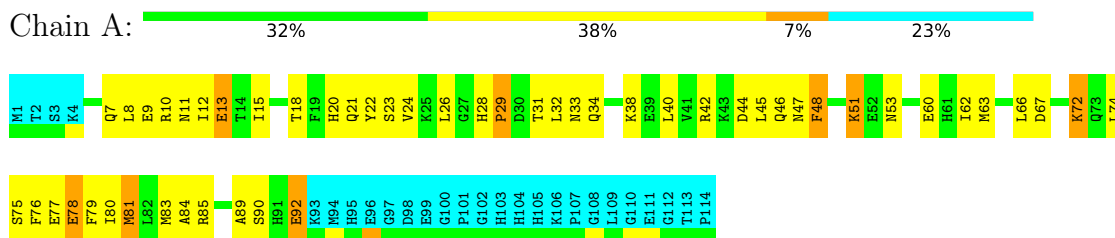
- Molecule 1: Protein S100-A9



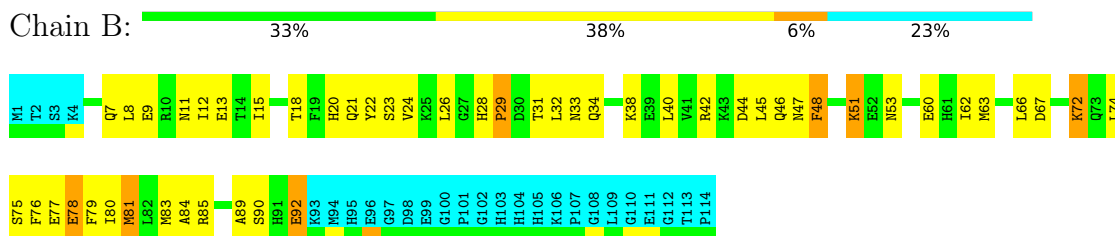


### 4.2.8 Score per residue for model 8

- Molecule 1: Protein S100-A9

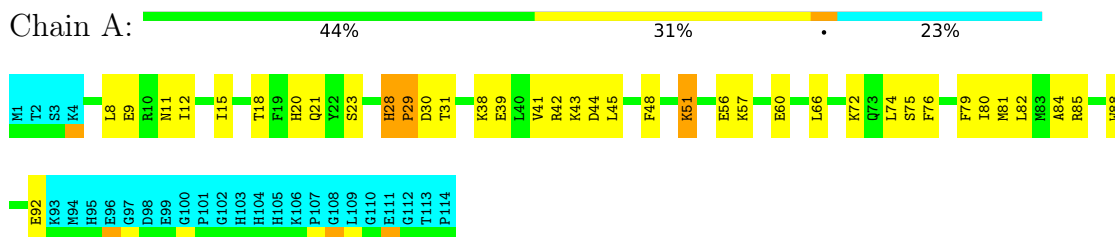


- Molecule 1: Protein S100-A9

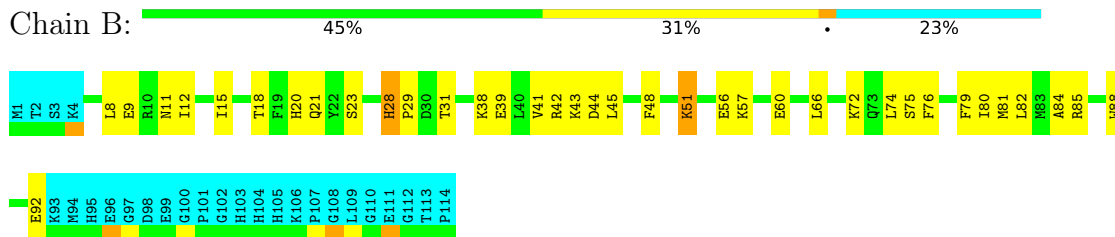


### 4.2.9 Score per residue for model 9

- Molecule 1: Protein S100-A9



- Molecule 1: Protein S100-A9



### 4.2.10 Score per residue for model 10

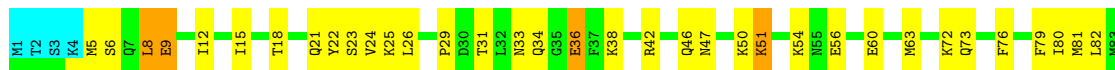
- Molecule 1: Protein S100-A9





• Molecule 1: Protein S100-A9

Chain B: 44% 30% • 23%



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	1.1
CNS	refinement	1.1

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	1201
Number of shifts mapped to atoms	1201
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.7
1	B	0.0±0.0	0.8±0.7
All	All	0	16

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	B	29	PRO	Peptide	6
1	A	29	PRO	Peptide	5
1	A	28	HIS	Peptide	3
1	B	28	HIS	Peptide	2

### 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	736	729	725	34±10
1	B	736	729	725	33±10
All	All	14720	14580	14500	550

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:34:GLN:HA	1:B:63:MET:SD	0.85	2.11	4	4
1:A:34:GLN:HA	1:A:63:MET:SD	0.85	2.11	4	4
1:A:80:ILE:HD13	1:B:84:ALA:HB2	0.77	1.55	8	1
1:A:84:ALA:HB2	1:B:80:ILE:HD13	0.77	1.56	8	1
1:A:81:MET:HA	1:B:80:ILE:HD12	0.75	1.58	8	1
1:A:80:ILE:HD12	1:B:81:MET:HA	0.75	1.58	8	1
1:A:8:LEU:HA	1:A:11:ASN:ND2	0.72	2.00	7	1
1:B:8:LEU:HA	1:B:11:ASN:ND2	0.72	2.00	7	1
1:B:77:GLU:O	1:B:80:ILE:HG12	0.71	1.85	8	1
1:A:77:GLU:O	1:A:80:ILE:HG12	0.71	1.85	8	1
1:A:23:SER:HB2	1:A:29:PRO:O	0.70	1.87	5	5
1:B:72:LYS:N	1:B:72:LYS:HE3	0.70	2.02	7	5
1:B:23:SER:HB2	1:B:29:PRO:O	0.70	1.87	5	5
1:A:72:LYS:N	1:A:72:LYS:HE3	0.69	2.02	7	5
1:B:76:PHE:HA	1:B:79:PHE:CE1	0.69	2.23	6	2
1:A:76:PHE:HA	1:A:79:PHE:CE1	0.68	2.23	6	2
1:A:80:ILE:HG21	1:B:84:ALA:HB2	0.67	1.66	2	9
1:A:84:ALA:HB2	1:B:80:ILE:HG21	0.67	1.66	10	9
1:B:18:THR:O	1:B:21:GLN:HG2	0.65	1.92	6	9
1:B:76:PHE:O	1:B:80:ILE:HG23	0.65	1.92	7	2
1:A:18:THR:O	1:A:21:GLN:HG2	0.64	1.92	6	9
1:A:28:HIS:N	1:A:29:PRO:HD3	0.63	2.09	6	1
1:A:76:PHE:O	1:A:80:ILE:HG23	0.63	1.92	7	2
1:A:15:ILE:HG13	1:B:11:ASN:ND2	0.62	2.07	8	1
1:B:28:HIS:N	1:B:29:PRO:HD3	0.62	2.09	6	1
1:A:11:ASN:ND2	1:B:15:ILE:HG13	0.62	2.08	8	1
1:A:15:ILE:HA	1:B:8:LEU:CD2	0.62	2.24	1	2
1:A:31:THR:OG1	1:A:73:GLN:HB3	0.62	1.95	1	3
1:A:80:ILE:HD12	1:B:84:ALA:HB2	0.62	1.70	7	1
1:B:31:THR:OG1	1:B:73:GLN:HB3	0.61	1.95	1	3
1:A:84:ALA:HB2	1:B:80:ILE:HD12	0.61	1.71	7	1
1:A:20:HIS:HA	1:A:23:SER:OG	0.61	1.96	4	3
1:A:48:PHE:HB2	1:B:9:GLU:OE2	0.61	1.96	8	1
1:B:20:HIS:HA	1:B:23:SER:OG	0.61	1.96	4	3
1:B:51:LYS:HD2	1:B:52:GLU:N	0.61	2.10	4	2
1:A:45:LEU:HA	1:B:9:GLU:OE1	0.61	1.96	5	1
1:B:46:GLN:O	1:B:50:LYS:HE3	0.60	1.95	7	1
1:A:42:ARG:HA	1:A:53:ASN:ND2	0.60	2.11	8	2
1:B:74:LEU:HB3	1:B:78:GLU:OE1	0.60	1.96	3	1
1:A:51:LYS:HD2	1:A:52:GLU:N	0.60	2.10	4	2
1:A:46:GLN:O	1:A:50:LYS:HE3	0.60	1.96	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:MET:HA	1:B:9:GLU:OE1	0.60	1.96	6	1
1:A:34:GLN:O	1:A:38:LYS:HD3	0.60	1.97	8	1
1:A:76:PHE:HA	1:A:79:PHE:CE2	0.60	2.32	2	2
1:A:8:LEU:CD2	1:B:15:ILE:HA	0.60	2.26	1	2
1:A:9:GLU:OE2	1:B:48:PHE:HB2	0.60	1.96	8	1
1:B:76:PHE:HA	1:B:79:PHE:CE2	0.59	2.32	10	2
1:A:74:LEU:HB3	1:A:78:GLU:OE1	0.59	1.96	3	1
1:B:42:ARG:HA	1:B:53:ASN:ND2	0.59	2.12	8	2
1:A:17:ASN:HA	1:A:20:HIS:CE1	0.59	2.32	4	1
1:B:34:GLN:O	1:B:38:LYS:HD3	0.59	1.97	8	1
1:A:9:GLU:OE1	1:B:45:LEU:HA	0.59	1.96	5	1
1:A:76:PHE:O	1:A:80:ILE:HB	0.59	1.98	9	3
1:B:17:ASN:HA	1:B:20:HIS:CE1	0.59	2.33	4	1
1:B:39:GLU:O	1:B:43:LYS:HG2	0.59	1.98	6	3
1:A:5:MET:HA	1:A:9:GLU:OE1	0.58	1.97	6	1
1:A:39:GLU:O	1:A:43:LYS:HG2	0.58	1.99	6	3
1:A:80:ILE:CD1	1:B:84:ALA:HB2	0.58	2.28	7	1
1:B:76:PHE:O	1:B:80:ILE:HB	0.58	1.99	9	3
1:A:88:TRP:O	1:A:92:GLU:HG2	0.58	1.99	4	6
1:B:8:LEU:O	1:B:12:ILE:HG13	0.58	1.99	4	10
1:B:88:TRP:O	1:B:92:GLU:HG2	0.58	1.99	4	5
1:A:9:GLU:CD	1:B:48:PHE:HB2	0.58	2.19	4	3
1:A:84:ALA:HB2	1:B:80:ILE:CD1	0.58	2.28	7	1
1:A:8:LEU:O	1:A:12:ILE:HG13	0.57	1.99	4	10
1:A:48:PHE:HB2	1:B:9:GLU:CD	0.57	2.20	4	3
1:B:47:ASN:O	1:B:50:LYS:HD2	0.57	2.00	2	1
1:A:48:PHE:HB2	1:B:9:GLU:OE1	0.57	2.00	5	1
1:B:42:ARG:O	1:B:46:GLN:HB3	0.56	2.00	10	9
1:A:9:GLU:OE1	1:B:48:PHE:HB2	0.56	2.00	5	1
1:A:84:ALA:HB2	1:B:80:ILE:CG2	0.56	2.31	3	5
1:A:76:PHE:HA	1:A:79:PHE:CZ	0.56	2.35	2	3
1:A:66:LEU:HB3	1:A:78:GLU:CG	0.56	2.31	3	1
1:A:18:THR:HB	1:B:8:LEU:HD21	0.56	1.77	1	1
1:A:42:ARG:O	1:A:46:GLN:HB3	0.56	2.01	10	8
1:B:76:PHE:HA	1:B:79:PHE:CZ	0.56	2.35	2	3
1:B:66:LEU:HB3	1:B:78:GLU:CG	0.56	2.31	3	1
1:A:47:ASN:O	1:A:50:LYS:HD2	0.55	2.00	2	1
1:A:38:LYS:O	1:A:42:ARG:HB2	0.55	2.02	9	1
1:B:38:LYS:O	1:B:42:ARG:HB2	0.55	2.02	9	1
1:A:44:ASP:O	1:B:9:GLU:HG3	0.55	2.02	3	2
1:A:80:ILE:CG2	1:B:84:ALA:HB2	0.54	2.31	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:28:HIS:H	1:B:29:PRO:CD	0.54	2.15	9	1
1:A:15:ILE:HD12	1:B:15:ILE:HD12	0.54	1.80	4	4
1:A:9:GLU:OE2	1:B:45:LEU:HA	0.53	2.02	4	2
1:A:28:HIS:H	1:A:29:PRO:CD	0.53	2.16	9	1
1:A:20:HIS:O	1:A:24:VAL:HB	0.53	2.04	4	1
1:A:8:LEU:HD21	1:B:18:THR:HB	0.53	1.78	1	1
1:A:50:LYS:HG2	1:A:51:LYS:N	0.53	2.18	2	1
1:A:66:LEU:HB3	1:A:78:GLU:HG2	0.53	1.79	3	1
1:B:66:LEU:HB3	1:B:78:GLU:HG2	0.53	1.80	3	1
1:B:78:GLU:O	1:B:81:MET:HG2	0.53	2.04	1	1
1:B:50:LYS:HG2	1:B:51:LYS:N	0.53	2.18	2	1
1:A:9:GLU:HG3	1:B:44:ASP:O	0.53	2.04	3	2
1:A:81:MET:O	1:A:85:ARG:HG3	0.52	2.03	1	7
1:A:45:LEU:HA	1:B:9:GLU:OE2	0.52	2.03	8	2
1:A:47:ASN:ND2	1:B:5:MET:HA	0.52	2.19	1	2
1:B:79:PHE:O	1:B:82:LEU:HB3	0.52	2.04	1	4
1:A:23:SER:OG	1:A:32:LEU:HG	0.52	2.05	8	1
1:A:78:GLU:O	1:A:81:MET:HG2	0.52	2.03	1	1
1:B:81:MET:O	1:B:85:ARG:HG3	0.52	2.03	1	7
1:B:28:HIS:N	1:B:29:PRO:CD	0.52	2.72	6	2
1:A:24:VAL:HA	1:A:29:PRO:HB3	0.52	1.81	8	6
1:A:79:PHE:O	1:A:82:LEU:HB3	0.52	2.04	1	4
1:B:20:HIS:O	1:B:24:VAL:HB	0.52	2.04	4	1
1:B:89:ALA:O	1:B:92:GLU:HG3	0.52	2.05	8	2
1:A:28:HIS:N	1:A:29:PRO:CD	0.52	2.72	6	2
1:B:23:SER:OG	1:B:32:LEU:HG	0.52	2.05	8	1
1:B:24:VAL:HA	1:B:29:PRO:HB3	0.51	1.81	8	6
1:A:8:LEU:HB3	1:B:44:ASP:CG	0.51	2.26	4	1
1:A:44:ASP:CG	1:B:8:LEU:HB3	0.51	2.25	4	1
1:A:11:ASN:OD1	1:B:15:ILE:HG13	0.51	2.05	9	1
1:A:89:ALA:O	1:A:92:GLU:HG3	0.51	2.06	8	2
1:A:15:ILE:HG13	1:B:11:ASN:OD1	0.51	2.06	9	1
1:A:80:ILE:HG12	1:B:80:ILE:HG12	0.51	1.83	7	1
1:A:81:MET:SD	1:A:85:ARG:HD2	0.50	2.46	8	1
1:B:38:LYS:O	1:B:42:ARG:HG3	0.50	2.06	3	2
1:A:80:ILE:O	1:A:83:MET:HB2	0.50	2.07	7	1
1:B:81:MET:SD	1:B:85:ARG:HD2	0.50	2.46	8	1
1:A:77:GLU:O	1:A:80:ILE:HG22	0.50	2.07	1	4
1:A:15:ILE:HA	1:B:8:LEU:CD1	0.49	2.37	2	1
1:B:51:LYS:N	1:B:51:LYS:HD2	0.49	2.22	1	1
1:A:80:ILE:HD13	1:B:84:ALA:CB	0.49	2.35	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ILE:HG23	1:B:80:ILE:HG23	0.49	1.84	9	3
1:A:5:MET:HA	1:B:47:ASN:ND2	0.49	2.21	10	2
1:B:80:ILE:O	1:B:83:MET:HB2	0.49	2.07	7	1
1:A:84:ALA:CB	1:B:80:ILE:HD13	0.49	2.36	8	1
1:B:77:GLU:O	1:B:80:ILE:HG22	0.49	2.08	1	4
1:A:38:LYS:O	1:A:42:ARG:HG3	0.49	2.07	3	2
1:A:15:ILE:HG13	1:B:11:ASN:HD22	0.49	1.68	8	1
1:B:26:LEU:HD11	1:B:33:ASN:ND2	0.49	2.22	8	2
1:A:51:LYS:N	1:A:51:LYS:HD2	0.49	2.23	1	1
1:B:24:VAL:CA	1:B:29:PRO:HB3	0.49	2.38	8	5
1:A:31:THR:CB	1:A:73:GLN:HB3	0.49	2.37	3	1
1:B:31:THR:HG22	1:B:75:SER:CA	0.49	2.38	9	1
1:A:24:VAL:CA	1:A:29:PRO:HB3	0.49	2.38	8	5
1:A:11:ASN:OD1	1:B:15:ILE:HG12	0.49	2.07	7	1
1:B:31:THR:CB	1:B:73:GLN:HB3	0.49	2.37	3	1
1:B:31:THR:HG21	1:B:73:GLN:OE1	0.49	2.08	4	1
1:B:75:SER:HB3	1:B:78:GLU:OE1	0.49	2.08	6	1
1:A:8:LEU:CD1	1:B:15:ILE:HA	0.48	2.38	2	1
1:A:46:GLN:HA	1:A:53:ASN:ND2	0.48	2.23	7	1
1:A:26:LEU:HD11	1:A:33:ASN:ND2	0.48	2.23	8	2
1:A:75:SER:HB3	1:A:78:GLU:OE1	0.48	2.08	6	1
1:B:20:HIS:CD2	1:B:29:PRO:HG3	0.48	2.44	8	1
1:A:15:ILE:HG12	1:B:11:ASN:OD1	0.48	2.08	7	1
1:A:31:THR:HG22	1:A:75:SER:CA	0.48	2.39	9	1
1:A:11:ASN:HD22	1:B:15:ILE:HG13	0.48	1.69	8	1
1:A:6:SER:HB2	1:A:9:GLU:OE1	0.48	2.09	10	1
1:A:11:ASN:HA	1:B:11:ASN:ND2	0.47	2.23	1	1
1:A:56:GLU:O	1:A:60:GLU:HG2	0.47	2.09	10	3
1:B:21:GLN:HG3	1:B:22:TYR:N	0.47	2.24	3	1
1:A:64:GLU:HA	1:A:67:ASP:CB	0.47	2.39	6	3
1:B:56:GLU:O	1:B:60:GLU:HG2	0.47	2.09	10	3
1:A:81:MET:CA	1:B:80:ILE:HD12	0.47	2.36	8	1
1:B:25:LYS:HD2	1:B:36:GLU:CG	0.47	2.40	10	1
1:A:31:THR:HG21	1:A:73:GLN:OE1	0.47	2.09	4	1
1:B:46:GLN:O	1:B:50:LYS:HA	0.47	2.10	6	2
1:B:46:GLN:HA	1:B:53:ASN:ND2	0.47	2.23	7	1
1:A:20:HIS:CD2	1:A:29:PRO:HG3	0.47	2.43	8	1
1:A:80:ILE:HG13	1:B:80:ILE:HG13	0.47	1.87	9	1
1:A:90:SER:OG	1:B:16:ILE:HD13	0.47	2.10	4	1
1:A:74:LEU:HB3	1:A:78:GLU:CD	0.47	2.30	8	1
1:A:21:GLN:HG3	1:A:22:TYR:N	0.47	2.24	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ILE:HD13	1:B:90:SER:OG	0.47	2.10	4	1
1:A:81:MET:HA	1:B:80:ILE:CD1	0.47	2.37	8	1
1:A:11:ASN:ND2	1:B:11:ASN:HA	0.47	2.24	1	1
1:B:74:LEU:HB3	1:B:78:GLU:CD	0.47	2.30	8	1
1:A:11:ASN:ND2	1:B:14:THR:HB	0.47	2.25	1	2
1:A:80:ILE:HD13	1:A:81:MET:N	0.47	2.25	7	1
1:A:14:THR:HB	1:B:11:ASN:ND2	0.47	2.25	1	2
1:A:80:ILE:HD12	1:B:81:MET:CA	0.47	2.36	8	1
1:A:46:GLN:O	1:A:50:LYS:HA	0.46	2.10	10	2
1:B:80:ILE:HD13	1:B:81:MET:N	0.46	2.25	7	1
1:B:59:ILE:O	1:B:63:MET:HB2	0.46	2.10	3	1
1:B:74:LEU:HB3	1:B:78:GLU:OE2	0.46	2.10	8	1
1:B:64:GLU:O	1:B:67:ASP:HB3	0.46	2.09	1	1
1:A:25:LYS:HD2	1:A:36:GLU:CG	0.46	2.40	10	1
1:B:33:ASN:HB3	1:B:36:GLU:OE2	0.46	2.11	3	1
1:B:6:SER:HB2	1:B:9:GLU:OE1	0.46	2.09	10	1
1:A:59:ILE:O	1:A:63:MET:HB2	0.46	2.10	3	1
1:A:33:ASN:HB2	1:A:36:GLU:OE1	0.46	2.10	4	1
1:A:34:GLN:HA	1:A:63:MET:CG	0.46	2.40	1	1
1:B:64:GLU:HA	1:B:67:ASP:CB	0.46	2.40	6	3
1:A:74:LEU:HB3	1:A:78:GLU:OE2	0.46	2.10	8	1
1:B:66:LEU:CD1	1:B:82:LEU:HB2	0.46	2.40	9	1
1:A:79:PHE:O	1:A:83:MET:HG2	0.46	2.10	3	2
1:A:8:LEU:HD12	1:B:18:THR:HG21	0.46	1.88	7	1
1:B:34:GLN:HA	1:B:63:MET:CG	0.46	2.41	1	1
1:B:88:TRP:O	1:B:91:HIS:HB3	0.46	2.11	1	2
1:B:33:ASN:HB2	1:B:36:GLU:OE1	0.46	2.10	4	1
1:A:66:LEU:CD1	1:A:82:LEU:HB2	0.46	2.40	9	1
1:A:51:LYS:HD2	1:A:51:LYS:H	0.46	1.70	1	1
1:A:88:TRP:O	1:A:91:HIS:HB3	0.45	2.11	1	2
1:A:21:GLN:O	1:A:24:VAL:HG12	0.45	2.12	4	2
1:B:51:LYS:HD2	1:B:51:LYS:H	0.45	1.70	1	1
1:A:33:ASN:HB3	1:A:36:GLU:OE2	0.45	2.11	3	1
1:A:64:GLU:O	1:A:67:ASP:HB3	0.45	2.11	1	1
1:A:31:THR:HA	1:A:74:LEU:O	0.45	2.11	3	3
1:B:77:GLU:HA	1:B:80:ILE:HD12	0.45	1.88	7	1
1:A:80:ILE:CD1	1:B:81:MET:HA	0.45	2.37	8	1
1:A:76:PHE:CE1	1:B:88:TRP:HB2	0.45	2.47	9	1
1:B:28:HIS:H	1:B:29:PRO:HD2	0.45	1.70	9	1
1:B:31:THR:HA	1:B:74:LEU:O	0.45	2.12	3	3
1:B:21:GLN:O	1:B:24:VAL:HG12	0.45	2.12	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:HB2	1:A:43:LYS:NZ	0.45	2.27	2	1
1:A:88:TRP:HB2	1:B:76:PHE:CE1	0.45	2.47	9	1
1:A:51:LYS:HD3	1:A:51:LYS:H	0.45	1.71	2	4
1:B:63:MET:O	1:B:67:ASP:HB2	0.45	2.12	3	1
1:A:23:SER:O	1:A:29:PRO:HB2	0.45	2.12	6	1
1:A:48:PHE:HB2	1:B:9:GLU:HG3	0.45	1.88	7	1
1:A:75:SER:O	1:A:78:GLU:HB3	0.45	2.12	8	1
1:A:77:GLU:HA	1:A:80:ILE:HD12	0.44	1.88	7	1
1:A:63:MET:O	1:A:67:ASP:HB2	0.44	2.12	3	1
1:B:79:PHE:O	1:B:83:MET:HG2	0.44	2.11	3	2
1:B:22:TYR:O	1:B:36:GLU:HG2	0.44	2.12	10	1
1:B:43:LYS:HB2	1:B:43:LYS:NZ	0.44	2.27	2	1
1:A:64:GLU:HA	1:A:67:ASP:HB3	0.44	1.89	4	1
1:B:42:ARG:HA	1:B:53:ASN:HD21	0.44	1.72	8	1
1:B:75:SER:O	1:B:78:GLU:HB3	0.44	2.12	8	1
1:A:7:GLN:O	1:A:11:ASN:HB2	0.44	2.13	8	1
1:B:9:GLU:H	1:B:9:GLU:CD	0.44	2.16	10	1
1:A:9:GLU:HG3	1:B:48:PHE:HB2	0.44	1.89	7	1
1:A:9:GLU:H	1:A:9:GLU:CD	0.44	2.16	10	1
1:A:51:LYS:HD2	1:A:52:GLU:H	0.44	1.73	7	1
1:A:42:ARG:HA	1:A:53:ASN:HD21	0.44	1.71	8	1
1:B:67:ASP:OD2	1:B:70:ALA:HA	0.44	2.13	1	1
1:B:51:LYS:HD2	1:B:52:GLU:H	0.44	1.73	7	1
1:A:22:TYR:O	1:A:36:GLU:HG2	0.44	2.12	10	1
1:B:64:GLU:HA	1:B:67:ASP:HB3	0.43	1.90	4	2
1:A:22:TYR:CD2	1:A:40:LEU:HD23	0.43	2.48	8	2
1:B:51:LYS:HD3	1:B:51:LYS:H	0.43	1.71	2	3
1:B:23:SER:O	1:B:29:PRO:HB2	0.43	2.12	6	1
1:B:26:LEU:HD11	1:B:33:ASN:HD22	0.43	1.72	10	1
1:A:67:ASP:OD2	1:A:70:ALA:HA	0.43	2.13	1	1
1:B:11:ASN:O	1:B:15:ILE:HG13	0.43	2.12	4	1
1:B:5:MET:SD	1:B:5:MET:N	0.43	2.91	10	1
1:B:41:VAL:HG13	1:B:49:LEU:HD12	0.43	1.89	7	1
1:A:5:MET:SD	1:A:5:MET:N	0.43	2.91	10	1
1:B:23:SER:HB3	1:B:31:THR:O	0.43	2.14	1	1
1:A:5:MET:HA	1:A:9:GLU:OE2	0.43	2.13	3	1
1:B:5:MET:HA	1:B:9:GLU:OE2	0.43	2.13	3	1
1:A:80:ILE:HD13	1:A:81:MET:H	0.43	1.74	7	1
1:B:80:ILE:HD13	1:B:81:MET:H	0.43	1.74	7	1
1:A:23:SER:HB3	1:A:31:THR:O	0.43	2.14	1	1
1:A:18:THR:HG21	1:B:8:LEU:HD12	0.43	1.90	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:22:TYR:CE1	1:B:40:LEU:HD23	0.43	2.49	7	1
1:B:31:THR:HB	1:B:73:GLN:HB3	0.43	1.91	3	1
1:A:11:ASN:O	1:A:15:ILE:HG13	0.43	2.12	4	1
1:A:50:LYS:HG3	1:A:51:LYS:N	0.43	2.29	4	1
1:B:22:TYR:CD2	1:B:40:LEU:HD23	0.43	2.48	8	2
1:B:17:ASN:HA	1:B:20:HIS:NE2	0.43	2.29	4	1
1:A:22:TYR:CE1	1:A:40:LEU:HD23	0.43	2.49	7	1
1:A:41:VAL:HG13	1:A:49:LEU:HD12	0.43	1.89	7	1
1:A:31:THR:HB	1:A:73:GLN:HB3	0.42	1.90	3	1
1:A:67:ASP:OD2	1:A:72:LYS:HE3	0.42	2.15	2	1
1:A:76:PHE:CB	1:B:87:THR:HG21	0.42	2.44	5	1
1:B:29:PRO:O	1:B:31:THR:N	0.42	2.52	5	2
1:A:26:LEU:HD11	1:A:33:ASN:HD22	0.42	1.72	10	1
1:A:5:MET:HG2	1:A:9:GLU:OE1	0.42	2.14	1	1
1:B:67:ASP:OD2	1:B:72:LYS:HE3	0.42	2.14	2	1
1:A:28:HIS:H	1:A:29:PRO:HD2	0.42	1.73	9	1
1:B:39:GLU:HG3	1:B:43:LYS:HZ2	0.42	1.74	7	1
1:B:7:GLN:O	1:B:11:ASN:HB2	0.42	2.13	8	1
1:B:5:MET:HG2	1:B:9:GLU:OE1	0.42	2.14	1	1
1:A:44:ASP:OD2	1:B:6:SER:HB3	0.42	2.15	4	1
1:A:34:GLN:O	1:A:38:LYS:HG3	0.42	2.15	5	1
1:A:77:GLU:O	1:A:80:ILE:HD13	0.42	2.15	7	1
1:A:80:ILE:CG1	1:A:81:MET:N	0.42	2.82	8	1
1:B:80:ILE:CG1	1:B:81:MET:N	0.42	2.82	8	1
1:A:17:ASN:HA	1:A:20:HIS:NE2	0.42	2.29	4	1
1:B:63:MET:O	1:B:74:LEU:HD21	0.42	2.14	8	1
1:B:77:GLU:O	1:B:80:ILE:HD13	0.41	2.15	7	1
1:A:80:ILE:HB	1:B:80:ILE:O	0.41	2.15	8	1
1:B:34:GLN:O	1:B:38:LYS:HG3	0.41	2.14	5	1
1:A:45:LEU:HD23	1:B:9:GLU:OE1	0.41	2.15	8	1
1:A:63:MET:O	1:A:74:LEU:HD21	0.41	2.14	8	1
1:A:6:SER:HB3	1:B:44:ASP:OD2	0.41	2.15	4	1
1:B:63:MET:CE	1:B:74:LEU:HG	0.41	2.45	7	2
1:B:31:THR:HG22	1:B:75:SER:HA	0.41	1.92	9	1
1:A:29:PRO:O	1:A:31:THR:N	0.41	2.52	5	2
1:B:50:LYS:HG3	1:B:51:LYS:N	0.41	2.29	4	1
1:A:87:THR:HG21	1:B:76:PHE:CB	0.41	2.44	5	1
1:B:52:GLU:HG2	1:B:58:VAL:HG11	0.41	1.93	7	1
1:A:63:MET:CE	1:A:74:LEU:HG	0.41	2.46	8	2
1:A:10:ARG:O	1:A:13:GLU:HG3	0.41	2.15	8	1
1:A:5:MET:HG3	1:B:47:ASN:ND2	0.41	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:GLU:OE1	1:B:45:LEU:HD23	0.41	2.16	8	1
1:A:16:ILE:O	1:A:20:HIS:HB2	0.41	2.16	2	1
1:A:8:LEU:HB3	1:B:44:ASP:OD2	0.41	2.15	4	1
1:A:41:VAL:HA	1:A:45:LEU:HB2	0.41	1.92	9	2
1:B:33:ASN:HB2	1:B:36:GLU:OE2	0.41	2.16	6	1
1:B:16:ILE:O	1:B:20:HIS:HB2	0.41	2.16	2	1
1:A:90:SER:OG	1:B:16:ILE:HG21	0.41	2.16	4	1
1:A:52:GLU:HG2	1:A:58:VAL:HG11	0.41	1.93	7	1
1:A:63:MET:HE1	1:A:74:LEU:HG	0.41	1.92	7	1
1:A:39:GLU:HG2	1:A:43:LYS:CE	0.41	2.46	2	1
1:A:16:ILE:HG21	1:B:90:SER:OG	0.41	2.16	4	1
1:B:23:SER:OG	1:B:29:PRO:HB2	0.41	2.16	4	1
1:A:33:ASN:HB2	1:A:36:GLU:OE2	0.41	2.16	6	1
1:A:80:ILE:O	1:B:80:ILE:HB	0.41	2.15	8	1
1:B:85:ARG:HA	1:B:88:TRP:CD2	0.40	2.51	5	1
1:A:85:ARG:HA	1:A:88:TRP:CD2	0.40	2.51	5	1
1:A:38:LYS:CE	1:A:60:GLU:HG2	0.40	2.46	8	1
1:A:62:ILE:O	1:A:66:LEU:HB2	0.40	2.16	8	1
1:B:51:LYS:H	1:B:51:LYS:HD3	0.40	1.76	8	1
1:B:62:ILE:O	1:B:66:LEU:HB2	0.40	2.16	8	1
1:B:42:ARG:HG2	1:B:53:ASN:OD1	0.40	2.17	2	1
1:A:23:SER:OG	1:A:29:PRO:HB2	0.40	2.16	4	1
1:A:23:SER:HB3	1:A:29:PRO:O	0.40	2.16	8	1
1:A:31:THR:HG22	1:A:75:SER:HA	0.40	1.92	9	1
1:B:41:VAL:HA	1:B:45:LEU:HB2	0.40	1.92	9	1
1:B:19:PHE:CE1	1:B:79:PHE:HE2	0.40	2.35	7	1
1:B:38:LYS:CE	1:B:60:GLU:HG2	0.40	2.47	8	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	88/114 (77%)	85±1 (96±1%)	2±1 (3±1%)	1±1 (1±1%)	24	71
1	B	88/114 (77%)	85±1 (96±1%)	2±1 (3±1%)	1±1 (1±1%)	24	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1760/2280 (77%)	1698 (96%)	48 (3%)	14 (1%)	24 71

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	67	ASP	4
1	B	67	ASP	4
1	A	28	HIS	2
1	B	28	HIS	2
1	A	5	MET	1
1	B	5	MET	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	83/103 (81%)	77±1 (93±1%)	6±1 (7±1%)	19 68
1	B	83/103 (81%)	78±1 (93±2%)	6±1 (7±2%)	20 69
All	All	1660/2060 (81%)	1548 (93%)	112 (7%)	20 68

All 52 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	72	LYS	10
1	B	72	LYS	10
1	A	51	LYS	8
1	B	51	LYS	8
1	A	31	THR	4
1	A	48	PHE	4
1	B	31	THR	4
1	B	48	PHE	4
1	A	63	MET	3
1	B	63	MET	3
1	A	43	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	B	43	LYS	2
1	A	57	LYS	2
1	B	57	LYS	2
1	A	81	MET	2
1	B	81	MET	2
1	A	13	GLU	2
1	B	13	GLU	2
1	A	44	ASP	2
1	B	44	ASP	2
1	A	8	LEU	2
1	B	8	LEU	2
1	A	50	LYS	1
1	B	50	LYS	1
1	A	21	GLN	1
1	A	38	LYS	1
1	B	21	GLN	1
1	B	38	LYS	1
1	A	65	ASP	1
1	B	65	ASP	1
1	A	52	GLU	1
1	B	52	GLU	1
1	A	69	ASN	1
1	A	79	PHE	1
1	B	69	ASN	1
1	B	79	PHE	1
1	A	80	ILE	1
1	A	83	MET	1
1	B	80	ILE	1
1	B	83	MET	1
1	A	78	GLU	1
1	A	92	GLU	1
1	B	78	GLU	1
1	B	92	GLU	1
1	A	29	PRO	1
1	A	30	ASP	1
1	A	9	GLU	1
1	A	36	GLU	1
1	A	54	LYS	1
1	B	9	GLU	1
1	B	36	GLU	1
1	B	54	LYS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 40% for the well-defined parts and 38% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *NMR-STAR31.str*

#### 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	1201
Number of shifts mapped to atoms	1201
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	105	$-0.41 \pm 0.21$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	98	$0.01 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	104	$-0.13 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	98	$2.95 \pm 0.32$	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 40%, i.e. 1026 atoms were assigned a chemical shift out of a possible 2542. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	419/880 (48%)	166/354 (47%)	170/352 (48%)	83/174 (48%)
Sidechain	607/1456 (42%)	411/934 (44%)	196/464 (42%)	0/58 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	0/206 (0%)	0/102 (0%)	0/86 (0%)	0/18 (0%)
Overall	1026/2542 (40%)	577/1390 (42%)	366/902 (41%)	83/250 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 38%, i.e. 1201 atoms were assigned a chemical shift out of a possible 3168. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	509/1140 (45%)	202/464 (44%)	209/456 (46%)	98/220 (45%)
Sidechain	692/1758 (39%)	466/1128 (41%)	226/566 (40%)	0/64 (0%)
Aromatic	0/270 (0%)	0/134 (0%)	0/102 (0%)	0/34 (0%)
Overall	1201/3168 (38%)	668/1726 (39%)	435/1124 (39%)	98/318 (31%)

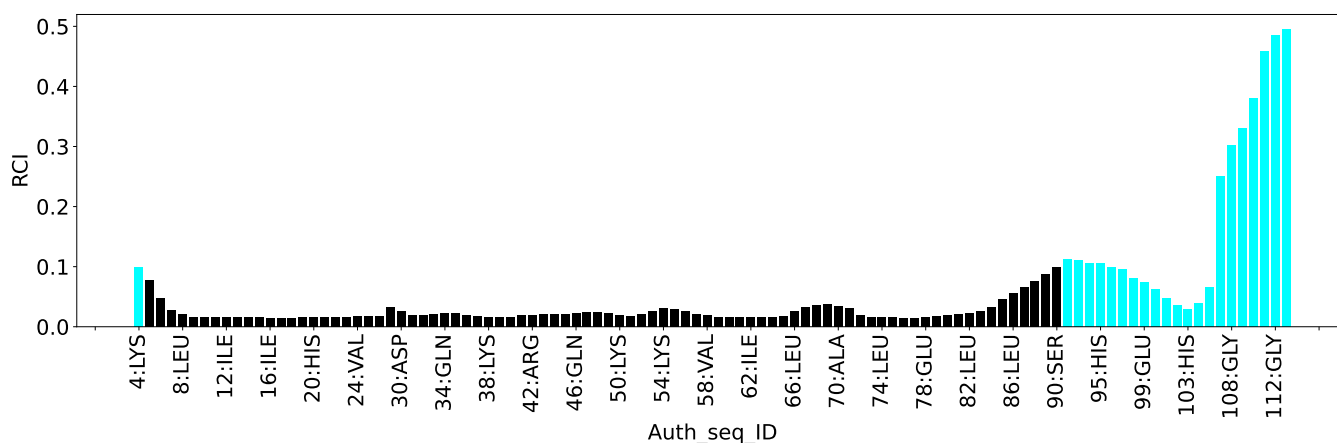
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 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	3714
Intra-residue ( $ i-j =0$ )	660
Sequential ( $ i-j =1$ )	832
Medium range ( $ i-j >1$ and $ i-j <5$ )	1048
Long range ( $ i-j \geq 5$ )	790
Inter-chain	298
Hydrogen bond restraints	86
Disulfide bond restraints	0
Total dihedral-angle restraints	210
Number of unmapped restraints	0
Number of restraints per residue	17.2
Number of long range restraints per residue <sup>1</sup>	3.5

<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)	77.6	0.2
0.2-0.5 (Medium)	37.6	0.46
>0.5 (Large)	5.0	6.05

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	51.0	10.0
10.0-20.0 (Medium)	4.7	20.0
>20.0 (Large)	4.5	158.8

## 9 Distance violation analysis i

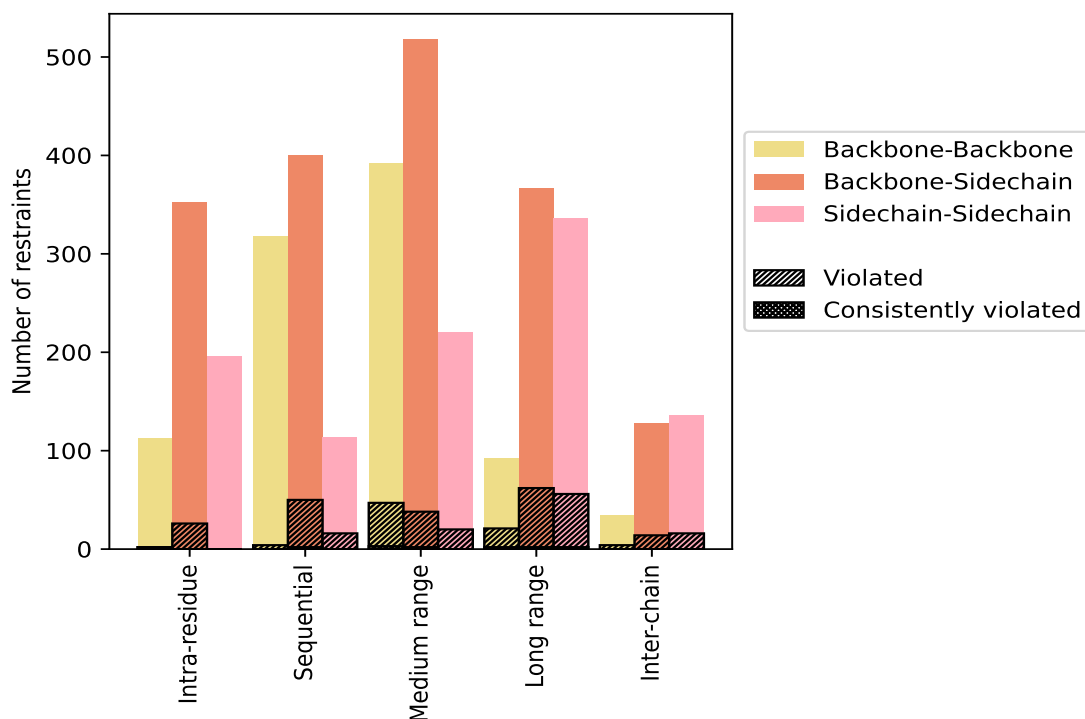
### 9.1 Summary of distance violations i

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 ( i-j =0)</b>	<b>660</b>	<b>17.8</b>	<b>28</b>	<b>4.2</b>	<b>0.8</b>	<b>2</b>	<b>0.3</b>	<b>0.1</b>
Backbone-Backbone	112	3.0	2	1.8	0.1	2	1.8	0.1
Backbone-Sidechain	352	9.5	26	7.4	0.7	0	0.0	0.0
Sidechain-Sidechain	196	5.3	0	0.0	0.0	0	0.0	0.0
<b>Sequential ( i-j =1)</b>	<b>832</b>	<b>22.4</b>	<b>70</b>	<b>8.4</b>	<b>1.9</b>	<b>2</b>	<b>0.2</b>	<b>0.1</b>
Backbone-Backbone	318	8.6	4	1.3	0.1	0	0.0	0.0
Backbone-Sidechain	400	10.8	50	12.5	1.3	2	0.5	0.1
Sidechain-Sidechain	114	3.1	16	14.0	0.4	0	0.0	0.0
<b>Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</b>	<b>1048</b>	<b>28.2</b>	<b>90</b>	<b>8.6</b>	<b>2.4</b>	<b>5</b>	<b>0.5</b>	<b>0.1</b>
Backbone-Backbone	310	8.3	32	10.3	0.9	3	1.0	0.1
Backbone-Sidechain	518	13.9	38	7.3	1.0	2	0.4	0.1
Sidechain-Sidechain	220	5.9	20	9.1	0.5	0	0.0	0.0
<b>Long range ( i-j ≥5)</b>	<b>790</b>	<b>21.3</b>	<b>136</b>	<b>17.2</b>	<b>3.7</b>	<b>6</b>	<b>0.8</b>	<b>0.2</b>
Backbone-Backbone	88	2.4	18	20.5	0.5	2	2.3	0.1
Backbone-Sidechain	366	9.9	62	16.9	1.7	2	0.5	0.1
Sidechain-Sidechain	336	9.0	56	16.7	1.5	2	0.6	0.1
<b>Inter-chain</b>	<b>298</b>	<b>8.0</b>	<b>34</b>	<b>11.4</b>	<b>0.9</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
Backbone-Backbone	34	0.9	4	11.8	0.1	0	0.0	0.0
Backbone-Sidechain	128	3.4	14	10.9	0.4	0	0.0	0.0
Sidechain-Sidechain	136	3.7	16	11.8	0.4	0	0.0	0.0
<b>Hydrogen bond</b>	<b>86</b>	<b>2.3</b>	<b>18</b>	<b>20.9</b>	<b>0.5</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Disulfide bond</b>	<b>0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>	<b>0</b>	<b>0.0</b>	<b>0.0</b>
<b>Total</b>	<b>3714</b>	<b>100.0</b>	<b>376</b>	<b>10.1</b>	<b>10.1</b>	<b>15</b>	<b>0.4</b>	<b>0.4</b>
Backbone-Backbone	948	25.5	78	8.2	2.1	7	0.7	0.2
Backbone-Sidechain	1764	47.5	190	10.8	5.1	6	0.3	0.2
Sidechain-Sidechain	1002	27.0	108	10.8	2.9	2	0.2	0.1

<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 disulfied bonds are counted in their appropriate category on the x-axis

## 9.2 Distance violation statistics for each model [i](#)

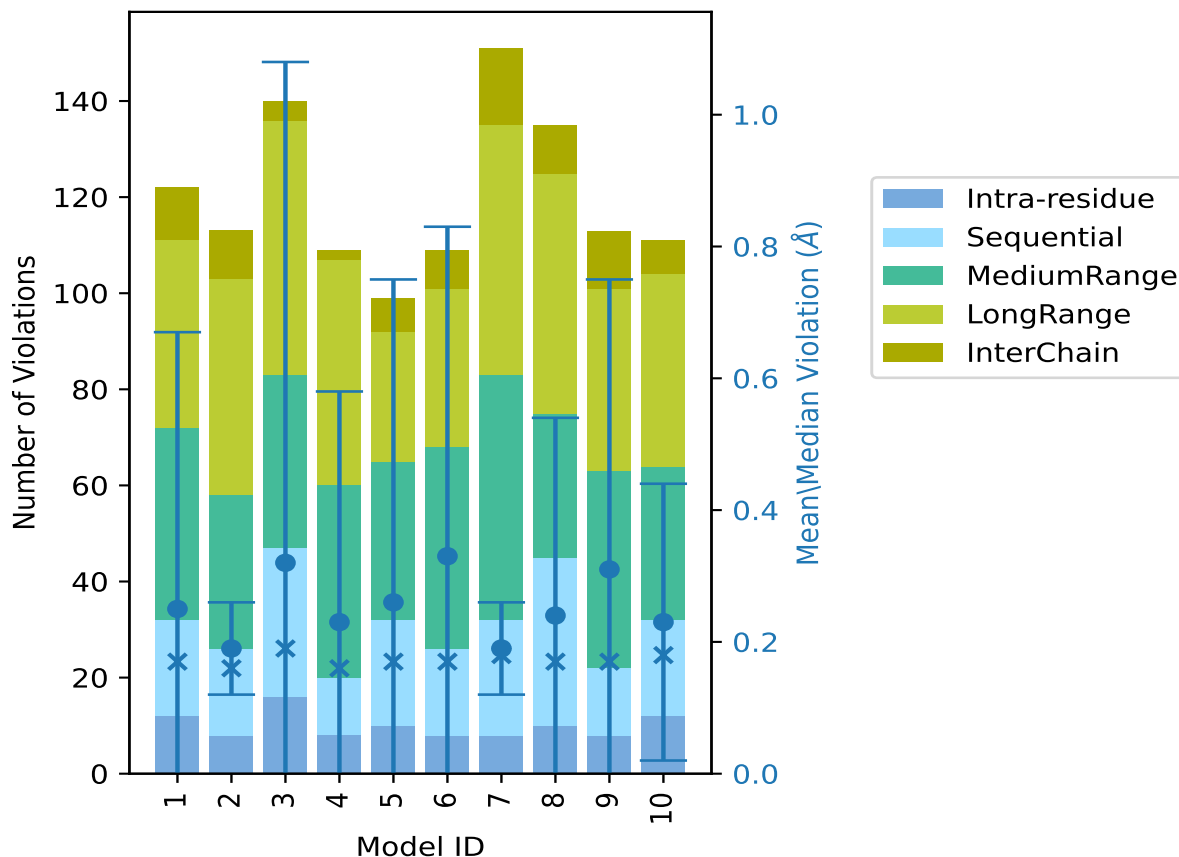
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <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	12	20	40	39	11	122	0.25	3.42	0.42	0.17
2	8	18	32	45	10	113	0.19	0.46	0.07	0.16
3	16	31	36	53	4	140	0.32	6.05	0.76	0.19
4	8	12	40	47	2	109	0.23	2.66	0.35	0.16
5	10	22	33	27	7	99	0.26	3.6	0.49	0.17
6	8	18	42	33	8	109	0.33	3.04	0.5	0.17
7	8	24	51	52	16	151	0.19	0.35	0.07	0.18
8	10	35	30	50	10	135	0.24	2.46	0.3	0.17
9	8	14	41	38	12	113	0.31	2.73	0.44	0.17
10	12	20	32	40	7	111	0.23	1.37	0.21	0.18

<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, 3270(IR:632, SQ:762, MR:958, LR:654, IC:264) 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>	%
10	23	30	52	15	130	1	10.0
4	23	14	23	11	75	2	20.0
4	1	8	21	0	34	3	30.0
2	9	12	7	0	30	4	40.0

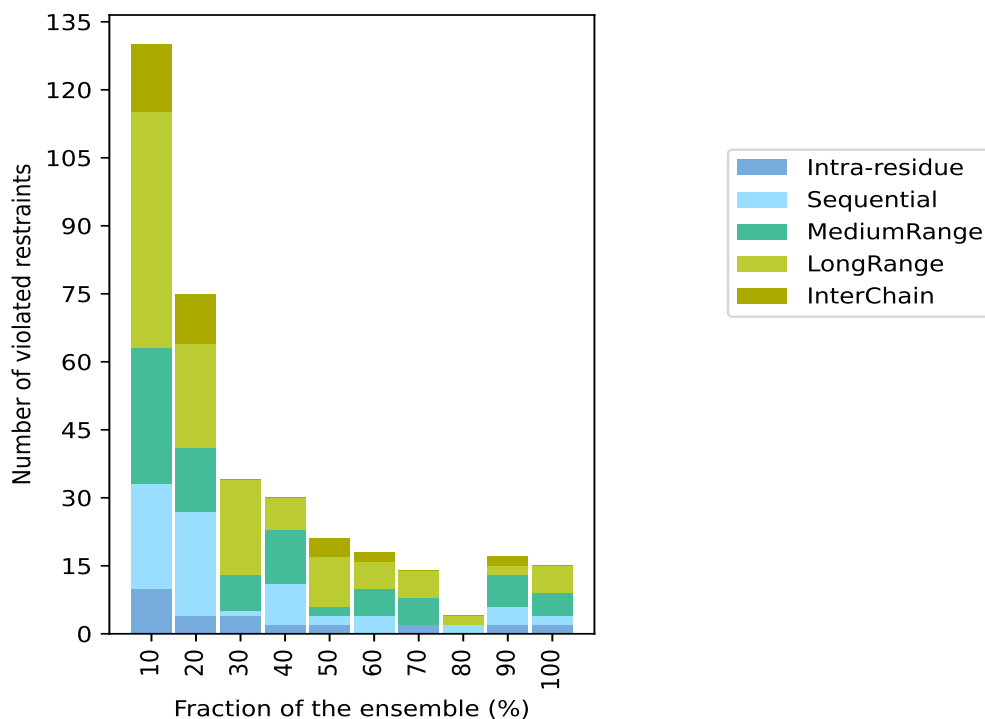
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
2	2	2	11	4	21	5	50.0
0	4	6	6	2	18	6	60.0
2	0	6	6	0	14	7	70.0
0	2	0	2	0	4	8	80.0
2	4	7	2	2	17	9	90.0
2	2	5	6	0	15	10	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

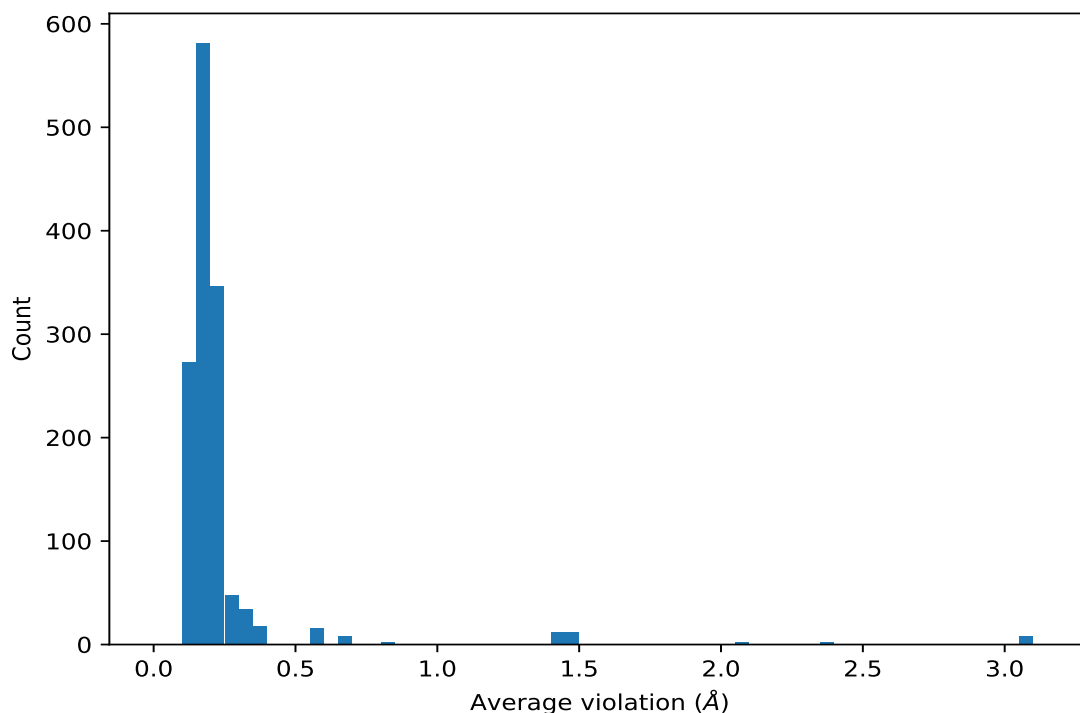
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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)
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	10	0.3	0.06	0.3
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	10	0.3	0.06	0.3
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	10	0.29	0.06	0.3
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	10	0.29	0.06	0.3
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	10	0.26	0.08	0.26
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	10	0.26	0.08	0.26
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	10	0.26	0.08	0.26
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	10	0.26	0.08	0.26
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	10	0.26	0.08	0.26
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	10	0.26	0.08	0.26
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	10	0.26	0.08	0.26
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	10	0.26	0.08	0.26
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	10	0.26	0.08	0.26
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	10	0.26	0.08	0.26
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	10	0.26	0.08	0.26
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	10	0.26	0.08	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	10	0.26	0.05	0.26
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	10	0.26	0.05	0.26
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	10	0.26	0.05	0.26
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	10	0.26	0.05	0.26
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	10	0.21	0.05	0.18
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	10	0.21	0.05	0.18
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	10	0.21	0.05	0.22
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	10	0.21	0.05	0.22
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	10	0.21	0.03	0.2
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	10	0.21	0.03	0.2
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	10	0.21	0.03	0.2
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	10	0.21	0.03	0.2
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	10	0.21	0.03	0.2
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	10	0.21	0.03	0.2
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	10	0.2	0.03	0.2
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	10	0.2	0.03	0.2
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	10	0.2	0.03	0.2
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	10	0.2	0.03	0.2
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	10	0.2	0.03	0.2
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	10	0.2	0.03	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	10	0.18	0.04	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	10	0.18	0.04	0.2
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	10	0.18	0.04	0.2
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	10	0.18	0.04	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	10	0.18	0.04	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	10	0.18	0.04	0.2
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	10	0.18	0.04	0.19
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	10	0.18	0.04	0.19
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	10	0.18	0.04	0.19
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	10	0.18	0.04	0.19
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	10	0.18	0.04	0.19
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	10	0.18	0.04	0.19
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	10	0.16	0.03	0.17
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	9	2.07	1.34	2.65
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	9	2.07	1.34	2.66
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	9	0.35	0.29	0.26
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	9	0.35	0.29	0.26
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	9	0.35	0.29	0.26
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	9	0.35	0.29	0.26
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	9	0.23	0.04	0.22

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	9	0.23	0.04	0.22
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	9	0.23	0.04	0.22
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	9	0.23	0.04	0.22
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	9	0.23	0.04	0.22
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	9	0.23	0.04	0.22
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	9	0.23	0.04	0.22
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	9	0.23	0.04	0.22
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	9	0.23	0.04	0.22
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	9	0.23	0.04	0.22
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	9	0.23	0.04	0.22
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	9	0.23	0.04	0.22
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	9	0.23	0.04	0.22
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	9	0.23	0.04	0.22
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	9	0.23	0.04	0.22
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	9	0.23	0.04	0.22
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	9	0.21	0.07	0.17
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	9	0.21	0.07	0.17
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	9	0.21	0.07	0.17
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	9	0.21	0.07	0.17
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	9	0.2	0.07	0.17
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	9	0.2	0.07	0.17
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	9	0.2	0.07	0.17
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	9	0.2	0.07	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	9	0.17	0.05	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	9	0.17	0.05	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	9	0.17	0.05	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	9	0.17	0.05	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	9	0.17	0.05	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	9	0.17	0.05	0.17
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	9	0.17	0.05	0.17
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	9	0.17	0.05	0.17
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	9	0.17	0.05	0.17
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	9	0.17	0.05	0.17
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	9	0.17	0.05	0.17
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	9	0.17	0.05	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	9	0.17	0.05	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	9	0.17	0.05	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	9	0.17	0.05	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	9	0.17	0.05	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	9	0.17	0.05	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	9	0.17	0.05	0.17
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	9	0.17	0.05	0.17
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	9	0.17	0.05	0.17
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	9	0.17	0.05	0.17
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	9	0.17	0.05	0.17
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	9	0.17	0.05	0.17
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	9	0.17	0.05	0.17
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	9	0.17	0.03	0.17
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	9	0.17	0.03	0.17
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	9	0.17	0.02	0.17
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	9	0.17	0.02	0.17
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	9	0.17	0.02	0.17
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	9	0.17	0.02	0.17
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	9	0.17	0.02	0.17
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	9	0.17	0.02	0.17
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	9	0.17	0.02	0.17
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	9	0.17	0.02	0.17
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	9	0.17	0.03	0.17
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	9	0.17	0.03	0.17
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	9	0.17	0.03	0.17
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	9	0.16	0.06	0.13
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	9	0.16	0.06	0.13
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	9	0.16	0.06	0.13
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	9	0.16	0.06	0.13
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	9	0.16	0.06	0.13
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	9	0.16	0.06	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	9	0.16	0.06	0.13
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	9	0.16	0.06	0.13
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	9	0.16	0.06	0.13
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	9	0.16	0.06	0.13
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	9	0.16	0.06	0.13
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	9	0.16	0.06	0.13
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	9	0.16	0.06	0.13
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	9	0.16	0.06	0.13
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	9	0.16	0.06	0.13
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	9	0.16	0.06	0.13
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	8	0.22	0.07	0.2
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	8	0.22	0.07	0.2
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	8	0.2	0.06	0.2
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	8	0.2	0.06	0.2
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	8	0.15	0.02	0.15
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	7	0.33	0.17	0.24
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	7	0.33	0.17	0.24
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	7	0.26	0.23	0.16
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	7	0.26	0.23	0.16
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	7	0.25	0.23	0.16
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	7	0.25	0.23	0.16
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	7	0.2	0.08	0.21
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	7	0.2	0.08	0.21
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	7	0.2	0.08	0.21
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	7	0.2	0.08	0.21
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	7	0.2	0.03	0.2
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	7	0.2	0.04	0.21
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	7	0.2	0.04	0.21
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	7	0.2	0.03	0.21
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	7	0.2	0.03	0.21
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	7	0.19	0.06	0.17
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	7	0.19	0.06	0.17
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	7	0.19	0.06	0.17
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	7	0.19	0.06	0.17
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	7	0.19	0.06	0.17
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	7	0.19	0.06	0.17
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	7	0.19	0.06	0.17
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	7	0.19	0.06	0.17
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	7	0.19	0.06	0.17
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	7	0.19	0.06	0.17
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	7	0.19	0.06	0.17
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	7	0.19	0.06	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	7	0.18	0.06	0.16
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	7	0.18	0.06	0.16
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	7	0.18	0.06	0.16
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	7	0.18	0.06	0.16
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	7	0.18	0.06	0.16
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	7	0.18	0.06	0.16
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	7	0.18	0.06	0.16
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	7	0.18	0.06	0.16
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	7	0.17	0.04	0.19
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	7	0.17	0.03	0.18
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	7	0.14	0.03	0.13
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA2	6	0.58	0.19	0.46
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA3	6	0.58	0.19	0.46
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA2	6	0.58	0.19	0.46
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA3	6	0.58	0.19	0.46
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA2	6	0.58	0.19	0.46
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA3	6	0.58	0.19	0.46
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA2	6	0.58	0.19	0.46
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA3	6	0.58	0.19	0.46
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA2	6	0.58	0.18	0.46
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA3	6	0.58	0.18	0.46
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA2	6	0.58	0.18	0.46
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA3	6	0.58	0.18	0.46
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA2	6	0.58	0.18	0.46
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA3	6	0.58	0.18	0.46
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA2	6	0.58	0.18	0.46
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA3	6	0.58	0.18	0.46
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD2	6	0.2	0.08	0.17
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD3	6	0.2	0.08	0.17
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD2	6	0.2	0.08	0.17
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD3	6	0.2	0.08	0.17
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG2	6	0.2	0.08	0.17
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG3	6	0.2	0.08	0.17
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG2	6	0.2	0.08	0.17
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG3	6	0.2	0.08	0.17
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB2	6	0.2	0.08	0.17
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB3	6	0.2	0.08	0.17
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB2	6	0.2	0.08	0.17
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB3	6	0.2	0.08	0.17
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD2	6	0.2	0.08	0.17
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD3	6	0.2	0.08	0.17
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD2	6	0.2	0.08	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD3	6	0.2	0.08	0.17
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD2	6	0.2	0.08	0.17
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD3	6	0.2	0.08	0.17
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD2	6	0.2	0.08	0.17
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD3	6	0.2	0.08	0.17
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG2	6	0.2	0.08	0.17
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG3	6	0.2	0.08	0.17
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG2	6	0.2	0.08	0.17
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG3	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB2	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB3	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB2	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB3	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD2	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD3	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD2	6	0.2	0.08	0.17
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD3	6	0.2	0.08	0.17
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB2	6	0.16	0.04	0.16
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB3	6	0.16	0.04	0.16
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB2	6	0.16	0.04	0.16
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB3	6	0.16	0.04	0.16
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB2	6	0.16	0.04	0.16
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB3	6	0.16	0.04	0.16
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB2	6	0.16	0.04	0.16
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB3	6	0.16	0.04	0.16
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB2	6	0.16	0.04	0.16
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB3	6	0.16	0.04	0.16
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB2	6	0.16	0.04	0.16
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB3	6	0.16	0.04	0.16
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB2	6	0.16	0.04	0.16
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB3	6	0.16	0.04	0.16
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB2	6	0.16	0.04	0.16
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB3	6	0.16	0.04	0.16
(1,477)	1:A:37:PHE:HB2	1:A:74:LEU:HG	6	0.16	0.04	0.16
(1,477)	1:A:37:PHE:HB3	1:A:74:LEU:HG	6	0.16	0.04	0.16
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB2	6	0.16	0.04	0.16
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB3	6	0.16	0.04	0.16
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB2	6	0.16	0.04	0.16
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB3	6	0.16	0.04	0.16
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB2	6	0.16	0.04	0.16
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB3	6	0.16	0.04	0.16
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB2	6	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB3	6	0.16	0.04	0.16
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB2	6	0.16	0.04	0.16
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB3	6	0.16	0.04	0.16
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB2	6	0.16	0.04	0.16
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB3	6	0.16	0.04	0.16
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB2	6	0.16	0.04	0.16
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB3	6	0.16	0.04	0.16
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB2	6	0.16	0.04	0.16
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB3	6	0.16	0.04	0.16
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB2	6	0.16	0.04	0.16
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB3	6	0.16	0.04	0.16
(1,478)	1:B:37:PHE:HB2	1:B:74:LEU:HG	6	0.16	0.04	0.16
(1,478)	1:B:37:PHE:HB3	1:B:74:LEU:HG	6	0.16	0.04	0.16
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB2	6	0.16	0.04	0.16
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB3	6	0.16	0.04	0.16
(1,357)	1:A:46:GLN:HB2	1:A:39:GLU:HA	6	0.16	0.02	0.16
(1,357)	1:A:46:GLN:HB3	1:A:39:GLU:HA	6	0.16	0.02	0.16
(1,357)	1:A:46:GLN:HB2	1:A:40:LEU:HA	6	0.16	0.02	0.16
(1,357)	1:A:46:GLN:HB3	1:A:40:LEU:HA	6	0.16	0.02	0.16
(1,357)	1:A:77:GLU:HB2	1:A:31:THR:HB	6	0.16	0.02	0.16
(1,357)	1:A:77:GLU:HB3	1:A:31:THR:HB	6	0.16	0.02	0.16
(1,358)	1:B:46:GLN:HB2	1:B:39:GLU:HA	6	0.16	0.02	0.16
(1,358)	1:B:46:GLN:HB3	1:B:39:GLU:HA	6	0.16	0.02	0.16
(1,358)	1:B:46:GLN:HB2	1:B:40:LEU:HA	6	0.16	0.02	0.16
(1,358)	1:B:46:GLN:HB3	1:B:40:LEU:HA	6	0.16	0.02	0.16
(1,358)	1:B:77:GLU:HB2	1:B:31:THR:HB	6	0.16	0.02	0.16
(1,358)	1:B:77:GLU:HB3	1:B:31:THR:HB	6	0.16	0.02	0.16
(1,1390)	1:B:5:MET:H	1:A:110:GLY:H	6	0.16	0.07	0.12
(1,1390)	1:B:12:ILE:H	1:B:19:PHE:H	6	0.16	0.07	0.12
(1,1390)	1:B:19:PHE:H	1:B:44:ASP:H	6	0.16	0.07	0.12
(1,1390)	1:B:19:PHE:H	1:A:12:ILE:H	6	0.16	0.07	0.12
(1,1390)	1:B:10:ARG:H	1:B:5:MET:H	6	0.16	0.07	0.12
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB2	6	0.16	0.05	0.15
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB3	6	0.16	0.05	0.15
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB2	6	0.16	0.05	0.15
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB3	6	0.16	0.05	0.15
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB2	6	0.16	0.05	0.15
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB3	6	0.16	0.05	0.15
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB2	6	0.16	0.05	0.15
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB3	6	0.16	0.05	0.15
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB2	6	0.16	0.05	0.15
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB3	6	0.16	0.05	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB2	6	0.16	0.05	0.15
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB3	6	0.16	0.05	0.15
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG2	6	0.14	0.03	0.15
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG3	6	0.14	0.03	0.15
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD22	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD21	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD23	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD12	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD11	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD13	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD22	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD21	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD23	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD12	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD11	6	0.14	0.04	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD13	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD22	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD21	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD23	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD12	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD11	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD13	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD22	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD21	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD23	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD12	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD11	6	0.14	0.04	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD13	6	0.14	0.04	0.13
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG22	6	0.14	0.02	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG21	6	0.14	0.02	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG23	6	0.14	0.02	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG12	6	0.14	0.02	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG11	6	0.14	0.02	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG13	6	0.14	0.02	0.14
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD12	6	0.14	0.02	0.14
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD11	6	0.14	0.02	0.14
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD13	6	0.14	0.02	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG22	6	0.14	0.02	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG21	6	0.14	0.02	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG23	6	0.14	0.02	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG12	6	0.14	0.02	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG11	6	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG13	6	0.14	0.02	0.14
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD12	6	0.14	0.02	0.14
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD11	6	0.14	0.02	0.14
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD13	6	0.14	0.02	0.14
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD22	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD21	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD23	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD12	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD11	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD13	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD22	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD21	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD23	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD12	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD11	6	0.13	0.03	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD13	6	0.13	0.03	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD22	6	0.13	0.03	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD21	6	0.13	0.03	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD23	6	0.13	0.03	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD12	6	0.13	0.03	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD11	6	0.13	0.03	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD13	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD22	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD21	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD23	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD12	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD11	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD13	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD22	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD21	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD23	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD12	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD11	6	0.13	0.03	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD13	6	0.13	0.03	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD22	6	0.13	0.03	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD21	6	0.13	0.03	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD23	6	0.13	0.03	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD12	6	0.13	0.03	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD11	6	0.13	0.03	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD13	6	0.13	0.03	0.12
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD2	5	0.39	0.37	0.25
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD3	5	0.39	0.37	0.25

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD2	5	0.39	0.37	0.25
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD3	5	0.39	0.37	0.25
(1,24)	1:B:65:ASP:HA	1:B:72:LYS:HA	5	0.39	0.37	0.25
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA2	5	0.39	0.24	0.37
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA3	5	0.39	0.24	0.37
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA2	5	0.39	0.24	0.37
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA3	5	0.39	0.24	0.37
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD2	5	0.39	0.37	0.24
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD3	5	0.39	0.37	0.24
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD2	5	0.39	0.37	0.24
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD3	5	0.39	0.37	0.24
(1,23)	1:A:65:ASP:HA	1:A:72:LYS:HA	5	0.39	0.37	0.24
(1,1705)	1:A:24:VAL:H	1:A:17:ASN:HA	5	0.23	0.09	0.19
(1,1705)	1:A:78:GLU:H	1:A:67:ASP:HA	5	0.23	0.09	0.19
(1,1706)	1:B:24:VAL:H	1:B:17:ASN:HA	5	0.23	0.09	0.19
(1,1706)	1:B:78:GLU:H	1:B:67:ASP:HA	5	0.23	0.09	0.19
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG21	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG22	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG23	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG21	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG22	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG23	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG21	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG22	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG23	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB1	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB1	5	0.23	0.03	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB1	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG2	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG3	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG21	1:B:80:ILE:HB	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG22	1:B:80:ILE:HB	5	0.23	0.03	0.21
(1,1078)	1:B:31:THR:HG23	1:B:80:ILE:HB	5	0.23	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG21	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG22	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG23	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG21	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG22	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG23	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG21	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG22	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG23	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB1	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB1	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB1	5	0.22	0.03	0.21

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG2	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG3	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG21	1:A:80:ILE:HB	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG22	1:A:80:ILE:HB	5	0.22	0.03	0.21
(1,1077)	1:A:31:THR:HG23	1:A:80:ILE:HB	5	0.22	0.03	0.21
(3,252)	1:B:33:ASN:HB2	1:B:72:LYS:HA	5	0.18	0.06	0.16
(3,252)	1:B:33:ASN:HB3	1:B:72:LYS:HA	5	0.18	0.06	0.16
(1,1389)	1:A:5:MET:H	1:B:110:GLY:H	5	0.18	0.06	0.14
(1,1389)	1:A:12:ILE:H	1:A:19:PHE:H	5	0.18	0.06	0.14
(1,1389)	1:A:19:PHE:H	1:A:44:ASP:H	5	0.18	0.06	0.14
(1,1389)	1:A:19:PHE:H	1:B:12:ILE:H	5	0.18	0.06	0.14
(1,1389)	1:A:10:ARG:H	1:A:5:MET:H	5	0.18	0.06	0.14
(3,251)	1:A:33:ASN:HB2	1:A:72:LYS:HA	5	0.18	0.06	0.16
(3,251)	1:A:33:ASN:HB3	1:A:72:LYS:HA	5	0.18	0.06	0.16
(3,33)	1:A:87:THR:HG21	1:A:88:TRP:HA	5	0.16	0.06	0.15
(3,33)	1:A:87:THR:HG22	1:A:88:TRP:HA	5	0.16	0.06	0.15
(3,33)	1:A:87:THR:HG23	1:A:88:TRP:HA	5	0.16	0.06	0.15
(3,34)	1:B:87:THR:HG21	1:B:88:TRP:HA	5	0.16	0.06	0.15
(3,34)	1:B:87:THR:HG22	1:B:88:TRP:HA	5	0.16	0.06	0.15
(3,34)	1:B:87:THR:HG23	1:B:88:TRP:HA	5	0.16	0.06	0.15
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG2	5	0.16	0.02	0.15
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG3	5	0.16	0.02	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG21	5	0.15	0.01	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG22	5	0.15	0.01	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG23	5	0.15	0.01	0.15
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB2	5	0.15	0.07	0.12
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB3	5	0.15	0.07	0.12
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG2	5	0.15	0.07	0.12
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG3	5	0.15	0.07	0.12
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG21	5	0.15	0.02	0.15
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG22	5	0.15	0.02	0.15
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG23	5	0.15	0.02	0.15
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB2	5	0.15	0.07	0.12
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB3	5	0.15	0.07	0.12
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG2	5	0.15	0.07	0.12
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG3	5	0.15	0.07	0.12
(2,26)	1:A:22:TYR:H	1:A:18:THR:O	5	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD22	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD21	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD23	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD12	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD11	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD13	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD22	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD21	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD23	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD12	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD11	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD13	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD12	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD11	5	0.14	0.03	0.14
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD13	5	0.14	0.03	0.14
(3,320)	1:B:51:LYS:HE2	1:B:51:LYS:H	5	0.14	0.03	0.12
(3,320)	1:B:51:LYS:HE3	1:B:51:LYS:H	5	0.14	0.03	0.12
(3,319)	1:A:51:LYS:HE2	1:A:51:LYS:H	5	0.14	0.03	0.12
(3,319)	1:A:51:LYS:HE3	1:A:51:LYS:H	5	0.14	0.03	0.12
(1,1195)	1:A:98:ASP:HA	1:A:95:HIS:HB3	4	0.66	0.48	0.63
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB2	4	0.66	0.48	0.63
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB3	4	0.66	0.48	0.63
(1,1196)	1:B:98:ASP:HA	1:B:95:HIS:HB3	4	0.66	0.48	0.63
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB2	4	0.66	0.48	0.63
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB3	4	0.66	0.48	0.63
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA2	4	0.34	0.19	0.25
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA3	4	0.34	0.19	0.25
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA2	4	0.34	0.19	0.25
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA3	4	0.34	0.19	0.25
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA2	4	0.34	0.19	0.25
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA3	4	0.34	0.19	0.25
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA2	4	0.34	0.19	0.25
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA3	4	0.34	0.19	0.25
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA2	4	0.34	0.2	0.24
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA3	4	0.34	0.2	0.24
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA2	4	0.34	0.2	0.24
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA3	4	0.34	0.2	0.24
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA2	4	0.34	0.2	0.24
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA3	4	0.34	0.2	0.24
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA2	4	0.34	0.2	0.24
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA3	4	0.34	0.2	0.24
(3,1427)	1:A:86:LEU:H	1:A:86:LEU:HG	4	0.34	0.03	0.34

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,1428)	1:B:86:LEU:H	1:B:86:LEU:HG	4	0.34	0.03	0.34
(3,486)	1:B:96:GLU:HG2	1:B:97:GLY:H	4	0.23	0.09	0.23
(3,486)	1:B:96:GLU:HG3	1:B:97:GLY:H	4	0.23	0.09	0.23
(1,1857)	1:A:108:GLY:H	1:A:111:GLU:HA	4	0.22	0.06	0.2
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA2	4	0.22	0.06	0.2
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA3	4	0.22	0.06	0.2
(1,1857)	1:A:110:GLY:H	1:A:111:GLU:HA	4	0.22	0.06	0.2
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA2	4	0.22	0.06	0.2
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA3	4	0.22	0.06	0.2
(1,1858)	1:B:108:GLY:H	1:B:111:GLU:HA	4	0.22	0.06	0.2
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA2	4	0.22	0.06	0.2
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA3	4	0.22	0.06	0.2
(1,1858)	1:B:110:GLY:H	1:B:111:GLU:HA	4	0.22	0.06	0.2
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA2	4	0.22	0.06	0.2
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA3	4	0.22	0.06	0.2
(4,259)	1:A:113:THR:H	1:A:107:PRO:HA	4	0.22	0.04	0.22
(4,260)	1:B:113:THR:H	1:B:107:PRO:HA	4	0.22	0.04	0.22
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG2	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG3	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG2	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG3	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG2	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG3	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG2	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG3	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG2	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG3	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG2	4	0.2	0.06	0.2
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG3	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG2	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG3	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG2	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG3	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG2	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG3	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG2	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG3	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG2	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG3	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG2	4	0.2	0.06	0.2
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG3	4	0.2	0.06	0.2
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA2	4	0.2	0.08	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA3	4	0.2	0.08	0.18
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA2	4	0.2	0.08	0.18
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA3	4	0.2	0.08	0.18
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA2	4	0.2	0.08	0.18
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA3	4	0.2	0.08	0.18
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA2	4	0.2	0.08	0.18
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA3	4	0.2	0.08	0.18
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB2	4	0.18	0.06	0.18
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB3	4	0.18	0.06	0.18
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB2	4	0.18	0.06	0.18
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB3	4	0.18	0.06	0.18
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB2	4	0.18	0.06	0.18
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB3	4	0.18	0.06	0.18
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB2	4	0.18	0.06	0.18
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB3	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE2	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE3	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE2	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE3	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD2	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD3	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD2	4	0.18	0.06	0.18
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD3	4	0.18	0.06	0.18
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB2	4	0.18	0.06	0.18
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB3	4	0.18	0.06	0.18
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB2	4	0.18	0.06	0.18
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB3	4	0.18	0.06	0.18
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB2	4	0.18	0.06	0.18
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB3	4	0.18	0.06	0.18
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB2	4	0.18	0.06	0.18
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB3	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE2	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE3	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE2	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE3	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD2	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD3	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD2	4	0.18	0.06	0.18
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD3	4	0.18	0.06	0.18
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG12	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG13	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE2	4	0.17	0.03	0.15

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE1	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE3	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG12	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG13	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE2	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE1	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE3	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB2	4	0.17	0.03	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB3	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG12	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG13	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE2	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE1	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE3	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG12	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG13	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE2	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE1	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE3	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB2	4	0.17	0.03	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB3	4	0.17	0.03	0.15
(2,4)	1:A:74:LEU:N	1:A:32:LEU:O	4	0.16	0.06	0.14
(3,863)	1:A:74:LEU:H	1:A:31:THR:HB	4	0.16	0.02	0.16
(3,864)	1:B:74:LEU:H	1:B:31:THR:HB	4	0.16	0.02	0.16
(1,1589)	1:A:10:ARG:H	1:A:12:ILE:HA	4	0.16	0.05	0.13
(1,1589)	1:A:51:LYS:H	1:A:46:GLN:HA	4	0.16	0.05	0.13
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD22	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD21	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD23	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD12	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD11	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD13	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD22	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD21	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD23	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD12	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD11	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD13	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD12	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD11	4	0.15	0.03	0.16
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD13	4	0.15	0.03	0.16
(1,1590)	1:B:10:ARG:H	1:B:12:ILE:HA	4	0.15	0.05	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1590)	1:B:51:LYS:H	1:B:46:GLN:HA	4	0.15	0.05	0.13
(4,63)	1:A:32:LEU:HG	1:A:31:THR:HB	4	0.14	0.05	0.12
(4,64)	1:B:32:LEU:HG	1:B:31:THR:HB	4	0.14	0.05	0.12
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB2	4	0.13	0.01	0.12
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB3	4	0.13	0.01	0.12
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB2	4	0.13	0.01	0.12
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB3	4	0.13	0.01	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD12	4	0.12	0.0	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD11	4	0.12	0.0	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD13	4	0.12	0.0	0.12
(1,771)	1:A:59:ILE:HD12	1:A:62:ILE:HA	4	0.12	0.0	0.12
(1,771)	1:A:59:ILE:HD11	1:A:62:ILE:HA	4	0.12	0.0	0.12
(1,771)	1:A:59:ILE:HD13	1:A:62:ILE:HA	4	0.12	0.0	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD12	4	0.12	0.0	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD11	4	0.12	0.0	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD13	4	0.12	0.0	0.12
(1,772)	1:B:59:ILE:HD12	1:B:62:ILE:HA	4	0.12	0.0	0.12
(1,772)	1:B:59:ILE:HD11	1:B:62:ILE:HA	4	0.12	0.0	0.12
(1,772)	1:B:59:ILE:HD13	1:B:62:ILE:HA	4	0.12	0.0	0.12
(4,257)	1:A:108:GLY:H	1:A:111:GLU:HA	3	0.8	0.09	0.83
(4,258)	1:B:108:GLY:H	1:B:111:GLU:HA	3	0.8	0.09	0.83
(3,1474)	1:B:100:GLY:H	1:B:98:ASP:HA	3	0.68	0.49	0.41
(3,1473)	1:A:100:GLY:H	1:A:98:ASP:HA	3	0.68	0.49	0.4
(3,485)	1:A:96:GLU:HG2	1:A:97:GLY:H	3	0.28	0.07	0.27
(3,485)	1:A:96:GLU:HG3	1:A:97:GLY:H	3	0.28	0.07	0.27
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG2	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG3	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG2	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG3	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG2	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG3	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG2	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG3	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG2	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG3	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG2	3	0.26	0.1	0.33
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG3	3	0.26	0.1	0.33
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG2	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG3	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG2	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG3	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG2	3	0.26	0.1	0.32

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG3	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG2	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG3	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG2	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG3	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG2	3	0.26	0.1	0.32
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG3	3	0.26	0.1	0.32
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD22	3	0.24	0.06	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD21	3	0.24	0.06	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD23	3	0.24	0.06	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD12	3	0.24	0.06	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD11	3	0.24	0.06	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD13	3	0.24	0.06	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD22	3	0.24	0.06	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD21	3	0.24	0.06	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD23	3	0.24	0.06	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD12	3	0.24	0.06	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD11	3	0.24	0.06	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD13	3	0.24	0.06	0.2
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB2	3	0.21	0.06	0.17
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB3	3	0.21	0.06	0.17
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB2	3	0.21	0.06	0.17
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB3	3	0.21	0.06	0.17
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG2	3	0.21	0.04	0.2
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG3	3	0.21	0.04	0.2
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG2	3	0.21	0.04	0.2
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG3	3	0.21	0.04	0.2
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG2	3	0.21	0.04	0.2
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG3	3	0.21	0.04	0.2
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG2	3	0.21	0.04	0.2
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG3	3	0.21	0.04	0.2
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD2	3	0.2	0.05	0.21
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD3	3	0.2	0.05	0.21
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD2	3	0.2	0.05	0.21
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD3	3	0.2	0.05	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD22	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD21	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD23	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD12	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD11	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD13	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD22	3	0.19	0.03	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD21	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD23	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD12	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD11	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD13	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD22	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD21	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD23	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD12	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD11	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD13	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD22	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD21	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD23	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD12	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD11	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD13	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD22	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD21	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD23	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD12	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD11	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD13	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD22	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD21	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD23	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD12	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD11	3	0.19	0.03	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD13	3	0.19	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD22	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD21	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD23	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD12	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD11	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD13	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD22	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD21	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD23	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD12	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD11	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD13	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD22	3	0.18	0.03	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD21	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD23	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD12	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD11	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD13	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD22	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD21	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD23	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD12	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD11	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD13	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD22	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD21	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD23	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD12	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD11	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD13	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD22	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD21	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD23	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD12	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD11	3	0.18	0.03	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD13	3	0.18	0.03	0.2
(2,86)	1:A:94:MET:H	1:A:90:SER:O	3	0.18	0.03	0.18
(1,987)	1:A:48:PHE:HB2	1:A:93:LYS:H	3	0.17	0.05	0.14
(1,987)	1:A:48:PHE:HB3	1:A:93:LYS:H	3	0.17	0.05	0.14
(1,987)	1:A:48:PHE:HB2	1:A:109:LEU:H	3	0.17	0.05	0.14
(1,987)	1:A:48:PHE:HB3	1:A:109:LEU:H	3	0.17	0.05	0.14
(1,987)	1:A:48:PHE:HB2	1:B:5:MET:H	3	0.17	0.05	0.14
(1,987)	1:A:48:PHE:HB3	1:B:5:MET:H	3	0.17	0.05	0.14
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB2	3	0.17	0.05	0.14
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB3	3	0.17	0.05	0.14
(1,988)	1:B:48:PHE:HB2	1:B:93:LYS:H	3	0.17	0.05	0.14
(1,988)	1:B:48:PHE:HB3	1:B:93:LYS:H	3	0.17	0.05	0.14
(1,988)	1:B:48:PHE:HB2	1:B:109:LEU:H	3	0.17	0.05	0.14
(1,988)	1:B:48:PHE:HB3	1:B:109:LEU:H	3	0.17	0.05	0.14
(1,988)	1:B:48:PHE:HB2	1:A:5:MET:H	3	0.17	0.05	0.14
(1,988)	1:B:48:PHE:HB3	1:A:5:MET:H	3	0.17	0.05	0.14
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB2	3	0.17	0.05	0.14
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB3	3	0.17	0.05	0.14
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG22	3	0.16	0.02	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG21	3	0.16	0.02	0.17

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG23	3	0.16	0.02	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD12	3	0.16	0.02	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD11	3	0.16	0.02	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD13	3	0.16	0.02	0.17
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD12	3	0.16	0.02	0.17
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD11	3	0.16	0.02	0.17
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD13	3	0.16	0.02	0.17
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD12	3	0.16	0.02	0.17
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD11	3	0.16	0.02	0.17
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD13	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG22	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG21	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG23	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD12	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD11	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD13	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD12	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD11	3	0.16	0.02	0.17
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD13	3	0.16	0.02	0.17
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD12	3	0.16	0.02	0.17
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD11	3	0.16	0.02	0.17
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD13	3	0.16	0.02	0.17
(1,1819)	1:A:21:GLN:H	1:A:40:LEU:HG	3	0.16	0.07	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB2	3	0.16	0.07	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB1	3	0.16	0.07	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB3	3	0.16	0.07	0.11
(1,1820)	1:B:21:GLN:H	1:B:40:LEU:HG	3	0.16	0.07	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB2	3	0.16	0.07	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB1	3	0.16	0.07	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB3	3	0.16	0.07	0.11
(2,79)	1:A:91:HIS:N	1:A:87:THR:O	3	0.15	0.02	0.14
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB2	3	0.14	0.04	0.12
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB3	3	0.14	0.04	0.12
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB2	3	0.14	0.04	0.12
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB3	3	0.14	0.04	0.12
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB2	3	0.14	0.04	0.12
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB3	3	0.14	0.04	0.12
(1,19)	1:A:92:GLU:HA	1:A:109:LEU:HG	3	0.14	0.04	0.12
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG2	3	0.14	0.04	0.12
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG3	3	0.14	0.04	0.12
(1,19)	1:A:93:LYS:HA	1:A:109:LEU:HG	3	0.14	0.04	0.12
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB2	3	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB3	3	0.14	0.02	0.14
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE2	3	0.14	0.02	0.14
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE3	3	0.14	0.02	0.14
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB2	3	0.14	0.02	0.14
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB3	3	0.14	0.02	0.14
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE2	3	0.14	0.02	0.14
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE3	3	0.14	0.02	0.14
(3,132)	1:B:78:GLU:HB2	1:B:31:THR:HA	3	0.14	0.03	0.13
(3,132)	1:B:78:GLU:HB3	1:B:31:THR:HA	3	0.14	0.03	0.13
(3,131)	1:A:78:GLU:HB2	1:A:31:THR:HA	3	0.14	0.02	0.13
(3,131)	1:A:78:GLU:HB3	1:A:31:THR:HA	3	0.14	0.02	0.13
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG2	3	0.13	0.02	0.12
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG3	3	0.13	0.02	0.12
(2,2)	1:A:32:LEU:N	1:A:74:LEU:O	3	0.13	0.02	0.12
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG2	3	0.13	0.02	0.12
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG3	3	0.13	0.02	0.12
(1,1158)	1:B:20:HIS:H	1:B:32:LEU:HG	3	0.13	0.0	0.13
(1,1158)	1:B:21:GLN:H	1:B:32:LEU:HG	3	0.13	0.0	0.13
(1,1158)	1:B:32:LEU:HG	1:B:41:VAL:H	3	0.13	0.0	0.13
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD22	3	0.13	0.02	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD21	3	0.13	0.02	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD23	3	0.13	0.02	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD12	3	0.13	0.02	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD11	3	0.13	0.02	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD13	3	0.13	0.02	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD22	3	0.13	0.02	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD21	3	0.13	0.02	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD23	3	0.13	0.02	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD12	3	0.13	0.02	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD11	3	0.13	0.02	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD13	3	0.13	0.02	0.12
(1,1157)	1:A:20:HIS:H	1:A:32:LEU:HG	3	0.12	0.0	0.12
(1,1157)	1:A:21:GLN:H	1:A:32:LEU:HG	3	0.12	0.0	0.12
(1,1157)	1:A:32:LEU:HG	1:A:41:VAL:H	3	0.12	0.0	0.12
(2,21)	1:A:20:HIS:N	1:A:16:ILE:O	3	0.12	0.01	0.12
(3,793)	1:A:107:PRO:HG2	1:A:93:LYS:HG2	2	3.08	2.96	3.08
(3,793)	1:A:107:PRO:HG2	1:A:93:LYS:HG3	2	3.08	2.96	3.08
(3,793)	1:A:107:PRO:HG3	1:A:93:LYS:HG2	2	3.08	2.96	3.08
(3,793)	1:A:107:PRO:HG3	1:A:93:LYS:HG3	2	3.08	2.96	3.08
(3,794)	1:B:107:PRO:HG2	1:B:93:LYS:HG2	2	3.08	2.96	3.08
(3,794)	1:B:107:PRO:HG2	1:B:93:LYS:HG3	2	3.08	2.96	3.08
(3,794)	1:B:107:PRO:HG3	1:B:93:LYS:HG2	2	3.08	2.96	3.08

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,794)	1:B:107:PRO:HG3	1:B:93:LYS:HG3	2	3.08	2.96	3.08
(3,534)	1:B:24:VAL:HA	1:B:29:PRO:HA	2	2.39	0.34	2.39
(3,533)	1:A:24:VAL:HA	1:A:29:PRO:HA	2	2.37	0.32	2.37
(3,738)	1:B:24:VAL:HG22	1:B:29:PRO:HB2	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG22	1:B:29:PRO:HB3	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG21	1:B:29:PRO:HB2	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG21	1:B:29:PRO:HB3	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG23	1:B:29:PRO:HB2	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG23	1:B:29:PRO:HB3	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG12	1:B:29:PRO:HB2	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG12	1:B:29:PRO:HB3	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG11	1:B:29:PRO:HB2	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG11	1:B:29:PRO:HB3	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG13	1:B:29:PRO:HB2	2	1.45	0.37	1.45
(3,738)	1:B:24:VAL:HG13	1:B:29:PRO:HB3	2	1.45	0.37	1.45
(3,737)	1:A:24:VAL:HG22	1:A:29:PRO:HB2	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG22	1:A:29:PRO:HB3	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG21	1:A:29:PRO:HB2	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG21	1:A:29:PRO:HB3	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG23	1:A:29:PRO:HB2	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG23	1:A:29:PRO:HB3	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG12	1:A:29:PRO:HB2	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG12	1:A:29:PRO:HB3	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG11	1:A:29:PRO:HB2	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG11	1:A:29:PRO:HB3	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG13	1:A:29:PRO:HB2	2	1.44	0.36	1.44
(3,737)	1:A:24:VAL:HG13	1:A:29:PRO:HB3	2	1.44	0.36	1.44
(3,628)	1:B:48:PHE:HB2	1:A:9:GLU:HG2	2	0.32	0.04	0.32
(3,628)	1:B:48:PHE:HB2	1:A:9:GLU:HG3	2	0.32	0.04	0.32
(3,628)	1:B:48:PHE:HB3	1:A:9:GLU:HG2	2	0.32	0.04	0.32
(3,628)	1:B:48:PHE:HB3	1:A:9:GLU:HG3	2	0.32	0.04	0.32
(3,627)	1:A:48:PHE:HB2	1:B:9:GLU:HG2	2	0.32	0.03	0.32
(3,627)	1:A:48:PHE:HB2	1:B:9:GLU:HG3	2	0.32	0.03	0.32
(3,627)	1:A:48:PHE:HB3	1:B:9:GLU:HG2	2	0.32	0.03	0.32
(3,627)	1:A:48:PHE:HB3	1:B:9:GLU:HG3	2	0.32	0.03	0.32
(3,618)	1:B:57:LYS:HA	1:B:57:LYS:HG2	2	0.32	0.01	0.32
(3,618)	1:B:57:LYS:HA	1:B:57:LYS:HG3	2	0.32	0.01	0.32
(3,617)	1:A:57:LYS:HA	1:A:57:LYS:HG2	2	0.31	0.01	0.31
(3,617)	1:A:57:LYS:HA	1:A:57:LYS:HG3	2	0.31	0.01	0.31
(1,1227)	1:A:76:PHE:H	1:A:32:LEU:HB2	2	0.23	0.01	0.23
(1,1227)	1:A:76:PHE:H	1:A:32:LEU:HB3	2	0.23	0.01	0.23
(1,1227)	1:A:76:PHE:H	1:A:80:ILE:HB	2	0.23	0.01	0.23

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1228)	1:B:76:PHE:H	1:B:32:LEU:HB2	2	0.23	0.01	0.23
(1,1228)	1:B:76:PHE:H	1:B:32:LEU:HB3	2	0.23	0.01	0.23
(1,1228)	1:B:76:PHE:H	1:B:80:ILE:HB	2	0.23	0.01	0.23
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE2	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE1	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE3	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE2	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE1	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE3	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE2	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE1	2	0.23	0.06	0.23
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE3	2	0.23	0.06	0.23
(1,224)	1:B:62:ILE:HG22	1:B:66:LEU:HG	2	0.23	0.06	0.23
(1,224)	1:B:62:ILE:HG21	1:B:66:LEU:HG	2	0.23	0.06	0.23
(1,224)	1:B:62:ILE:HG23	1:B:66:LEU:HG	2	0.23	0.06	0.23
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE2	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE1	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE3	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE2	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE1	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE3	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE2	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE1	2	0.22	0.06	0.22
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE3	2	0.22	0.06	0.22
(1,223)	1:A:62:ILE:HG22	1:A:66:LEU:HG	2	0.22	0.06	0.22
(1,223)	1:A:62:ILE:HG21	1:A:66:LEU:HG	2	0.22	0.06	0.22
(1,223)	1:A:62:ILE:HG23	1:A:66:LEU:HG	2	0.22	0.06	0.22
(3,503)	1:A:111:GLU:HA	1:A:107:PRO:HB2	2	0.22	0.08	0.22
(3,503)	1:A:111:GLU:HA	1:A:107:PRO:HB3	2	0.22	0.08	0.22
(3,504)	1:B:111:GLU:HA	1:B:107:PRO:HB2	2	0.22	0.08	0.22
(3,504)	1:B:111:GLU:HA	1:B:107:PRO:HB3	2	0.22	0.08	0.22
(3,865)	1:A:52:GLU:H	1:A:51:LYS:HG2	2	0.21	0.09	0.21
(3,865)	1:A:52:GLU:H	1:A:51:LYS:HG3	2	0.21	0.09	0.21
(1,41)	1:A:64:GLU:HG2	1:A:61:HIS:HB2	2	0.2	0.04	0.2
(1,41)	1:A:64:GLU:HG2	1:A:61:HIS:HB3	2	0.2	0.04	0.2
(1,41)	1:A:64:GLU:HG3	1:A:61:HIS:HB2	2	0.2	0.04	0.2
(1,41)	1:A:64:GLU:HG3	1:A:61:HIS:HB3	2	0.2	0.04	0.2
(1,41)	1:A:78:GLU:HG2	1:A:76:PHE:HA	2	0.2	0.04	0.2
(1,41)	1:A:78:GLU:HG3	1:A:76:PHE:HA	2	0.2	0.04	0.2
(1,42)	1:B:64:GLU:HG2	1:B:61:HIS:HB2	2	0.2	0.04	0.2
(1,42)	1:B:64:GLU:HG2	1:B:61:HIS:HB3	2	0.2	0.04	0.2
(1,42)	1:B:64:GLU:HG3	1:B:61:HIS:HB2	2	0.2	0.04	0.2

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,42)	1:B:64:GLU:HG3	1:B:61:HIS:HB3	2	0.2	0.04	0.2
(1,42)	1:B:78:GLU:HG2	1:B:76:PHE:HA	2	0.2	0.04	0.2
(1,42)	1:B:78:GLU:HG3	1:B:76:PHE:HA	2	0.2	0.04	0.2
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE2	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE1	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE3	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:B:10:ARG:HB2	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:B:10:ARG:HB3	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:B:12:ILE:HB	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:A:8:LEU:HB2	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:A:8:LEU:HB3	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:A:83:MET:HB2	2	0.2	0.02	0.2
(1,1382)	1:B:18:THR:H	1:A:83:MET:HB3	2	0.2	0.02	0.2
(3,49)	1:A:78:GLU:HG2	1:A:77:GLU:H	2	0.2	0.03	0.2
(3,49)	1:A:78:GLU:HG3	1:A:77:GLU:H	2	0.2	0.03	0.2
(3,50)	1:B:78:GLU:HG2	1:B:77:GLU:H	2	0.2	0.03	0.2
(3,50)	1:B:78:GLU:HG3	1:B:77:GLU:H	2	0.2	0.03	0.2
(3,866)	1:B:52:GLU:H	1:B:51:LYS:HG2	2	0.2	0.09	0.2
(3,866)	1:B:52:GLU:H	1:B:51:LYS:HG3	2	0.2	0.09	0.2
(3,199)	1:A:46:GLN:HB2	1:A:43:LYS:HA	2	0.2	0.04	0.2
(3,199)	1:A:46:GLN:HB3	1:A:43:LYS:HA	2	0.2	0.04	0.2
(3,200)	1:B:46:GLN:HB2	1:B:43:LYS:HA	2	0.2	0.04	0.2
(3,200)	1:B:46:GLN:HB3	1:B:43:LYS:HA	2	0.2	0.04	0.2
(1,1825)	1:A:21:GLN:H	1:A:17:ASN:HB2	2	0.2	0.05	0.2
(1,1825)	1:A:21:GLN:H	1:A:17:ASN:HB3	2	0.2	0.05	0.2
(1,1825)	1:A:94:MET:H	1:A:93:LYS:HE2	2	0.2	0.05	0.2
(1,1825)	1:A:94:MET:H	1:A:93:LYS:HE3	2	0.2	0.05	0.2
(1,1825)	1:A:94:MET:H	1:A:95:HIS:HB3	2	0.2	0.05	0.2
(1,1825)	1:A:98:ASP:H	1:A:95:HIS:HB3	2	0.2	0.05	0.2
(1,1825)	1:A:16:ILE:H	1:A:17:ASN:HB2	2	0.2	0.05	0.2
(1,1825)	1:A:16:ILE:H	1:A:17:ASN:HB3	2	0.2	0.05	0.2
(1,1826)	1:B:21:GLN:H	1:B:17:ASN:HB2	2	0.2	0.05	0.2
(1,1826)	1:B:21:GLN:H	1:B:17:ASN:HB3	2	0.2	0.05	0.2
(1,1826)	1:B:94:MET:H	1:B:93:LYS:HE2	2	0.2	0.05	0.2
(1,1826)	1:B:94:MET:H	1:B:93:LYS:HE3	2	0.2	0.05	0.2
(1,1826)	1:B:94:MET:H	1:B:95:HIS:HB3	2	0.2	0.05	0.2
(1,1826)	1:B:98:ASP:H	1:B:95:HIS:HB3	2	0.2	0.05	0.2
(1,1826)	1:B:16:ILE:H	1:B:17:ASN:HB2	2	0.2	0.05	0.2
(1,1826)	1:B:16:ILE:H	1:B:17:ASN:HB3	2	0.2	0.05	0.2
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE2	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE1	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE3	2	0.19	0.03	0.19

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1381)	1:A:18:THR:H	1:A:10:ARG:HB2	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:A:10:ARG:HB3	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:A:12:ILE:HB	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:B:8:LEU:HB2	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:B:8:LEU:HB3	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:B:83:MET:HB2	2	0.19	0.03	0.19
(1,1381)	1:A:18:THR:H	1:B:83:MET:HB3	2	0.19	0.03	0.19
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD22	2	0.19	0.07	0.19
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD21	2	0.19	0.07	0.19
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD23	2	0.19	0.07	0.19
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD12	2	0.19	0.07	0.19
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD11	2	0.19	0.07	0.19
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD13	2	0.19	0.07	0.19
(3,500)	1:B:32:LEU:HG	1:B:23:SER:HB2	2	0.19	0.01	0.19
(3,500)	1:B:32:LEU:HG	1:B:23:SER:HB3	2	0.19	0.01	0.19
(1,402)	1:B:38:LYS:HD2	1:B:57:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:38:LYS:HD2	1:B:57:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:38:LYS:HD3	1:B:57:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:38:LYS:HD3	1:B:57:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:38:LYS:HD2	1:B:72:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:38:LYS:HD2	1:B:72:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:38:LYS:HD3	1:B:72:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:38:LYS:HD3	1:B:72:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB2	1:B:19:PHE:HB2	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB2	1:B:19:PHE:HB3	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB3	1:B:19:PHE:HB2	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB3	1:B:19:PHE:HB3	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB2	1:B:51:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB2	1:B:51:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB3	1:B:51:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB3	1:B:51:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB2	1:A:4:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB2	1:A:4:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB3	1:A:4:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:42:ARG:HB3	1:A:4:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:85:ARG:HB2	1:B:51:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:85:ARG:HB2	1:B:51:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:85:ARG:HB3	1:B:51:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:85:ARG:HB3	1:B:51:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:85:ARG:HB2	1:A:30:ASP:HB2	2	0.18	0.05	0.18
(1,402)	1:B:85:ARG:HB2	1:A:30:ASP:HB3	2	0.18	0.05	0.18
(1,402)	1:B:85:ARG:HB3	1:A:30:ASP:HB2	2	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,402)	1:B:85:ARG:HB3	1:A:30:ASP:HB3	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB2	1:B:51:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB2	1:B:51:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB3	1:B:51:LYS:HE2	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB3	1:B:51:LYS:HE3	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB2	1:A:30:ASP:HB2	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB2	1:A:30:ASP:HB3	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB3	1:A:30:ASP:HB2	2	0.18	0.05	0.18
(1,402)	1:B:92:GLU:HB3	1:A:30:ASP:HB3	2	0.18	0.05	0.18
(1,1797)	1:A:5:MET:H	1:A:4:LYS:HE2	2	0.18	0.02	0.18
(1,1797)	1:A:5:MET:H	1:A:4:LYS:HE3	2	0.18	0.02	0.18
(1,1797)	1:A:16:ILE:H	1:A:17:ASN:HB2	2	0.18	0.02	0.18
(1,1797)	1:A:16:ILE:H	1:A:17:ASN:HB3	2	0.18	0.02	0.18
(1,1797)	1:A:94:MET:H	1:A:93:LYS:HE2	2	0.18	0.02	0.18
(1,1797)	1:A:94:MET:H	1:A:93:LYS:HE3	2	0.18	0.02	0.18
(1,1797)	1:A:109:LEU:H	1:A:93:LYS:HE2	2	0.18	0.02	0.18
(1,1797)	1:A:109:LEU:H	1:A:93:LYS:HE3	2	0.18	0.02	0.18
(1,1798)	1:B:5:MET:H	1:B:4:LYS:HE2	2	0.18	0.02	0.18
(1,1798)	1:B:5:MET:H	1:B:4:LYS:HE3	2	0.18	0.02	0.18
(1,1798)	1:B:16:ILE:H	1:B:17:ASN:HB2	2	0.18	0.02	0.18
(1,1798)	1:B:16:ILE:H	1:B:17:ASN:HB3	2	0.18	0.02	0.18
(1,1798)	1:B:94:MET:H	1:B:93:LYS:HE2	2	0.18	0.02	0.18
(1,1798)	1:B:94:MET:H	1:B:93:LYS:HE3	2	0.18	0.02	0.18
(1,1798)	1:B:109:LEU:H	1:B:93:LYS:HE2	2	0.18	0.02	0.18
(1,1798)	1:B:109:LEU:H	1:B:93:LYS:HE3	2	0.18	0.02	0.18
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD22	2	0.18	0.08	0.18
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD21	2	0.18	0.08	0.18
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD23	2	0.18	0.08	0.18
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD12	2	0.18	0.08	0.18
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD11	2	0.18	0.08	0.18
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD13	2	0.18	0.08	0.18
(3,499)	1:A:32:LEU:HG	1:A:23:SER:HB2	2	0.18	0.02	0.18
(3,499)	1:A:32:LEU:HG	1:A:23:SER:HB3	2	0.18	0.02	0.18
(1,401)	1:A:38:LYS:HD2	1:A:57:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:38:LYS:HD2	1:A:57:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:38:LYS:HD3	1:A:57:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:38:LYS:HD3	1:A:57:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:38:LYS:HD2	1:A:72:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:38:LYS:HD2	1:A:72:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:38:LYS:HD3	1:A:72:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:38:LYS:HD3	1:A:72:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB2	1:A:19:PHE:HB2	2	0.18	0.06	0.18

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,401)	1:A:42:ARG:HB2	1:A:19:PHE:HB3	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB3	1:A:19:PHE:HB2	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB3	1:A:19:PHE:HB3	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB2	1:A:51:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB2	1:A:51:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB3	1:A:51:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB3	1:A:51:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB2	1:B:4:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB2	1:B:4:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB3	1:B:4:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:42:ARG:HB3	1:B:4:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB2	1:A:51:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB2	1:A:51:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB3	1:A:51:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB3	1:A:51:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB2	1:B:30:ASP:HB2	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB2	1:B:30:ASP:HB3	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB3	1:B:30:ASP:HB2	2	0.18	0.06	0.18
(1,401)	1:A:85:ARG:HB3	1:B:30:ASP:HB3	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB2	1:A:51:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB2	1:A:51:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB3	1:A:51:LYS:HE2	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB3	1:A:51:LYS:HE3	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB2	1:B:30:ASP:HB2	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB2	1:B:30:ASP:HB3	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB3	1:B:30:ASP:HB2	2	0.18	0.06	0.18
(1,401)	1:A:92:GLU:HB3	1:B:30:ASP:HB3	2	0.18	0.06	0.18
(3,461)	1:A:5:MET:HB2	1:A:4:LYS:HE2	2	0.18	0.03	0.18
(3,461)	1:A:5:MET:HB2	1:A:4:LYS:HE3	2	0.18	0.03	0.18
(3,461)	1:A:5:MET:HB3	1:A:4:LYS:HE2	2	0.18	0.03	0.18
(3,461)	1:A:5:MET:HB3	1:A:4:LYS:HE3	2	0.18	0.03	0.18
(3,462)	1:B:5:MET:HB2	1:B:4:LYS:HE2	2	0.18	0.03	0.18
(3,462)	1:B:5:MET:HB2	1:B:4:LYS:HE3	2	0.18	0.03	0.18
(3,462)	1:B:5:MET:HB3	1:B:4:LYS:HE2	2	0.18	0.03	0.18
(3,462)	1:B:5:MET:HB3	1:B:4:LYS:HE3	2	0.18	0.03	0.18
(3,195)	1:A:46:GLN:HA	1:A:50:LYS:HG2	2	0.17	0.04	0.17
(3,195)	1:A:46:GLN:HA	1:A:50:LYS:HG3	2	0.17	0.04	0.17
(3,196)	1:B:46:GLN:HA	1:B:50:LYS:HG2	2	0.17	0.04	0.17
(3,196)	1:B:46:GLN:HA	1:B:50:LYS:HG3	2	0.17	0.04	0.17
(1,20)	1:B:65:ASP:HA	1:B:74:LEU:HB2	2	0.16	0.04	0.16
(1,20)	1:B:65:ASP:HA	1:B:74:LEU:HB3	2	0.16	0.04	0.16
(1,20)	1:B:65:ASP:HA	1:B:82:LEU:HB2	2	0.16	0.04	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,20)	1:B:65:ASP:HA	1:B:82:LEU:HB3	2	0.16	0.04	0.16
(1,20)	1:B:92:GLU:HA	1:B:86:LEU:HB2	2	0.16	0.04	0.16
(1,20)	1:B:92:GLU:HA	1:B:86:LEU:HB3	2	0.16	0.04	0.16
(1,20)	1:B:92:GLU:HA	1:B:109:LEU:HG	2	0.16	0.04	0.16
(1,20)	1:B:93:LYS:HA	1:B:51:LYS:HG2	2	0.16	0.04	0.16
(1,20)	1:B:93:LYS:HA	1:B:51:LYS:HG3	2	0.16	0.04	0.16
(1,20)	1:B:93:LYS:HA	1:B:109:LEU:HG	2	0.16	0.04	0.16
(1,917)	1:A:87:THR:HA	1:A:92:GLU:HG2	2	0.16	0.04	0.16
(1,917)	1:A:87:THR:HA	1:A:92:GLU:HG3	2	0.16	0.04	0.16
(1,917)	1:A:87:THR:HA	1:B:9:GLU:HB2	2	0.16	0.04	0.16
(1,917)	1:A:87:THR:HA	1:B:9:GLU:HB3	2	0.16	0.04	0.16
(1,917)	1:A:87:THR:HA	1:B:12:ILE:HB	2	0.16	0.04	0.16
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD12	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD11	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD13	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD12	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD11	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD13	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD12	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD11	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD13	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD12	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD11	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD13	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD12	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD11	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD13	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD12	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD11	2	0.16	0.02	0.16
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD13	2	0.16	0.02	0.16
(1,918)	1:B:87:THR:HA	1:B:92:GLU:HG2	2	0.16	0.05	0.16
(1,918)	1:B:87:THR:HA	1:B:92:GLU:HG3	2	0.16	0.05	0.16
(1,918)	1:B:87:THR:HA	1:A:9:GLU:HB2	2	0.16	0.05	0.16
(1,918)	1:B:87:THR:HA	1:A:9:GLU:HB3	2	0.16	0.05	0.16
(1,918)	1:B:87:THR:HA	1:A:12:ILE:HB	2	0.16	0.05	0.16
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD12	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD11	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD13	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD12	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD11	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD13	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD12	2	0.16	0.02	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD11	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD13	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD12	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD11	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD13	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD12	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD11	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD13	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD12	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD11	2	0.16	0.02	0.16
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD13	2	0.16	0.02	0.16
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG21	2	0.16	0.02	0.16
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG22	2	0.16	0.02	0.16
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG23	2	0.16	0.02	0.16
(3,1363)	1:A:69:ASN:H	1:A:68:THR:HB	2	0.16	0.04	0.16
(3,1364)	1:B:69:ASN:H	1:B:68:THR:HB	2	0.16	0.04	0.16
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG21	2	0.15	0.02	0.15
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG22	2	0.15	0.02	0.15
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG23	2	0.15	0.02	0.15
(2,62)	1:A:81:MET:H	1:A:77:GLU:O	2	0.15	0.02	0.15
(4,111)	1:A:76:PHE:H	1:A:31:THR:H	2	0.15	0.03	0.15
(1,353)	1:A:58:VAL:HG22	1:A:54:LYS:HA	2	0.14	0.03	0.14
(1,353)	1:A:58:VAL:HG21	1:A:54:LYS:HA	2	0.14	0.03	0.14
(1,353)	1:A:58:VAL:HG23	1:A:54:LYS:HA	2	0.14	0.03	0.14
(1,353)	1:A:58:VAL:HG12	1:A:54:LYS:HA	2	0.14	0.03	0.14
(1,353)	1:A:58:VAL:HG11	1:A:54:LYS:HA	2	0.14	0.03	0.14
(1,353)	1:A:58:VAL:HG13	1:A:54:LYS:HA	2	0.14	0.03	0.14
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG21	2	0.14	0.03	0.14
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG22	2	0.14	0.03	0.14
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG23	2	0.14	0.03	0.14
(1,354)	1:B:58:VAL:HG22	1:B:54:LYS:HA	2	0.14	0.03	0.14
(1,354)	1:B:58:VAL:HG21	1:B:54:LYS:HA	2	0.14	0.03	0.14
(1,354)	1:B:58:VAL:HG23	1:B:54:LYS:HA	2	0.14	0.03	0.14
(1,354)	1:B:58:VAL:HG12	1:B:54:LYS:HA	2	0.14	0.03	0.14
(1,354)	1:B:58:VAL:HG11	1:B:54:LYS:HA	2	0.14	0.03	0.14
(1,354)	1:B:58:VAL:HG13	1:B:54:LYS:HA	2	0.14	0.03	0.14
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG21	2	0.14	0.03	0.14
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG22	2	0.14	0.03	0.14
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG23	2	0.14	0.03	0.14
(1,1098)	1:B:59:ILE:HG22	1:B:42:ARG:HD2	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG22	1:B:42:ARG:HD3	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG21	1:B:42:ARG:HD2	2	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,1098)	1:B:59:ILE:HG21	1:B:42:ARG:HD3	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG23	1:B:42:ARG:HD2	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG23	1:B:42:ARG:HD3	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG22	1:B:79:PHE:HB2	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG22	1:B:79:PHE:HB3	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG21	1:B:79:PHE:HB2	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG21	1:B:79:PHE:HB3	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG23	1:B:79:PHE:HB2	2	0.14	0.01	0.14
(1,1098)	1:B:59:ILE:HG23	1:B:79:PHE:HB3	2	0.14	0.01	0.14
(1,1331)	1:A:12:ILE:H	1:A:14:THR:H	2	0.14	0.02	0.14
(1,1331)	1:A:12:ILE:H	1:A:15:ILE:H	2	0.14	0.02	0.14
(1,1332)	1:B:12:ILE:H	1:B:14:THR:H	2	0.14	0.02	0.14
(1,1332)	1:B:12:ILE:H	1:B:15:ILE:H	2	0.14	0.02	0.14
(4,112)	1:B:76:PHE:H	1:B:31:THR:H	2	0.14	0.03	0.14
(1,1097)	1:A:59:ILE:HG22	1:A:42:ARG:HD2	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG22	1:A:42:ARG:HD3	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG21	1:A:42:ARG:HD2	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG21	1:A:42:ARG:HD3	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG23	1:A:42:ARG:HD2	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG23	1:A:42:ARG:HD3	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG22	1:A:79:PHE:HB2	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG22	1:A:79:PHE:HB3	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG21	1:A:79:PHE:HB2	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG21	1:A:79:PHE:HB3	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG23	1:A:79:PHE:HB2	2	0.14	0.02	0.14
(1,1097)	1:A:59:ILE:HG23	1:A:79:PHE:HB3	2	0.14	0.02	0.14
(3,345)	1:A:5:MET:H	1:A:4:LYS:HG2	2	0.14	0.02	0.14
(3,345)	1:A:5:MET:H	1:A:4:LYS:HG3	2	0.14	0.02	0.14
(3,346)	1:B:5:MET:H	1:B:4:LYS:HG2	2	0.14	0.01	0.14
(3,346)	1:B:5:MET:H	1:B:4:LYS:HG3	2	0.14	0.01	0.14
(1,651)	1:A:93:LYS:H	1:A:92:GLU:HB2	2	0.12	0.01	0.12
(1,651)	1:A:93:LYS:H	1:A:92:GLU:HB3	2	0.12	0.01	0.12
(1,651)	1:A:100:GLY:H	1:A:99:GLU:HB2	2	0.12	0.01	0.12
(1,651)	1:A:100:GLY:H	1:A:99:GLU:HB3	2	0.12	0.01	0.12
(1,652)	1:B:93:LYS:H	1:B:92:GLU:HB2	2	0.12	0.01	0.12
(1,652)	1:B:93:LYS:H	1:B:92:GLU:HB3	2	0.12	0.01	0.12
(1,652)	1:B:100:GLY:H	1:B:99:GLU:HB2	2	0.12	0.01	0.12
(1,652)	1:B:100:GLY:H	1:B:99:GLU:HB3	2	0.12	0.01	0.12
(1,1405)	1:A:20:HIS:H	1:B:8:LEU:HB2	2	0.12	0.01	0.12
(1,1405)	1:A:20:HIS:H	1:B:8:LEU:HB3	2	0.12	0.01	0.12
(1,1405)	1:A:20:HIS:H	1:A:25:LYS:HB2	2	0.12	0.01	0.12
(1,1405)	1:A:20:HIS:H	1:A:25:LYS:HB3	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)
(1,1405)	1:A:20:HIS:H	1:A:32:LEU:HG	2	0.12	0.01	0.12
(1,1405)	1:A:20:HIS:H	1:A:36:GLU:HB2	2	0.12	0.01	0.12
(1,1405)	1:A:20:HIS:H	1:A:36:GLU:HB3	2	0.12	0.01	0.12
(4,235)	1:A:81:MET:H	1:B:81:MET:H	2	0.12	0.02	0.12
(4,236)	1:B:81:MET:H	1:A:81:MET:H	2	0.12	0.02	0.12
(1,567)	1:A:42:ARG:HA	1:A:43:LYS:HE2	2	0.12	0.0	0.12
(1,567)	1:A:42:ARG:HA	1:A:43:LYS:HE3	2	0.12	0.0	0.12
(1,567)	1:A:42:ARG:HA	1:A:50:LYS:HE2	2	0.12	0.0	0.12
(1,567)	1:A:42:ARG:HA	1:A:50:LYS:HE3	2	0.12	0.0	0.12
(1,567)	1:A:42:ARG:HA	1:A:54:LYS:HE2	2	0.12	0.0	0.12
(1,567)	1:A:42:ARG:HA	1:A:54:LYS:HE3	2	0.12	0.0	0.12
(1,1406)	1:B:20:HIS:H	1:A:8:LEU:HB2	2	0.12	0.01	0.12
(1,1406)	1:B:20:HIS:H	1:A:8:LEU:HB3	2	0.12	0.01	0.12
(1,1406)	1:B:20:HIS:H	1:B:25:LYS:HB2	2	0.12	0.01	0.12
(1,1406)	1:B:20:HIS:H	1:B:25:LYS:HB3	2	0.12	0.01	0.12
(1,1406)	1:B:20:HIS:H	1:B:32:LEU:HG	2	0.12	0.01	0.12
(1,1406)	1:B:20:HIS:H	1:B:36:GLU:HB2	2	0.12	0.01	0.12
(1,1406)	1:B:20:HIS:H	1:B:36:GLU:HB3	2	0.12	0.01	0.12
(1,1555)	1:A:46:GLN:H	1:A:45:LEU:HG	2	0.12	0.0	0.12
(1,1555)	1:A:38:LYS:H	1:A:32:LEU:HB2	2	0.12	0.0	0.12
(1,1555)	1:A:38:LYS:H	1:A:32:LEU:HB3	2	0.12	0.0	0.12
(1,1555)	1:A:44:ASP:H	1:A:45:LEU:HG	2	0.12	0.0	0.12
(1,1556)	1:B:46:GLN:H	1:B:45:LEU:HG	2	0.12	0.0	0.12
(1,1556)	1:B:38:LYS:H	1:B:32:LEU:HB2	2	0.12	0.0	0.12
(1,1556)	1:B:38:LYS:H	1:B:32:LEU:HB3	2	0.12	0.0	0.12
(1,1556)	1:B:44:ASP:H	1:B:45:LEU:HG	2	0.12	0.0	0.12
(3,340)	1:B:57:LYS:HG2	1:B:56:GLU:HB2	2	0.12	0.01	0.12
(3,340)	1:B:57:LYS:HG2	1:B:56:GLU:HB3	2	0.12	0.01	0.12
(3,340)	1:B:57:LYS:HG3	1:B:56:GLU:HB2	2	0.12	0.01	0.12
(3,340)	1:B:57:LYS:HG3	1:B:56:GLU:HB3	2	0.12	0.01	0.12
(3,601)	1:A:46:GLN:HG2	1:B:4:LYS:HE2	2	0.12	0.01	0.12
(3,601)	1:A:46:GLN:HG2	1:B:4:LYS:HE3	2	0.12	0.01	0.12
(3,601)	1:A:46:GLN:HG3	1:B:4:LYS:HE2	2	0.12	0.01	0.12
(3,601)	1:A:46:GLN:HG3	1:B:4:LYS:HE3	2	0.12	0.01	0.12
(3,1343)	1:A:66:LEU:H	1:A:66:LEU:HG	2	0.12	0.01	0.12
(3,1344)	1:B:66:LEU:H	1:B:66:LEU:HG	2	0.12	0.01	0.12
(1,568)	1:B:42:ARG:HA	1:B:43:LYS:HE2	2	0.12	0.0	0.12
(1,568)	1:B:42:ARG:HA	1:B:43:LYS:HE3	2	0.12	0.0	0.12
(1,568)	1:B:42:ARG:HA	1:B:50:LYS:HE2	2	0.12	0.0	0.12
(1,568)	1:B:42:ARG:HA	1:B:50:LYS:HE3	2	0.12	0.0	0.12
(1,568)	1:B:42:ARG:HA	1:B:54:LYS:HE2	2	0.12	0.0	0.12
(1,568)	1:B:42:ARG:HA	1:B:54:LYS:HE3	2	0.12	0.0	0.12

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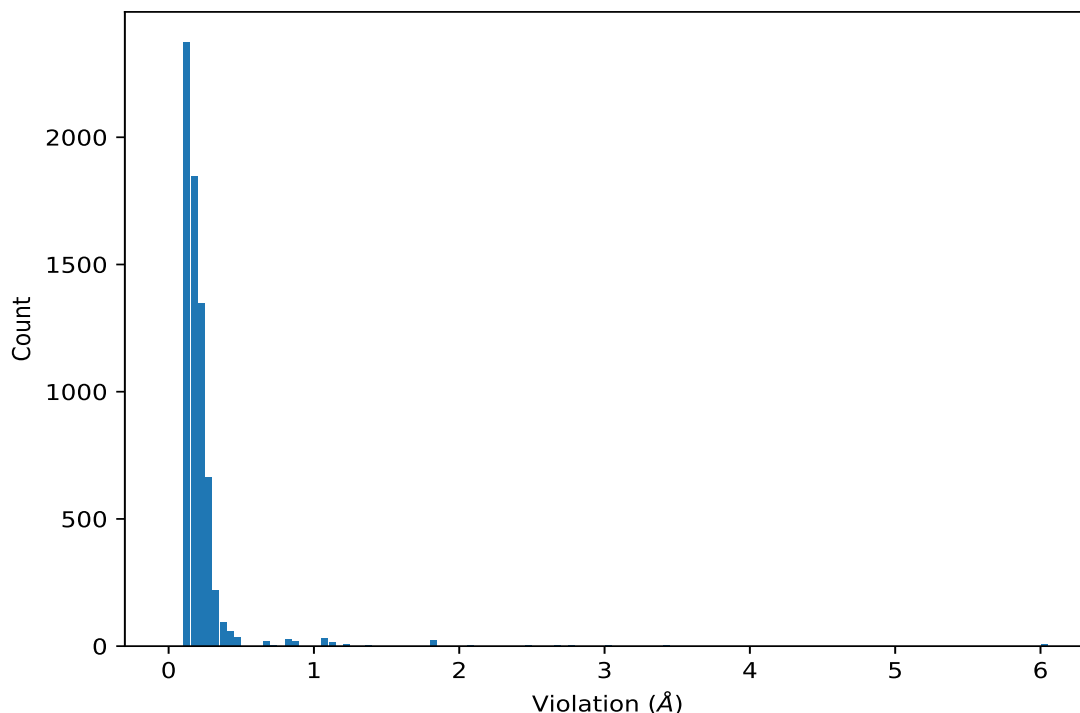
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,84)	1:A:93:LYS:H	1:A:89:ALA:O	2	0.12	0.0	0.12
(4,231)	1:A:79:PHE:H	1:A:80:ILE:HB	2	0.12	0.0	0.12
(4,232)	1:B:79:PHE:H	1:B:80:ILE:HB	2	0.12	0.0	0.12

<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)
(3,794)	1:B:107:PRO:HG2	1:B:93:LYS:HG2	3	6.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,794)	1:B:107:PRO:HG2	1:B:93:LYS:HG3	3	6.05
(3,794)	1:B:107:PRO:HG3	1:B:93:LYS:HG2	3	6.05
(3,794)	1:B:107:PRO:HG3	1:B:93:LYS:HG3	3	6.05
(3,793)	1:A:107:PRO:HG2	1:A:93:LYS:HG2	3	6.05
(3,793)	1:A:107:PRO:HG2	1:A:93:LYS:HG3	3	6.05
(3,793)	1:A:107:PRO:HG3	1:A:93:LYS:HG2	3	6.05
(3,793)	1:A:107:PRO:HG3	1:A:93:LYS:HG3	3	6.05
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	5	3.6
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	5	3.59
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	1	3.42
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	1	3.42
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	6	3.04
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	6	3.04
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	3	2.77
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	3	2.77
(3,534)	1:B:24:VAL:HA	1:B:29:PRO:HA	9	2.73
(3,533)	1:A:24:VAL:HA	1:A:29:PRO:HA	9	2.69
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	4	2.66
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	4	2.65
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	8	2.46
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	8	2.46
(3,534)	1:B:24:VAL:HA	1:B:29:PRO:HA	6	2.05
(3,533)	1:A:24:VAL:HA	1:A:29:PRO:HA	6	2.05
(3,738)	1:B:24:VAL:HG22	1:B:29:PRO:HB2	9	1.82
(3,738)	1:B:24:VAL:HG22	1:B:29:PRO:HB3	9	1.82
(3,738)	1:B:24:VAL:HG21	1:B:29:PRO:HB2	9	1.82
(3,738)	1:B:24:VAL:HG21	1:B:29:PRO:HB3	9	1.82
(3,738)	1:B:24:VAL:HG23	1:B:29:PRO:HB2	9	1.82
(3,738)	1:B:24:VAL:HG23	1:B:29:PRO:HB3	9	1.82
(3,738)	1:B:24:VAL:HG12	1:B:29:PRO:HB2	9	1.82
(3,738)	1:B:24:VAL:HG12	1:B:29:PRO:HB3	9	1.82
(3,738)	1:B:24:VAL:HG11	1:B:29:PRO:HB2	9	1.82
(3,738)	1:B:24:VAL:HG11	1:B:29:PRO:HB3	9	1.82
(3,738)	1:B:24:VAL:HG13	1:B:29:PRO:HB2	9	1.82
(3,738)	1:B:24:VAL:HG13	1:B:29:PRO:HB3	9	1.82
(3,737)	1:A:24:VAL:HG22	1:A:29:PRO:HB2	9	1.81
(3,737)	1:A:24:VAL:HG22	1:A:29:PRO:HB3	9	1.81
(3,737)	1:A:24:VAL:HG21	1:A:29:PRO:HB2	9	1.81
(3,737)	1:A:24:VAL:HG21	1:A:29:PRO:HB3	9	1.81
(3,737)	1:A:24:VAL:HG23	1:A:29:PRO:HB2	9	1.81
(3,737)	1:A:24:VAL:HG23	1:A:29:PRO:HB3	9	1.81
(3,737)	1:A:24:VAL:HG12	1:A:29:PRO:HB2	9	1.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,737)	1:A:24:VAL:HG12	1:A:29:PRO:HB3	9	1.81
(3,737)	1:A:24:VAL:HG11	1:A:29:PRO:HB2	9	1.81
(3,737)	1:A:24:VAL:HG11	1:A:29:PRO:HB3	9	1.81
(3,737)	1:A:24:VAL:HG13	1:A:29:PRO:HB2	9	1.81
(3,737)	1:A:24:VAL:HG13	1:A:29:PRO:HB3	9	1.81
(3,1474)	1:B:100:GLY:H	1:B:98:ASP:HA	10	1.37
(3,1473)	1:A:100:GLY:H	1:A:98:ASP:HA	10	1.37
(1,1196)	1:B:98:ASP:HA	1:B:95:HIS:HB3	9	1.2
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB2	9	1.2
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB3	9	1.2
(1,1195)	1:A:98:ASP:HA	1:A:95:HIS:HB3	9	1.2
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB2	9	1.2
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB3	9	1.2
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	6	1.14
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	6	1.14
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	6	1.14
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	6	1.14
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD2	9	1.12
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD3	9	1.12
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD2	9	1.12
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD3	9	1.12
(1,24)	1:B:65:ASP:HA	1:B:72:LYS:HA	9	1.12
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD2	9	1.11
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD3	9	1.11
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD2	9	1.11
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD3	9	1.11
(1,23)	1:A:65:ASP:HA	1:A:72:LYS:HA	9	1.11
(3,738)	1:B:24:VAL:HG22	1:B:29:PRO:HB2	6	1.08
(3,738)	1:B:24:VAL:HG22	1:B:29:PRO:HB3	6	1.08
(3,738)	1:B:24:VAL:HG21	1:B:29:PRO:HB2	6	1.08
(3,738)	1:B:24:VAL:HG21	1:B:29:PRO:HB3	6	1.08
(3,738)	1:B:24:VAL:HG23	1:B:29:PRO:HB2	6	1.08
(3,738)	1:B:24:VAL:HG23	1:B:29:PRO:HB3	6	1.08
(3,738)	1:B:24:VAL:HG12	1:B:29:PRO:HB2	6	1.08
(3,738)	1:B:24:VAL:HG12	1:B:29:PRO:HB3	6	1.08
(3,738)	1:B:24:VAL:HG11	1:B:29:PRO:HB2	6	1.08
(3,738)	1:B:24:VAL:HG11	1:B:29:PRO:HB3	6	1.08
(3,738)	1:B:24:VAL:HG13	1:B:29:PRO:HB2	6	1.08
(3,738)	1:B:24:VAL:HG13	1:B:29:PRO:HB3	6	1.08
(3,737)	1:A:24:VAL:HG22	1:A:29:PRO:HB2	6	1.08
(3,737)	1:A:24:VAL:HG22	1:A:29:PRO:HB3	6	1.08
(3,737)	1:A:24:VAL:HG21	1:A:29:PRO:HB2	6	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,737)	1:A:24:VAL:HG21	1:A:29:PRO:HB3	6	1.08
(3,737)	1:A:24:VAL:HG23	1:A:29:PRO:HB2	6	1.08
(3,737)	1:A:24:VAL:HG23	1:A:29:PRO:HB3	6	1.08
(3,737)	1:A:24:VAL:HG12	1:A:29:PRO:HB2	6	1.08
(3,737)	1:A:24:VAL:HG12	1:A:29:PRO:HB3	6	1.08
(3,737)	1:A:24:VAL:HG11	1:A:29:PRO:HB2	6	1.08
(3,737)	1:A:24:VAL:HG11	1:A:29:PRO:HB3	6	1.08
(3,737)	1:A:24:VAL:HG13	1:A:29:PRO:HB2	6	1.08
(3,737)	1:A:24:VAL:HG13	1:A:29:PRO:HB3	6	1.08
(1,1196)	1:B:98:ASP:HA	1:B:95:HIS:HB3	10	1.08
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB2	10	1.08
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB3	10	1.08
(1,1195)	1:A:98:ASP:HA	1:A:95:HIS:HB3	10	1.08
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB2	10	1.08
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB3	10	1.08
(4,258)	1:B:108:GLY:H	1:B:111:GLU:HA	6	0.89
(4,257)	1:A:108:GLY:H	1:A:111:GLU:HA	6	0.89
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA2	4	0.86
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA3	4	0.86
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA2	4	0.86
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA3	4	0.86
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA2	4	0.86
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA3	4	0.86
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA2	4	0.86
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA3	4	0.86
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA2	4	0.85
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA3	4	0.85
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA2	4	0.85
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA3	4	0.85
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA2	4	0.85
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA3	4	0.85
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA2	4	0.85
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA3	4	0.85
(4,258)	1:B:108:GLY:H	1:B:111:GLU:HA	9	0.83
(4,257)	1:A:108:GLY:H	1:A:111:GLU:HA	9	0.83
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA2	5	0.83
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA3	5	0.83
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA2	5	0.83
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA3	5	0.83
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA2	5	0.83
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA3	5	0.83
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA2	5	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA3	5	0.83
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA2	5	0.83
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA3	5	0.83
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA2	5	0.83
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA3	5	0.83
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA2	5	0.83
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA3	5	0.83
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA2	5	0.83
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA3	5	0.83
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	8	0.82
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	8	0.82
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	8	0.82
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	8	0.82
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA2	6	0.81
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA3	6	0.81
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA2	6	0.8
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA3	6	0.8
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	8	0.73
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	8	0.72
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA2	8	0.68
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA3	8	0.68
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA2	8	0.68
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA3	8	0.68
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA2	8	0.68
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA3	8	0.68
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA2	8	0.68
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA3	8	0.68
(4,258)	1:B:108:GLY:H	1:B:111:GLU:HA	1	0.67
(4,257)	1:A:108:GLY:H	1:A:111:GLU:HA	1	0.67
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA2	8	0.67
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA3	8	0.67
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA2	8	0.67
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA3	8	0.67
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA2	8	0.67
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA3	8	0.67
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA2	8	0.67
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA3	8	0.67
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA2	9	0.46
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA3	9	0.46
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA2	9	0.46
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA3	9	0.46
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA2	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA3	2	0.46
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA2	2	0.46
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA3	2	0.46
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA2	2	0.46
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA3	2	0.46
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA2	2	0.46
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA3	2	0.46
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA2	3	0.46
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA3	3	0.46
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA2	3	0.46
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA3	3	0.46
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA2	3	0.46
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA3	3	0.46
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA2	3	0.46
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA3	3	0.46
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA2	2	0.46
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA3	2	0.46
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA2	2	0.46
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA3	2	0.46
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA2	2	0.46
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA3	2	0.46
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA2	2	0.46
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA3	2	0.46
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA2	3	0.45
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA3	3	0.45
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA2	3	0.45
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA3	3	0.45
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA2	3	0.45
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA3	3	0.45
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA2	3	0.45
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA3	3	0.45
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	4	0.44
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	4	0.44
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	4	0.44
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	4	0.44
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA2	8	0.44
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA3	8	0.44
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA2	8	0.44
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA3	8	0.44
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA2	8	0.44
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA3	8	0.44
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA2	8	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA3	8	0.44
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA2	10	0.44
(1,690)	1:B:107:PRO:HG2	1:B:108:GLY:HA3	10	0.44
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA2	10	0.44
(1,690)	1:B:107:PRO:HG3	1:B:108:GLY:HA3	10	0.44
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA2	10	0.44
(1,690)	1:B:107:PRO:HG2	1:B:112:GLY:HA3	10	0.44
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA2	10	0.44
(1,690)	1:B:107:PRO:HG3	1:B:112:GLY:HA3	10	0.44
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA2	8	0.44
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA3	8	0.44
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA2	8	0.44
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA3	8	0.44
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA2	8	0.44
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA3	8	0.44
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA2	8	0.44
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA3	8	0.44
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA2	10	0.44
(1,689)	1:A:107:PRO:HG2	1:A:108:GLY:HA3	10	0.44
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA2	10	0.44
(1,689)	1:A:107:PRO:HG3	1:A:108:GLY:HA3	10	0.44
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA2	10	0.44
(1,689)	1:A:107:PRO:HG2	1:A:112:GLY:HA3	10	0.44
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA2	10	0.44
(1,689)	1:A:107:PRO:HG3	1:A:112:GLY:HA3	10	0.44
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	1	0.42
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	1	0.42
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	1	0.42
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	1	0.42
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	1	0.42
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	1	0.42
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	1	0.42
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	1	0.42
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	1	0.42
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	1	0.42
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	1	0.42
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	1	0.42
(3,1474)	1:B:100:GLY:H	1:B:98:ASP:HA	9	0.41
(3,572)	1:B:78:GLU:HB2	1:B:66:LEU:HB2	3	0.4
(3,572)	1:B:78:GLU:HB2	1:B:66:LEU:HB3	3	0.4
(3,572)	1:B:78:GLU:HB3	1:B:66:LEU:HB2	3	0.4
(3,572)	1:B:78:GLU:HB3	1:B:66:LEU:HB3	3	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,571)	1:A:78:GLU:HB2	1:A:66:LEU:HB2	3	0.4
(3,571)	1:A:78:GLU:HB2	1:A:66:LEU:HB3	3	0.4
(3,571)	1:A:78:GLU:HB3	1:A:66:LEU:HB2	3	0.4
(3,571)	1:A:78:GLU:HB3	1:A:66:LEU:HB3	3	0.4
(3,1473)	1:A:100:GLY:H	1:A:98:ASP:HA	9	0.4
(3,1427)	1:A:86:LEU:H	1:A:86:LEU:HG	10	0.38
(1,1706)	1:B:24:VAL:H	1:B:17:ASN:HA	6	0.38
(1,1706)	1:B:78:GLU:H	1:B:67:ASP:HA	6	0.38
(1,1705)	1:A:24:VAL:H	1:A:17:ASN:HA	6	0.38
(1,1705)	1:A:78:GLU:H	1:A:67:ASP:HA	6	0.38
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	8	0.38
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	8	0.38
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	8	0.38
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	8	0.38
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	8	0.38
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	8	0.38
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	8	0.38
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	8	0.38
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	8	0.38
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	8	0.38
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	8	0.38
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	8	0.38
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	10	0.37
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	10	0.37
(3,485)	1:A:96:GLU:HG2	1:A:97:GLY:H	9	0.37
(3,485)	1:A:96:GLU:HG3	1:A:97:GLY:H	9	0.37
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA2	1	0.37
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA3	1	0.37
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA2	1	0.37
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA3	1	0.37
(3,1428)	1:B:86:LEU:H	1:B:86:LEU:HG	10	0.37
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	10	0.37
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	10	0.37
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	10	0.37
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	10	0.37
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	10	0.37
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	10	0.37
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	10	0.37
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	10	0.37
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD2	1	0.37
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD3	1	0.37
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD2	1	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD3	1	0.37
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG2	1	0.37
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG3	1	0.37
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG2	1	0.37
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG3	1	0.37
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB2	1	0.37
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB3	1	0.37
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB2	1	0.37
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB3	1	0.37
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD2	1	0.37
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD3	1	0.37
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD2	1	0.37
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD3	1	0.37
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD2	1	0.37
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD3	1	0.37
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD2	1	0.37
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD3	1	0.37
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG2	1	0.37
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG3	1	0.37
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG2	1	0.37
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG3	1	0.37
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB2	1	0.37
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB3	1	0.37
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB2	1	0.37
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB3	1	0.37
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD2	1	0.37
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD3	1	0.37
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD2	1	0.37
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD3	1	0.37
(3,628)	1:B:48:PHE:HB2	1:A:9:GLU:HG2	8	0.36
(3,628)	1:B:48:PHE:HB2	1:A:9:GLU:HG3	8	0.36
(3,628)	1:B:48:PHE:HB3	1:A:9:GLU:HG2	8	0.36
(3,628)	1:B:48:PHE:HB3	1:A:9:GLU:HG3	8	0.36
(3,486)	1:B:96:GLU:HG2	1:B:97:GLY:H	9	0.36
(3,486)	1:B:96:GLU:HG3	1:B:97:GLY:H	9	0.36
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	3	0.36
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	3	0.36
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	5	0.35
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	5	0.35
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	5	0.35
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	5	0.35
(3,627)	1:A:48:PHE:HB2	1:B:9:GLU:HG2	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,627)	1:A:48:PHE:HB2	1:B:9:GLU:HG3	8	0.35
(3,627)	1:A:48:PHE:HB3	1:B:9:GLU:HG2	8	0.35
(3,627)	1:A:48:PHE:HB3	1:B:9:GLU:HG3	8	0.35
(3,596)	1:B:72:LYS:HG2	1:B:72:LYS:HA	2	0.35
(3,596)	1:B:72:LYS:HG3	1:B:72:LYS:HA	2	0.35
(3,595)	1:A:72:LYS:HG2	1:A:72:LYS:HA	2	0.35
(3,595)	1:A:72:LYS:HG3	1:A:72:LYS:HA	2	0.35
(3,1428)	1:B:86:LEU:H	1:B:86:LEU:HG	1	0.35
(3,1427)	1:A:86:LEU:H	1:A:86:LEU:HG	1	0.35
(3,1406)	1:B:81:MET:H	1:B:80:ILE:HB	7	0.35
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	5	0.35
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	5	0.35
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	3	0.35
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	3	0.35
(3,1428)	1:B:86:LEU:H	1:B:86:LEU:HG	9	0.34
(3,1427)	1:A:86:LEU:H	1:A:86:LEU:HG	9	0.34
(3,1405)	1:A:81:MET:H	1:A:80:ILE:HB	7	0.34
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	5	0.34
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	5	0.34
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG2	7	0.34
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG3	7	0.34
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG2	7	0.34
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG3	7	0.34
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG2	7	0.34
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG3	7	0.34
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG2	7	0.34
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG3	7	0.34
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG2	7	0.34
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG3	7	0.34
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG2	7	0.34
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG3	7	0.34
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG2	7	0.34
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG3	7	0.34
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG2	7	0.34
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG3	7	0.34
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG2	7	0.34
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG3	7	0.34
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG2	7	0.34
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG3	7	0.34
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG2	7	0.34
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG3	7	0.34
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG2	7	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG3	7	0.34
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	7	0.33
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	7	0.33
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	3	0.33
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	3	0.33
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	7	0.33
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	7	0.33
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	3	0.33
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	3	0.33
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	7	0.33
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	7	0.33
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA2	6	0.33
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA3	6	0.33
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA2	6	0.33
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA3	6	0.33
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA2	6	0.33
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA3	6	0.33
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA2	6	0.33
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA3	6	0.33
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD22	3	0.33
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD21	3	0.33
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD23	3	0.33
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD12	3	0.33
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD11	3	0.33
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD13	3	0.33
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD22	3	0.33
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD21	3	0.33
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD23	3	0.33
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD12	3	0.33
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD11	3	0.33
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD13	3	0.33
(1,698)	1:B:74:LEU:HG	1:B:38:LYS:HG2	3	0.33
(1,698)	1:B:74:LEU:HG	1:B:38:LYS:HG3	3	0.33
(1,698)	1:B:74:LEU:HG	1:B:40:LEU:HB2	3	0.33
(1,698)	1:B:74:LEU:HG	1:B:40:LEU:HB3	3	0.33
(1,698)	1:B:107:PRO:HG2	1:B:93:LYS:HG2	3	0.33
(1,698)	1:B:107:PRO:HG2	1:B:93:LYS:HG3	3	0.33
(1,698)	1:B:107:PRO:HG3	1:B:93:LYS:HG2	3	0.33
(1,698)	1:B:107:PRO:HG3	1:B:93:LYS:HG3	3	0.33
(1,697)	1:A:74:LEU:HG	1:A:38:LYS:HG2	3	0.33
(1,697)	1:A:74:LEU:HG	1:A:38:LYS:HG3	3	0.33
(1,697)	1:A:74:LEU:HG	1:A:40:LEU:HB2	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:A:74:LEU:HG	1:A:40:LEU:HB3	3	0.33
(1,697)	1:A:107:PRO:HG2	1:A:93:LYS:HG2	3	0.33
(1,697)	1:A:107:PRO:HG2	1:A:93:LYS:HG3	3	0.33
(1,697)	1:A:107:PRO:HG3	1:A:93:LYS:HG2	3	0.33
(1,697)	1:A:107:PRO:HG3	1:A:93:LYS:HG3	3	0.33
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG2	1	0.33
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG3	1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG2	1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG3	1	0.33
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG2	1	0.33
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG3	1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG2	1	0.33
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG3	1	0.33
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG2	1	0.33
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG3	1	0.33
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG2	1	0.33
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG3	1	0.33
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	1	0.33
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	1	0.33
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	1	0.33
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	1	0.33
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	1	0.33
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	1	0.33
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	1	0.33
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	1	0.33
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	1	0.33
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	1	0.33
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	1	0.33
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	1	0.33
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	1	0.33
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	1	0.33
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	1	0.33
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	1	0.33
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	1	0.33
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	1	0.33
(1,1858)	1:B:108:GLY:H	1:B:111:GLU:HA	3	0.33
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA2	3	0.33
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA3	3	0.33
(1,1858)	1:B:110:GLY:H	1:B:111:GLU:HA	3	0.33
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA2	3	0.33
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA3	3	0.33
(1,1857)	1:A:108:GLY:H	1:A:111:GLU:HA	3	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA2	3	0.33
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA3	3	0.33
(1,1857)	1:A:110:GLY:H	1:A:111:GLU:HA	3	0.33
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA2	3	0.33
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA3	3	0.33
(1,1508)	1:B:39:GLU:H	1:B:41:VAL:HB	3	0.33
(1,1508)	1:B:67:ASP:H	1:B:64:GLU:HG2	3	0.33
(1,1508)	1:B:67:ASP:H	1:B:64:GLU:HG3	3	0.33
(1,1508)	1:B:67:ASP:H	1:B:78:GLU:HB2	3	0.33
(1,1508)	1:B:67:ASP:H	1:B:78:GLU:HB3	3	0.33
(1,1507)	1:A:39:GLU:H	1:A:41:VAL:HB	3	0.33
(1,1507)	1:A:67:ASP:H	1:A:64:GLU:HG2	3	0.33
(1,1507)	1:A:67:ASP:H	1:A:64:GLU:HG3	3	0.33
(1,1507)	1:A:67:ASP:H	1:A:78:GLU:HB2	3	0.33
(1,1507)	1:A:67:ASP:H	1:A:78:GLU:HB3	3	0.33
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	9	0.32
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	9	0.32
(3,712)	1:B:11:ASN:HB2	1:B:8:LEU:HA	7	0.32
(3,712)	1:B:11:ASN:HB3	1:B:8:LEU:HA	7	0.32
(3,711)	1:A:11:ASN:HB2	1:A:8:LEU:HA	7	0.32
(3,711)	1:A:11:ASN:HB3	1:A:8:LEU:HA	7	0.32
(3,618)	1:B:57:LYS:HA	1:B:57:LYS:HG2	8	0.32
(3,618)	1:B:57:LYS:HA	1:B:57:LYS:HG3	8	0.32
(3,617)	1:A:57:LYS:HA	1:A:57:LYS:HG2	8	0.32
(3,617)	1:A:57:LYS:HA	1:A:57:LYS:HG3	8	0.32
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	8	0.32
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	8	0.32
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG2	1	0.32
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG3	1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG2	1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG3	1	0.32
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG2	1	0.32
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG3	1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG2	1	0.32
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG3	1	0.32
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG2	1	0.32
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG3	1	0.32
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG2	1	0.32
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG3	1	0.32
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	10	0.32
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	10	0.32
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	10	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	10	0.32
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	1	0.32
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	1	0.32
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	1	0.32
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	1	0.32
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	1	0.32
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	1	0.32
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	1	0.32
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	1	0.32
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	1	0.32
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	1	0.32
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	1	0.32
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	1	0.32
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	1	0.32
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	1	0.32
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	1	0.32
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	1	0.32
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	1	0.32
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	1	0.32
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD2	1	0.32
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD3	1	0.32
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD2	1	0.32
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD3	1	0.32
(1,24)	1:B:65:ASP:HA	1:B:72:LYS:HA	1	0.32
(1,1816)	1:B:97:GLY:H	1:B:98:ASP:HA	7	0.32
(1,1816)	1:B:110:GLY:H	1:B:48:PHE:HA	7	0.32
(1,1815)	1:A:97:GLY:H	1:A:98:ASP:HA	7	0.32
(1,1815)	1:A:110:GLY:H	1:A:48:PHE:HA	7	0.32
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	6	0.31
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	6	0.31
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	6	0.31
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	6	0.31
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	6	0.31
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	6	0.31
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	9	0.31
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	9	0.31
(3,618)	1:B:57:LYS:HA	1:B:57:LYS:HG2	7	0.31
(3,618)	1:B:57:LYS:HA	1:B:57:LYS:HG3	7	0.31
(3,366)	1:B:85:ARG:HG2	1:A:77:GLU:HA	8	0.31
(3,366)	1:B:85:ARG:HG3	1:A:77:GLU:HA	8	0.31
(3,365)	1:A:85:ARG:HG2	1:B:77:GLU:HA	8	0.31
(3,365)	1:A:85:ARG:HG3	1:B:77:GLU:HA	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD2	1	0.31
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD3	1	0.31
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD2	1	0.31
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD3	1	0.31
(1,23)	1:A:65:ASP:HA	1:A:72:LYS:HA	1	0.31
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	2	0.3
(3,866)	1:B:52:GLU:H	1:B:51:LYS:HG2	2	0.3
(3,866)	1:B:52:GLU:H	1:B:51:LYS:HG3	2	0.3
(3,865)	1:A:52:GLU:H	1:A:51:LYS:HG2	2	0.3
(3,865)	1:A:52:GLU:H	1:A:51:LYS:HG3	2	0.3
(3,617)	1:A:57:LYS:HA	1:A:57:LYS:HG2	7	0.3
(3,617)	1:A:57:LYS:HA	1:A:57:LYS:HG3	7	0.3
(3,504)	1:B:111:GLU:HA	1:B:107:PRO:HB2	3	0.3
(3,504)	1:B:111:GLU:HA	1:B:107:PRO:HB3	3	0.3
(3,503)	1:A:111:GLU:HA	1:A:107:PRO:HB2	3	0.3
(3,503)	1:A:111:GLU:HA	1:A:107:PRO:HB3	3	0.3
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB2	9	0.3
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB3	9	0.3
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB2	9	0.3
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB3	9	0.3
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	6	0.3
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	6	0.3
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	2	0.29
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	8	0.29
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	8	0.29
(3,628)	1:B:48:PHE:HB2	1:A:9:GLU:HG2	5	0.29
(3,628)	1:B:48:PHE:HB2	1:A:9:GLU:HG3	5	0.29
(3,628)	1:B:48:PHE:HB3	1:A:9:GLU:HG2	5	0.29
(3,628)	1:B:48:PHE:HB3	1:A:9:GLU:HG3	5	0.29
(3,627)	1:A:48:PHE:HB2	1:B:9:GLU:HG2	5	0.29
(3,627)	1:A:48:PHE:HB2	1:B:9:GLU:HG3	5	0.29
(3,627)	1:A:48:PHE:HB3	1:B:9:GLU:HG2	5	0.29
(3,627)	1:A:48:PHE:HB3	1:B:9:GLU:HG3	5	0.29
(3,1428)	1:B:86:LEU:H	1:B:86:LEU:HG	3	0.29
(3,1427)	1:A:86:LEU:H	1:A:86:LEU:HG	3	0.29
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	10	0.29
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	10	0.29
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	10	0.29
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	10	0.29
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB2	7	0.29
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB3	7	0.29
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG2	7	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG3	7	0.29
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	2	0.29
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	2	0.29
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	2	0.29
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	2	0.29
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	2	0.29
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	2	0.29
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	2	0.29
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	2	0.29
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	2	0.29
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	2	0.29
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	2	0.29
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	2	0.29
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	5	0.29
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	5	0.29
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	5	0.29
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	5	0.29
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG2	6	0.29
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG3	6	0.29
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG2	6	0.29
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG3	6	0.29
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG2	6	0.29
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG3	6	0.29
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG2	6	0.29
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG3	6	0.29
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG2	6	0.29
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG3	6	0.29
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG2	6	0.29
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG3	6	0.29
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG2	6	0.29
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG3	6	0.29
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG2	6	0.29
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG3	6	0.29
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG2	6	0.29
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG3	6	0.29
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG2	6	0.29
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG3	6	0.29
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG2	6	0.29
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG3	6	0.29
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG2	6	0.29
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG3	6	0.29
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE2	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE1	1	0.29
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE3	1	0.29
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE2	1	0.29
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE1	1	0.29
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE3	1	0.29
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE2	1	0.29
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE1	1	0.29
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE3	1	0.29
(1,223)	1:A:62:ILE:HG22	1:A:66:LEU:HG	1	0.29
(1,223)	1:A:62:ILE:HG21	1:A:66:LEU:HG	1	0.29
(1,223)	1:A:62:ILE:HG23	1:A:66:LEU:HG	1	0.29
(1,1706)	1:B:24:VAL:H	1:B:17:ASN:HA	4	0.29
(1,1706)	1:B:78:GLU:H	1:B:67:ASP:HA	4	0.29
(1,1705)	1:A:24:VAL:H	1:A:17:ASN:HA	4	0.29
(1,1705)	1:A:78:GLU:H	1:A:67:ASP:HA	4	0.29
(1,1390)	1:B:5:MET:H	1:A:110:GLY:H	1	0.29
(1,1390)	1:B:12:ILE:H	1:B:19:PHE:H	1	0.29
(1,1390)	1:B:19:PHE:H	1:B:44:ASP:H	1	0.29
(1,1390)	1:B:19:PHE:H	1:A:12:ILE:H	1	0.29
(1,1390)	1:B:10:ARG:H	1:B:5:MET:H	1	0.29
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	3	0.29
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	3	0.29
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	3	0.29
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	3	0.29
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	3	0.29
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	3	0.29
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	9	0.29
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	9	0.29
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	9	0.29
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	9	0.29
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	9	0.29
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	9	0.29
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	3	0.29
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	3	0.29
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	3	0.29
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	3	0.29
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	3	0.29
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	3	0.29
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	9	0.29
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	9	0.29
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	9	0.29
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	9	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	9	0.29
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	9	0.29
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	10	0.28
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	10	0.28
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	10	0.28
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	10	0.28
(3,34)	1:B:87:THR:HG21	1:B:88:TRP:HA	5	0.28
(3,34)	1:B:87:THR:HG22	1:B:88:TRP:HA	5	0.28
(3,34)	1:B:87:THR:HG23	1:B:88:TRP:HA	5	0.28
(3,33)	1:A:87:THR:HG21	1:A:88:TRP:HA	5	0.28
(3,33)	1:A:87:THR:HG22	1:A:88:TRP:HA	5	0.28
(3,33)	1:A:87:THR:HG23	1:A:88:TRP:HA	5	0.28
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	7	0.28
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	2	0.28
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	7	0.28
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	2	0.28
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	7	0.28
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB2	7	0.28
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB3	7	0.28
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG2	7	0.28
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG3	7	0.28
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE2	1	0.28
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE1	1	0.28
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE3	1	0.28
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE2	1	0.28
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE1	1	0.28
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE3	1	0.28
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE2	1	0.28
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE1	1	0.28
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE3	1	0.28
(1,224)	1:B:62:ILE:HG22	1:B:66:LEU:HG	1	0.28
(1,224)	1:B:62:ILE:HG21	1:B:66:LEU:HG	1	0.28
(1,224)	1:B:62:ILE:HG23	1:B:66:LEU:HG	1	0.28
(1,1389)	1:A:5:MET:H	1:B:110:GLY:H	1	0.28
(1,1389)	1:A:12:ILE:H	1:A:19:PHE:H	1	0.28
(1,1389)	1:A:19:PHE:H	1:A:44:ASP:H	1	0.28
(1,1389)	1:A:19:PHE:H	1:B:12:ILE:H	1	0.28
(1,1389)	1:A:10:ARG:H	1:A:5:MET:H	1	0.28
(4,260)	1:B:113:THR:H	1:B:107:PRO:HA	7	0.27
(4,259)	1:A:113:THR:H	1:A:107:PRO:HA	7	0.27
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	1	0.27
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	1	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	1	0.27
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	1	0.27
(3,486)	1:B:96:GLU:HG2	1:B:97:GLY:H	7	0.27
(3,486)	1:B:96:GLU:HG3	1:B:97:GLY:H	7	0.27
(3,485)	1:A:96:GLU:HG2	1:A:97:GLY:H	7	0.27
(3,485)	1:A:96:GLU:HG3	1:A:97:GLY:H	7	0.27
(3,1474)	1:B:100:GLY:H	1:B:98:ASP:HA	7	0.27
(3,1473)	1:A:100:GLY:H	1:A:98:ASP:HA	7	0.27
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	2	0.27
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	2	0.27
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	2	0.27
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	2	0.27
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	7	0.27
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	9	0.27
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	10	0.27
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	9	0.27
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	10	0.27
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	10	0.27
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	10	0.27
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	10	0.27
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	10	0.27
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	10	0.27
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	10	0.27
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	10	0.27
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	10	0.27
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	10	0.27
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	10	0.27
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	10	0.27
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	10	0.27
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	10	0.27
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	10	0.27
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	10	0.27
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	10	0.27
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	10	0.27
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	10	0.27
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	10	0.27
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	10	0.27
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	10	0.27
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	10	0.27
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	10	0.27
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	10	0.27
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	10	0.27
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	10	0.27
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	10	0.27
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	10	0.27
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	10	0.27
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	10	0.27
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	10	0.27
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	10	0.27
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	10	0.27
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	10	0.27
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	10	0.27
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	3	0.27
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	3	0.27
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	3	0.27
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	3	0.27
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	3	0.27
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	3	0.27
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	3	0.27
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	3	0.27
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	3	0.27
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	3	0.27
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	3	0.27
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	3	0.27
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	3	0.27
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	3	0.27
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	3	0.27
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	3	0.27
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	4	0.27
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	4	0.27
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	4	0.27
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	4	0.27
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	4	0.27
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	4	0.27
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG2	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG3	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG2	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG3	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG2	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG3	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB2	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB3	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB2	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB3	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB2	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB3	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG21	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG22	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG23	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG21	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG22	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG23	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG21	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG22	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG23	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB2	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB1	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB3	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB2	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB1	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB3	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB2	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB1	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB3	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG2	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG3	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG2	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG3	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG2	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG3	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:80:ILE:HB	5	0.27
(1,1078)	1:B:31:THR:HG22	1:B:80:ILE:HB	5	0.27
(1,1078)	1:B:31:THR:HG23	1:B:80:ILE:HB	5	0.27
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG2	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG3	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG2	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG3	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG2	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG3	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB2	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB3	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB2	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB3	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB2	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB3	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG21	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG22	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG23	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG21	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG22	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG23	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG21	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG22	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG23	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB2	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB1	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB3	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB2	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB1	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB3	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB2	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB1	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB3	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG2	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG3	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG2	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG3	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG2	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG3	10	0.27
(1,1078)	1:B:31:THR:HG21	1:B:80:ILE:HB	10	0.27
(1,1078)	1:B:31:THR:HG22	1:B:80:ILE:HB	10	0.27
(1,1078)	1:B:31:THR:HG23	1:B:80:ILE:HB	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG2	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG3	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG2	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG3	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG2	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG3	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB2	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB3	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB2	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB3	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB2	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB3	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG21	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG22	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG23	10	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG21	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG22	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG23	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG21	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG22	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG23	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB2	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB1	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB3	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB2	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB1	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB3	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB2	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB1	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB3	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG2	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG3	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG2	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG3	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG2	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG3	10	0.27
(1,1077)	1:A:31:THR:HG21	1:A:80:ILE:HB	10	0.27
(1,1077)	1:A:31:THR:HG22	1:A:80:ILE:HB	10	0.27
(1,1077)	1:A:31:THR:HG23	1:A:80:ILE:HB	10	0.27
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	9	0.26
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	4	0.26
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	4	0.26
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	9	0.26
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB2	1	0.26
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB3	1	0.26
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB2	1	0.26
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB3	1	0.26
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB2	1	0.26
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB3	1	0.26
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB2	1	0.26
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB3	1	0.26
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB2	1	0.26
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB3	1	0.26
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB2	1	0.26
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB3	1	0.26
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD22	9	0.26
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD21	9	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD23	9	0.26
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD12	9	0.26
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD11	9	0.26
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD13	9	0.26
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD22	9	0.26
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD21	9	0.26
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD23	9	0.26
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD12	9	0.26
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD11	9	0.26
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD13	9	0.26
(3,252)	1:B:33:ASN:HB2	1:B:72:LYS:HA	9	0.26
(3,252)	1:B:33:ASN:HB3	1:B:72:LYS:HA	9	0.26
(3,251)	1:A:33:ASN:HB2	1:A:72:LYS:HA	9	0.26
(3,251)	1:A:33:ASN:HB3	1:A:72:LYS:HA	9	0.26
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG2	7	0.26
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG3	7	0.26
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG2	7	0.26
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG3	7	0.26
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG2	7	0.26
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG3	7	0.26
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG2	7	0.26
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG3	7	0.26
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	3	0.26
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	3	0.26
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	7	0.26
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	7	0.26
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	3	0.26
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	3	0.26
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	7	0.26
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	7	0.26
(2,4)	1:A:74:LEU:N	1:A:32:LEU:O	3	0.26
(1,940)	1:B:46:GLN:HG2	1:A:9:GLU:HA	10	0.26
(1,940)	1:B:46:GLN:HG3	1:A:9:GLU:HA	10	0.26
(1,940)	1:B:5:MET:HB2	1:B:9:GLU:HA	10	0.26
(1,940)	1:B:5:MET:HB3	1:B:9:GLU:HA	10	0.26
(1,939)	1:A:46:GLN:HG2	1:B:9:GLU:HA	10	0.26
(1,939)	1:A:46:GLN:HG3	1:B:9:GLU:HA	10	0.26
(1,939)	1:A:5:MET:HB2	1:A:9:GLU:HA	10	0.26
(1,939)	1:A:5:MET:HB3	1:A:9:GLU:HA	10	0.26
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	2	0.26
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	2	0.26
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	2	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	2	0.26
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	2	0.26
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	2	0.26
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	2	0.26
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	2	0.26
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	3	0.26
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	3	0.26
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	3	0.26
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	3	0.26
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	3	0.26
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	3	0.26
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	3	0.26
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	3	0.26
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	3	0.26
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	3	0.26
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	3	0.26
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	3	0.26
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	1	0.26
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	1	0.26
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	6	0.26
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	6	0.26
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	8	0.26
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	8	0.26
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	9	0.26
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	9	0.26
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	1	0.26
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	1	0.26
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	6	0.26
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	6	0.26
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	8	0.26
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	8	0.26
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	9	0.26
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	9	0.26
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	6	0.26
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	6	0.26
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	6	0.26
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	6	0.26
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	6	0.26
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	6	0.26
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	6	0.26
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	6	0.26
(1,1820)	1:B:21:GLN:H	1:B:40:LEU:HG	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB2	7	0.26
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB1	7	0.26
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB3	7	0.26
(1,1819)	1:A:21:GLN:H	1:A:40:LEU:HG	7	0.26
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB2	7	0.26
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB1	7	0.26
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB3	7	0.26
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	6	0.26
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	6	0.26
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	6	0.26
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	6	0.26
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	6	0.26
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	6	0.26
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	6	0.26
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	6	0.26
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	6	0.26
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	6	0.26
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	6	0.26
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	6	0.26
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	7	0.26
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	7	0.26
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	7	0.26
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	7	0.26
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	7	0.26
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	7	0.26
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	7	0.26
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	7	0.26
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	7	0.26
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	7	0.26
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	7	0.26
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	7	0.26
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	7	0.26
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	7	0.26
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	7	0.26
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	7	0.26
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB2	3	0.26
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB3	3	0.26
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB2	3	0.26
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB3	3	0.26
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB2	3	0.26
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB3	3	0.26
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB2	3	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB3	3	0.26
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE2	3	0.26
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE3	3	0.26
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE2	3	0.26
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE3	3	0.26
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD2	3	0.26
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD3	3	0.26
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD2	3	0.26
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD3	3	0.26
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB2	3	0.26
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB3	3	0.26
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB2	3	0.26
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB3	3	0.26
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB2	3	0.26
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB3	3	0.26
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB2	3	0.26
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB3	3	0.26
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE2	3	0.26
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE3	3	0.26
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE2	3	0.26
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE3	3	0.26
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD2	3	0.26
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD3	3	0.26
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD2	3	0.26
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD3	3	0.26
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	2	0.26
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	2	0.26
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	2	0.26
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	2	0.26
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	2	0.26
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	2	0.26
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	2	0.26
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	2	0.26
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	2	0.26
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	2	0.26
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	2	0.26
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	2	0.26
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	4	0.26
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	4	0.26
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	4	0.26
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	4	0.26
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	4	0.26
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG2	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG3	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG2	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG3	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG2	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG3	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB2	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB3	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB2	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB3	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB2	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB3	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG21	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG22	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG23	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG21	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG22	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG23	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG21	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG22	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG23	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB2	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB1	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB3	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB2	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB1	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB3	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB2	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB1	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB3	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG2	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG3	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG2	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG3	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG2	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG3	5	0.26
(1,1077)	1:A:31:THR:HG21	1:A:80:ILE:HB	5	0.26
(1,1077)	1:A:31:THR:HG22	1:A:80:ILE:HB	5	0.26
(1,1077)	1:A:31:THR:HG23	1:A:80:ILE:HB	5	0.26
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	2	0.25
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	2	0.25
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	2	0.25
(3,390)	1:B:51:LYS:H	1:B:51:LYS:HD2	3	0.25
(3,390)	1:B:51:LYS:H	1:B:51:LYS:HD3	3	0.25
(3,389)	1:A:51:LYS:H	1:A:51:LYS:HD2	3	0.25
(3,389)	1:A:51:LYS:H	1:A:51:LYS:HD3	3	0.25
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD2	4	0.25
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD3	4	0.25
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD2	4	0.25
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD3	4	0.25
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	10	0.25
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	10	0.25
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	10	0.25
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	10	0.25
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	7	0.25
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	7	0.25
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	7	0.25
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA2	6	0.25
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA3	6	0.25
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA2	6	0.25
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA3	6	0.25
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA2	6	0.25
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA3	6	0.25
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA2	6	0.25
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA3	6	0.25
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA2	3	0.25
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA3	3	0.25
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA2	3	0.25
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA3	3	0.25
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA2	3	0.25
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA3	3	0.25
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA2	3	0.25
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA3	3	0.25
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA2	6	0.25
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA3	6	0.25
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA2	6	0.25
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA3	6	0.25
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA2	6	0.25
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA3	6	0.25
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA2	6	0.25
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA3	6	0.25
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	2	0.25
(1,42)	1:B:64:GLU:HG2	1:B:61:HIS:HB2	6	0.25
(1,42)	1:B:64:GLU:HG2	1:B:61:HIS:HB3	6	0.25
(1,42)	1:B:64:GLU:HG3	1:B:61:HIS:HB2	6	0.25
(1,42)	1:B:64:GLU:HG3	1:B:61:HIS:HB3	6	0.25
(1,42)	1:B:78:GLU:HG2	1:B:76:PHE:HA	6	0.25
(1,42)	1:B:78:GLU:HG3	1:B:76:PHE:HA	6	0.25
(1,41)	1:A:64:GLU:HG2	1:A:61:HIS:HB2	6	0.25
(1,41)	1:A:64:GLU:HG2	1:A:61:HIS:HB3	6	0.25
(1,41)	1:A:64:GLU:HG3	1:A:61:HIS:HB2	6	0.25
(1,41)	1:A:64:GLU:HG3	1:A:61:HIS:HB3	6	0.25
(1,41)	1:A:78:GLU:HG2	1:A:76:PHE:HA	6	0.25
(1,41)	1:A:78:GLU:HG3	1:A:76:PHE:HA	6	0.25
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	10	0.25
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	10	0.25
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	10	0.25
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	10	0.25
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	10	0.25
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	10	0.25
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	10	0.25
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	10	0.25
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD2	2	0.25
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD3	2	0.25
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD2	2	0.25
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD3	2	0.25
(1,24)	1:B:65:ASP:HA	1:B:72:LYS:HA	2	0.25
(1,1826)	1:B:21:GLN:H	1:B:17:ASN:HB2	2	0.25
(1,1826)	1:B:21:GLN:H	1:B:17:ASN:HB3	2	0.25
(1,1826)	1:B:94:MET:H	1:B:93:LYS:HE2	2	0.25
(1,1826)	1:B:94:MET:H	1:B:93:LYS:HE3	2	0.25
(1,1826)	1:B:94:MET:H	1:B:95:HIS:HB3	2	0.25
(1,1826)	1:B:98:ASP:H	1:B:95:HIS:HB3	2	0.25
(1,1826)	1:B:16:ILE:H	1:B:17:ASN:HB2	2	0.25
(1,1826)	1:B:16:ILE:H	1:B:17:ASN:HB3	2	0.25
(1,1825)	1:A:21:GLN:H	1:A:17:ASN:HB2	2	0.25
(1,1825)	1:A:21:GLN:H	1:A:17:ASN:HB3	2	0.25
(1,1825)	1:A:94:MET:H	1:A:93:LYS:HE2	2	0.25
(1,1825)	1:A:94:MET:H	1:A:93:LYS:HE3	2	0.25
(1,1825)	1:A:94:MET:H	1:A:95:HIS:HB3	2	0.25
(1,1825)	1:A:98:ASP:H	1:A:95:HIS:HB3	2	0.25
(1,1825)	1:A:16:ILE:H	1:A:17:ASN:HB2	2	0.25
(1,1825)	1:A:16:ILE:H	1:A:17:ASN:HB3	2	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	7	0.25
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	7	0.25
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	7	0.25
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	7	0.25
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	7	0.25
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	7	0.25
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	7	0.25
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	7	0.25
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	7	0.25
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	7	0.25
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	7	0.25
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	7	0.25
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	5	0.24
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	10	0.24
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	10	0.24
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	2	0.24
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	5	0.24
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	1	0.24
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	1	0.24
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	1	0.24
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	1	0.24
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	1	0.24
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	1	0.24
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	6	0.24
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	6	0.24
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	6	0.24
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	6	0.24
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	6	0.24
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	6	0.24
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	1	0.24
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	1	0.24
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	1	0.24
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	1	0.24
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	1	0.24
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	1	0.24
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	6	0.24
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	6	0.24
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	6	0.24
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	6	0.24
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	6	0.24
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	6	0.24
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	9	0.24
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	9	0.24
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	9	0.24
(3,54)	1:B:39:GLU:HG2	1:B:43:LYS:HD2	4	0.24
(3,54)	1:B:39:GLU:HG2	1:B:43:LYS:HD3	4	0.24
(3,54)	1:B:39:GLU:HG3	1:B:43:LYS:HD2	4	0.24
(3,54)	1:B:39:GLU:HG3	1:B:43:LYS:HD3	4	0.24
(3,53)	1:A:39:GLU:HG2	1:A:43:LYS:HD2	4	0.24
(3,53)	1:A:39:GLU:HG2	1:A:43:LYS:HD3	4	0.24
(3,53)	1:A:39:GLU:HG3	1:A:43:LYS:HD2	4	0.24
(3,53)	1:A:39:GLU:HG3	1:A:43:LYS:HD3	4	0.24
(3,50)	1:B:78:GLU:HG2	1:B:77:GLU:H	3	0.24
(3,50)	1:B:78:GLU:HG3	1:B:77:GLU:H	3	0.24
(3,49)	1:A:78:GLU:HG2	1:A:77:GLU:H	3	0.24
(3,49)	1:A:78:GLU:HG3	1:A:77:GLU:H	3	0.24
(3,200)	1:B:46:GLN:HB2	1:B:43:LYS:HA	1	0.24
(3,200)	1:B:46:GLN:HB3	1:B:43:LYS:HA	1	0.24
(3,199)	1:A:46:GLN:HB2	1:A:43:LYS:HA	1	0.24
(3,199)	1:A:46:GLN:HB3	1:A:43:LYS:HA	1	0.24
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	4	0.24
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	4	0.24
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	4	0.24
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	4	0.24
(3,116)	1:B:75:SER:HB2	1:B:67:ASP:HA	9	0.24
(3,116)	1:B:75:SER:HB3	1:B:67:ASP:HA	9	0.24
(3,115)	1:A:75:SER:HB2	1:A:67:ASP:HA	9	0.24
(3,115)	1:A:75:SER:HB3	1:A:67:ASP:HA	9	0.24
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	7	0.24
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	7	0.24
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	1	0.24
(1,988)	1:B:48:PHE:HB2	1:B:93:LYS:H	5	0.24
(1,988)	1:B:48:PHE:HB3	1:B:93:LYS:H	5	0.24
(1,988)	1:B:48:PHE:HB2	1:B:109:LEU:H	5	0.24
(1,988)	1:B:48:PHE:HB3	1:B:109:LEU:H	5	0.24
(1,988)	1:B:48:PHE:HB2	1:A:5:MET:H	5	0.24
(1,988)	1:B:48:PHE:HB3	1:A:5:MET:H	5	0.24
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB2	5	0.24
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB3	5	0.24
(1,987)	1:A:48:PHE:HB2	1:A:93:LYS:H	5	0.24
(1,987)	1:A:48:PHE:HB3	1:A:93:LYS:H	5	0.24
(1,987)	1:A:48:PHE:HB2	1:A:109:LEU:H	5	0.24
(1,987)	1:A:48:PHE:HB3	1:A:109:LEU:H	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,987)	1:A:48:PHE:HB2	1:B:5:MET:H	5	0.24
(1,987)	1:A:48:PHE:HB3	1:B:5:MET:H	5	0.24
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB2	5	0.24
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB3	5	0.24
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA2	3	0.24
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA3	3	0.24
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA2	3	0.24
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA3	3	0.24
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA2	3	0.24
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA3	3	0.24
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA2	3	0.24
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA3	3	0.24
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	8	0.24
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	8	0.24
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	8	0.24
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	8	0.24
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	8	0.24
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	8	0.24
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	8	0.24
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	8	0.24
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	2	0.24
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	2	0.24
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB2	10	0.24
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB3	10	0.24
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB2	10	0.24
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB3	10	0.24
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB2	10	0.24
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB3	10	0.24
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB2	10	0.24
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB3	10	0.24
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB2	10	0.24
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB3	10	0.24
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB2	10	0.24
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB3	10	0.24
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB2	10	0.24
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB3	10	0.24
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB2	10	0.24
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB3	10	0.24
(1,478)	1:B:37:PHE:HB2	1:B:74:LEU:HG	10	0.24
(1,478)	1:B:37:PHE:HB3	1:B:74:LEU:HG	10	0.24
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB2	10	0.24
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB3	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB2	10	0.24
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB3	10	0.24
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB2	10	0.24
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB3	10	0.24
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB2	10	0.24
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB3	10	0.24
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB2	10	0.24
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB3	10	0.24
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB2	10	0.24
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB3	10	0.24
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB2	10	0.24
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB3	10	0.24
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB2	10	0.24
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB3	10	0.24
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB2	10	0.24
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB3	10	0.24
(1,477)	1:A:37:PHE:HB2	1:A:74:LEU:HG	10	0.24
(1,477)	1:A:37:PHE:HB3	1:A:74:LEU:HG	10	0.24
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB2	10	0.24
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB3	10	0.24
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG2	7	0.24
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG3	7	0.24
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG2	7	0.24
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG3	7	0.24
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG2	7	0.24
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG3	7	0.24
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG2	7	0.24
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG3	7	0.24
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG2	7	0.24
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG3	7	0.24
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG2	7	0.24
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG3	7	0.24
(1,402)	1:B:38:LYS:HD2	1:B:57:LYS:HE2	4	0.24
(1,402)	1:B:38:LYS:HD2	1:B:57:LYS:HE3	4	0.24
(1,402)	1:B:38:LYS:HD3	1:B:57:LYS:HE2	4	0.24
(1,402)	1:B:38:LYS:HD3	1:B:57:LYS:HE3	4	0.24
(1,402)	1:B:38:LYS:HD2	1:B:72:LYS:HE2	4	0.24
(1,402)	1:B:38:LYS:HD2	1:B:72:LYS:HE3	4	0.24
(1,402)	1:B:38:LYS:HD3	1:B:72:LYS:HE2	4	0.24
(1,402)	1:B:38:LYS:HD3	1:B:72:LYS:HE3	4	0.24
(1,402)	1:B:42:ARG:HB2	1:B:19:PHE:HB2	4	0.24
(1,402)	1:B:42:ARG:HB2	1:B:19:PHE:HB3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:B:42:ARG:HB3	1:B:19:PHE:HB2	4	0.24
(1,402)	1:B:42:ARG:HB3	1:B:19:PHE:HB3	4	0.24
(1,402)	1:B:42:ARG:HB2	1:B:51:LYS:HE2	4	0.24
(1,402)	1:B:42:ARG:HB2	1:B:51:LYS:HE3	4	0.24
(1,402)	1:B:42:ARG:HB3	1:B:51:LYS:HE2	4	0.24
(1,402)	1:B:42:ARG:HB3	1:B:51:LYS:HE3	4	0.24
(1,402)	1:B:42:ARG:HB2	1:A:4:LYS:HE2	4	0.24
(1,402)	1:B:42:ARG:HB2	1:A:4:LYS:HE3	4	0.24
(1,402)	1:B:42:ARG:HB3	1:A:4:LYS:HE2	4	0.24
(1,402)	1:B:42:ARG:HB3	1:A:4:LYS:HE3	4	0.24
(1,402)	1:B:85:ARG:HB2	1:B:51:LYS:HE2	4	0.24
(1,402)	1:B:85:ARG:HB2	1:B:51:LYS:HE3	4	0.24
(1,402)	1:B:85:ARG:HB3	1:B:51:LYS:HE2	4	0.24
(1,402)	1:B:85:ARG:HB3	1:B:51:LYS:HE3	4	0.24
(1,402)	1:B:85:ARG:HB2	1:A:30:ASP:HB2	4	0.24
(1,402)	1:B:85:ARG:HB2	1:A:30:ASP:HB3	4	0.24
(1,402)	1:B:85:ARG:HB3	1:A:30:ASP:HB2	4	0.24
(1,402)	1:B:85:ARG:HB3	1:A:30:ASP:HB3	4	0.24
(1,402)	1:B:92:GLU:HB2	1:B:51:LYS:HE2	4	0.24
(1,402)	1:B:92:GLU:HB2	1:B:51:LYS:HE3	4	0.24
(1,402)	1:B:92:GLU:HB3	1:B:51:LYS:HE2	4	0.24
(1,402)	1:B:92:GLU:HB3	1:B:51:LYS:HE3	4	0.24
(1,402)	1:B:92:GLU:HB2	1:A:30:ASP:HB2	4	0.24
(1,402)	1:B:92:GLU:HB2	1:A:30:ASP:HB3	4	0.24
(1,402)	1:B:92:GLU:HB3	1:A:30:ASP:HB2	4	0.24
(1,402)	1:B:92:GLU:HB3	1:A:30:ASP:HB3	4	0.24
(1,401)	1:A:38:LYS:HD2	1:A:57:LYS:HE2	4	0.24
(1,401)	1:A:38:LYS:HD2	1:A:57:LYS:HE3	4	0.24
(1,401)	1:A:38:LYS:HD3	1:A:57:LYS:HE2	4	0.24
(1,401)	1:A:38:LYS:HD3	1:A:57:LYS:HE3	4	0.24
(1,401)	1:A:38:LYS:HD2	1:A:72:LYS:HE2	4	0.24
(1,401)	1:A:38:LYS:HD2	1:A:72:LYS:HE3	4	0.24
(1,401)	1:A:38:LYS:HD3	1:A:72:LYS:HE2	4	0.24
(1,401)	1:A:38:LYS:HD3	1:A:72:LYS:HE3	4	0.24
(1,401)	1:A:42:ARG:HB2	1:A:19:PHE:HB2	4	0.24
(1,401)	1:A:42:ARG:HB2	1:A:19:PHE:HB3	4	0.24
(1,401)	1:A:42:ARG:HB3	1:A:19:PHE:HB2	4	0.24
(1,401)	1:A:42:ARG:HB3	1:A:19:PHE:HB3	4	0.24
(1,401)	1:A:42:ARG:HB2	1:A:51:LYS:HE2	4	0.24
(1,401)	1:A:42:ARG:HB2	1:A:51:LYS:HE3	4	0.24
(1,401)	1:A:42:ARG:HB3	1:A:51:LYS:HE2	4	0.24
(1,401)	1:A:42:ARG:HB3	1:A:51:LYS:HE3	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:A:42:ARG:HB2	1:B:4:LYS:HE2	4	0.24
(1,401)	1:A:42:ARG:HB2	1:B:4:LYS:HE3	4	0.24
(1,401)	1:A:42:ARG:HB3	1:B:4:LYS:HE2	4	0.24
(1,401)	1:A:42:ARG:HB3	1:B:4:LYS:HE3	4	0.24
(1,401)	1:A:85:ARG:HB2	1:A:51:LYS:HE2	4	0.24
(1,401)	1:A:85:ARG:HB2	1:A:51:LYS:HE3	4	0.24
(1,401)	1:A:85:ARG:HB3	1:A:51:LYS:HE2	4	0.24
(1,401)	1:A:85:ARG:HB3	1:A:51:LYS:HE3	4	0.24
(1,401)	1:A:85:ARG:HB2	1:B:30:ASP:HB2	4	0.24
(1,401)	1:A:85:ARG:HB2	1:B:30:ASP:HB3	4	0.24
(1,401)	1:A:85:ARG:HB3	1:B:30:ASP:HB2	4	0.24
(1,401)	1:A:85:ARG:HB3	1:B:30:ASP:HB3	4	0.24
(1,401)	1:A:92:GLU:HB2	1:A:51:LYS:HE2	4	0.24
(1,401)	1:A:92:GLU:HB2	1:A:51:LYS:HE3	4	0.24
(1,401)	1:A:92:GLU:HB3	1:A:51:LYS:HE2	4	0.24
(1,401)	1:A:92:GLU:HB3	1:A:51:LYS:HE3	4	0.24
(1,401)	1:A:92:GLU:HB2	1:B:30:ASP:HB2	4	0.24
(1,401)	1:A:92:GLU:HB2	1:B:30:ASP:HB3	4	0.24
(1,401)	1:A:92:GLU:HB3	1:B:30:ASP:HB2	4	0.24
(1,401)	1:A:92:GLU:HB3	1:B:30:ASP:HB3	4	0.24
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	2	0.24
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	2	0.24
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	2	0.24
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	2	0.24
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	2	0.24
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	2	0.24
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	2	0.24
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	2	0.24
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	2	0.24
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	2	0.24
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	2	0.24
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	2	0.24
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	2	0.24
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	2	0.24
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	2	0.24
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	2	0.24
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	2	0.24
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	2	0.24
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD2	2	0.24
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD3	2	0.24
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD2	2	0.24
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD3	2	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:A:65:ASP:HA	1:A:72:LYS:HA	2	0.24
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	7	0.24
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	7	0.24
(1,1589)	1:A:10:ARG:H	1:A:12:ILE:HA	7	0.24
(1,1589)	1:A:51:LYS:H	1:A:46:GLN:HA	7	0.24
(1,1228)	1:B:76:PHE:H	1:B:32:LEU:HB2	8	0.24
(1,1228)	1:B:76:PHE:H	1:B:32:LEU:HB3	8	0.24
(1,1228)	1:B:76:PHE:H	1:B:80:ILE:HB	8	0.24
(1,1227)	1:A:76:PHE:H	1:A:32:LEU:HB2	8	0.24
(1,1227)	1:A:76:PHE:H	1:A:32:LEU:HB3	8	0.24
(1,1227)	1:A:76:PHE:H	1:A:80:ILE:HB	8	0.24
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	8	0.24
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	8	0.24
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	8	0.24
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	8	0.24
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	8	0.24
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	8	0.24
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	8	0.24
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	8	0.24
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	8	0.24
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	8	0.24
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	8	0.24
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	8	0.24
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	8	0.24
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	8	0.24
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	8	0.24
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	8	0.24
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	8	0.24
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	8	0.24
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	8	0.24
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	8	0.24
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	8	0.24
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	8	0.24
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	8	0.24
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	8	0.24
(4,64)	1:B:32:LEU:HG	1:B:31:THR:HB	7	0.23
(4,63)	1:A:32:LEU:HG	1:A:31:THR:HB	7	0.23
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	1	0.23
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	2	0.23
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	1	0.23
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	8	0.23
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	8	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	4	0.23
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	4	0.23
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	4	0.23
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	4	0.23
(3,252)	1:B:33:ASN:HB2	1:B:72:LYS:HA	3	0.23
(3,252)	1:B:33:ASN:HB3	1:B:72:LYS:HA	3	0.23
(3,251)	1:A:33:ASN:HB2	1:A:72:LYS:HA	3	0.23
(3,251)	1:A:33:ASN:HB3	1:A:72:LYS:HA	3	0.23
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	2	0.23
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	2	0.23
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	2	0.23
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	2	0.23
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	1	0.23
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	2	0.23
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	1	0.23
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG12	3	0.23
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG13	3	0.23
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE2	3	0.23
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE1	3	0.23
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE3	3	0.23
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG12	3	0.23
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG13	3	0.23
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE2	3	0.23
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE1	3	0.23
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE3	3	0.23
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB2	3	0.23
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB3	3	0.23
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG12	3	0.23
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG13	3	0.23
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE2	3	0.23
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE1	3	0.23
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE3	3	0.23
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG12	3	0.23
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG13	3	0.23
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE2	3	0.23
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE1	3	0.23
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE3	3	0.23
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB2	3	0.23
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB3	3	0.23
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG2	7	0.23
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG3	7	0.23
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG2	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG3	7	0.23
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG2	7	0.23
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG3	7	0.23
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG2	7	0.23
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG3	7	0.23
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG2	7	0.23
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG3	7	0.23
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG2	7	0.23
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG3	7	0.23
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	9	0.23
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	9	0.23
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	9	0.23
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	9	0.23
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	9	0.23
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	9	0.23
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	9	0.23
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	9	0.23
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	9	0.23
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	9	0.23
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	9	0.23
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	9	0.23
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	9	0.23
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	9	0.23
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	9	0.23
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	9	0.23
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	9	0.23
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	9	0.23
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	2	0.23
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	2	0.23
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	2	0.23
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	2	0.23
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	2	0.23
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	2	0.23
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	2	0.23
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	2	0.23
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	2	0.23
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	2	0.23
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	2	0.23
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	2	0.23
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	2	0.23
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	2	0.23
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	2	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	2	0.23
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	2	0.23
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	2	0.23
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	9	0.23
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	9	0.23
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	9	0.23
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	9	0.23
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	9	0.23
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	9	0.23
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	9	0.23
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	9	0.23
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	9	0.23
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	9	0.23
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	9	0.23
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	9	0.23
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	9	0.23
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	9	0.23
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	9	0.23
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	9	0.23
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	9	0.23
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	9	0.23
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	7	0.23
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	7	0.23
(1,1590)	1:B:10:ARG:H	1:B:12:ILE:HA	7	0.23
(1,1590)	1:B:51:LYS:H	1:B:46:GLN:HA	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD22	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD21	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD23	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD12	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD11	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD13	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD22	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD21	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD23	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD12	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD11	7	0.23
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD13	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD22	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD21	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD23	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD12	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD11	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD13	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD22	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD21	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD23	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD12	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD11	7	0.23
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD13	7	0.23
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	5	0.23
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	5	0.23
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	5	0.23
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	5	0.23
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	5	0.23
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	5	0.23
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	5	0.23
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	5	0.23
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	5	0.23
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	5	0.23
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	5	0.23
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	5	0.23
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	5	0.23
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	5	0.23
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	5	0.23
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	5	0.23
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	5	0.23
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	5	0.23
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	5	0.23
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	5	0.23
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	5	0.23
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	5	0.23
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	5	0.23
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	5	0.23
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	8	0.22
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	8	0.22
(4,260)	1:B:113:THR:H	1:B:107:PRO:HA	3	0.22
(4,259)	1:A:113:THR:H	1:A:107:PRO:HA	3	0.22
(4,12)	1:B:98:ASP:HA	1:B:96:GLU:HA	4	0.22
(4,11)	1:A:98:ASP:HA	1:A:96:GLU:HA	4	0.22
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	8	0.22
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	8	0.22
(3,802)	1:B:29:PRO:HD2	1:B:30:ASP:HB2	9	0.22
(3,802)	1:B:29:PRO:HD2	1:B:30:ASP:HB3	9	0.22
(3,802)	1:B:29:PRO:HD3	1:B:30:ASP:HB2	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,802)	1:B:29:PRO:HD3	1:B:30:ASP:HB3	9	0.22
(3,256)	1:B:33:ASN:HB2	1:B:31:THR:HG21	6	0.22
(3,256)	1:B:33:ASN:HB2	1:B:31:THR:HG22	6	0.22
(3,256)	1:B:33:ASN:HB2	1:B:31:THR:HG23	6	0.22
(3,256)	1:B:33:ASN:HB3	1:B:31:THR:HG21	6	0.22
(3,256)	1:B:33:ASN:HB3	1:B:31:THR:HG22	6	0.22
(3,256)	1:B:33:ASN:HB3	1:B:31:THR:HG23	6	0.22
(3,255)	1:A:33:ASN:HB2	1:A:31:THR:HG21	6	0.22
(3,255)	1:A:33:ASN:HB2	1:A:31:THR:HG22	6	0.22
(3,255)	1:A:33:ASN:HB2	1:A:31:THR:HG23	6	0.22
(3,255)	1:A:33:ASN:HB3	1:A:31:THR:HG21	6	0.22
(3,255)	1:A:33:ASN:HB3	1:A:31:THR:HG22	6	0.22
(3,255)	1:A:33:ASN:HB3	1:A:31:THR:HG23	6	0.22
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	3	0.22
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	3	0.22
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	4	0.22
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	4	0.22
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	3	0.22
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	6	0.22
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	10	0.22
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	2	0.22
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	3	0.22
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	6	0.22
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	10	0.22
(2,86)	1:A:94:MET:H	1:A:90:SER:O	5	0.22
(1,507)	1:A:11:ASN:HB2	1:A:15:ILE:HG12	7	0.22
(1,507)	1:A:11:ASN:HB2	1:A:15:ILE:HG13	7	0.22
(1,507)	1:A:11:ASN:HB3	1:A:15:ILE:HG12	7	0.22
(1,507)	1:A:11:ASN:HB3	1:A:15:ILE:HG13	7	0.22
(1,507)	1:A:11:ASN:HB2	1:B:15:ILE:HG12	7	0.22
(1,507)	1:A:11:ASN:HB2	1:B:15:ILE:HG13	7	0.22
(1,507)	1:A:11:ASN:HB3	1:B:15:ILE:HG12	7	0.22
(1,507)	1:A:11:ASN:HB3	1:B:15:ILE:HG13	7	0.22
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	3	0.22
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	3	0.22
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	3	0.22
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	3	0.22
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	3	0.22
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	3	0.22
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	3	0.22
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	3	0.22
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	3	0.22
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	3	0.22
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	3	0.22
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	3	0.22
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	3	0.22
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	3	0.22
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	3	0.22
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	3	0.22
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	3	0.22
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	4	0.22
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	4	0.22
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	4	0.22
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	4	0.22
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	4	0.22
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	4	0.22
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	4	0.22
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	4	0.22
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	4	0.22
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	4	0.22
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	4	0.22
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	4	0.22
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	4	0.22
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	4	0.22
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	4	0.22
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	4	0.22
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	4	0.22
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	4	0.22
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	4	0.22
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	4	0.22
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	4	0.22
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	4	0.22
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	4	0.22
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	4	0.22
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	4	0.22
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	4	0.22
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	4	0.22
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	4	0.22
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	4	0.22
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	4	0.22
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	4	0.22
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	4	0.22
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	4	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	4	0.22
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	4	0.22
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	4	0.22
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	2	0.22
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	2	0.22
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	2	0.22
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	2	0.22
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	2	0.22
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	2	0.22
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	8	0.22
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	8	0.22
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	8	0.22
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	8	0.22
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	8	0.22
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	8	0.22
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	8	0.22
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	8	0.22
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	8	0.22
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	8	0.22
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	8	0.22
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	8	0.22
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE2	2	0.22
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE1	2	0.22
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE3	2	0.22
(1,1382)	1:B:18:THR:H	1:B:10:ARG:HB2	2	0.22
(1,1382)	1:B:18:THR:H	1:B:10:ARG:HB3	2	0.22
(1,1382)	1:B:18:THR:H	1:B:12:ILE:HB	2	0.22
(1,1382)	1:B:18:THR:H	1:A:8:LEU:HB2	2	0.22
(1,1382)	1:B:18:THR:H	1:A:8:LEU:HB3	2	0.22
(1,1382)	1:B:18:THR:H	1:A:83:MET:HB2	2	0.22
(1,1382)	1:B:18:THR:H	1:A:83:MET:HB3	2	0.22
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE2	2	0.22
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE1	2	0.22
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE3	2	0.22
(1,1381)	1:A:18:THR:H	1:A:10:ARG:HB2	2	0.22
(1,1381)	1:A:18:THR:H	1:A:10:ARG:HB3	2	0.22
(1,1381)	1:A:18:THR:H	1:A:12:ILE:HB	2	0.22
(1,1381)	1:A:18:THR:H	1:B:8:LEU:HB2	2	0.22
(1,1381)	1:A:18:THR:H	1:B:8:LEU:HB3	2	0.22
(1,1381)	1:A:18:THR:H	1:B:83:MET:HB2	2	0.22
(1,1381)	1:A:18:THR:H	1:B:83:MET:HB3	2	0.22
(1,1228)	1:B:76:PHE:H	1:B:32:LEU:HB2	7	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1228)	1:B:76:PHE:H	1:B:32:LEU:HB3	7	0.22
(1,1228)	1:B:76:PHE:H	1:B:80:ILE:HB	7	0.22
(1,1227)	1:A:76:PHE:H	1:A:32:LEU:HB2	7	0.22
(1,1227)	1:A:76:PHE:H	1:A:32:LEU:HB3	7	0.22
(1,1227)	1:A:76:PHE:H	1:A:80:ILE:HB	7	0.22
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	10	0.21
(4,260)	1:B:113:THR:H	1:B:107:PRO:HA	5	0.21
(4,259)	1:A:113:THR:H	1:A:107:PRO:HA	5	0.21
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	3	0.21
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	3	0.21
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	3	0.21
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	3	0.21
(3,462)	1:B:5:MET:HB2	1:B:4:LYS:HE2	10	0.21
(3,462)	1:B:5:MET:HB2	1:B:4:LYS:HE3	10	0.21
(3,462)	1:B:5:MET:HB3	1:B:4:LYS:HE2	10	0.21
(3,462)	1:B:5:MET:HB3	1:B:4:LYS:HE3	10	0.21
(3,461)	1:A:5:MET:HB2	1:A:4:LYS:HE2	10	0.21
(3,461)	1:A:5:MET:HB2	1:A:4:LYS:HE3	10	0.21
(3,461)	1:A:5:MET:HB3	1:A:4:LYS:HE2	10	0.21
(3,461)	1:A:5:MET:HB3	1:A:4:LYS:HE3	10	0.21
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	6	0.21
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	6	0.21
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	6	0.21
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	6	0.21
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	6	0.21
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	6	0.21
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	6	0.21
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	6	0.21
(3,196)	1:B:46:GLN:HA	1:B:50:LYS:HG2	2	0.21
(3,196)	1:B:46:GLN:HA	1:B:50:LYS:HG3	2	0.21
(3,195)	1:A:46:GLN:HA	1:A:50:LYS:HG2	2	0.21
(3,195)	1:A:46:GLN:HA	1:A:50:LYS:HG3	2	0.21
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD2	10	0.21
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD3	10	0.21
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD2	10	0.21
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD3	10	0.21
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	10	0.21
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	10	0.21
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	4	0.21
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	4	0.21
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	5	0.21
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	4	0.21
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	4	0.21
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	5	0.21
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	5	0.21
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	9	0.21
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	9	0.21
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	9	0.21
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	9	0.21
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	9	0.21
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	9	0.21
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	9	0.21
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	9	0.21
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	9	0.21
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	9	0.21
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	9	0.21
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	9	0.21
(1,508)	1:B:11:ASN:HB2	1:B:15:ILE:HG12	7	0.21
(1,508)	1:B:11:ASN:HB2	1:B:15:ILE:HG13	7	0.21
(1,508)	1:B:11:ASN:HB3	1:B:15:ILE:HG12	7	0.21
(1,508)	1:B:11:ASN:HB3	1:B:15:ILE:HG13	7	0.21
(1,508)	1:B:11:ASN:HB2	1:A:15:ILE:HG12	7	0.21
(1,508)	1:B:11:ASN:HB2	1:A:15:ILE:HG13	7	0.21
(1,508)	1:B:11:ASN:HB3	1:A:15:ILE:HG12	7	0.21
(1,508)	1:B:11:ASN:HB3	1:A:15:ILE:HG13	7	0.21
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	3	0.21
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	3	0.21
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	3	0.21
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	3	0.21
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	3	0.21
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	3	0.21
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	3	0.21
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	3	0.21
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	3	0.21
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	3	0.21
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	3	0.21
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	3	0.21
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	3	0.21
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	3	0.21
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	3	0.21
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	3	0.21
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	3	0.21
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	3	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:B:108:GLY:H	1:B:111:GLU:HA	5	0.21
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA2	5	0.21
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA3	5	0.21
(1,1858)	1:B:110:GLY:H	1:B:111:GLU:HA	5	0.21
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA2	5	0.21
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA3	5	0.21
(1,1857)	1:A:108:GLY:H	1:A:111:GLU:HA	5	0.21
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA2	5	0.21
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA3	5	0.21
(1,1857)	1:A:110:GLY:H	1:A:111:GLU:HA	5	0.21
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA2	5	0.21
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA3	5	0.21
(1,1798)	1:B:5:MET:H	1:B:4:LYS:HE2	3	0.21
(1,1798)	1:B:5:MET:H	1:B:4:LYS:HE3	3	0.21
(1,1798)	1:B:16:ILE:H	1:B:17:ASN:HB2	3	0.21
(1,1798)	1:B:16:ILE:H	1:B:17:ASN:HB3	3	0.21
(1,1798)	1:B:94:MET:H	1:B:93:LYS:HE2	3	0.21
(1,1798)	1:B:94:MET:H	1:B:93:LYS:HE3	3	0.21
(1,1798)	1:B:109:LEU:H	1:B:93:LYS:HE2	3	0.21
(1,1798)	1:B:109:LEU:H	1:B:93:LYS:HE3	3	0.21
(1,1797)	1:A:5:MET:H	1:A:4:LYS:HE2	3	0.21
(1,1797)	1:A:5:MET:H	1:A:4:LYS:HE3	3	0.21
(1,1797)	1:A:16:ILE:H	1:A:17:ASN:HB2	3	0.21
(1,1797)	1:A:16:ILE:H	1:A:17:ASN:HB3	3	0.21
(1,1797)	1:A:94:MET:H	1:A:93:LYS:HE2	3	0.21
(1,1797)	1:A:94:MET:H	1:A:93:LYS:HE3	3	0.21
(1,1797)	1:A:109:LEU:H	1:A:93:LYS:HE2	3	0.21
(1,1797)	1:A:109:LEU:H	1:A:93:LYS:HE3	3	0.21
(1,1710)	1:B:79:PHE:H	1:B:66:LEU:HD22	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:66:LEU:HD21	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:66:LEU:HD23	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:66:LEU:HD12	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:66:LEU:HD11	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:66:LEU:HD13	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:74:LEU:HD22	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:74:LEU:HD21	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:74:LEU:HD23	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:74:LEU:HD12	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:74:LEU:HD11	8	0.21
(1,1710)	1:B:79:PHE:H	1:B:74:LEU:HD13	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:66:LEU:HD22	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:66:LEU:HD21	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1709)	1:A:79:PHE:H	1:A:66:LEU:HD23	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:66:LEU:HD12	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:66:LEU:HD11	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:66:LEU:HD13	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:74:LEU:HD22	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:74:LEU:HD21	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:74:LEU:HD23	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:74:LEU:HD12	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:74:LEU:HD11	8	0.21
(1,1709)	1:A:79:PHE:H	1:A:74:LEU:HD13	8	0.21
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	3	0.21
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	3	0.21
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	3	0.21
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	3	0.21
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	3	0.21
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	3	0.21
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	2	0.21
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	2	0.21
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	2	0.21
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	2	0.21
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	2	0.21
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	2	0.21
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	3	0.21
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	3	0.21
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	3	0.21
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	3	0.21
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	3	0.21
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	3	0.21
(1,1390)	1:B:5:MET:H	1:A:110:GLY:H	10	0.21
(1,1390)	1:B:12:ILE:H	1:B:19:PHE:H	10	0.21
(1,1390)	1:B:19:PHE:H	1:B:44:ASP:H	10	0.21
(1,1390)	1:B:19:PHE:H	1:A:12:ILE:H	10	0.21
(1,1390)	1:B:10:ARG:H	1:B:5:MET:H	10	0.21
(1,1389)	1:A:5:MET:H	1:B:110:GLY:H	10	0.21
(1,1389)	1:A:12:ILE:H	1:A:19:PHE:H	10	0.21
(1,1389)	1:A:19:PHE:H	1:A:44:ASP:H	10	0.21
(1,1389)	1:A:19:PHE:H	1:B:12:ILE:H	10	0.21
(1,1389)	1:A:10:ARG:H	1:A:5:MET:H	10	0.21
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB2	1	0.21
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB3	1	0.21
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB2	1	0.21
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB3	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB2	1	0.21
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB3	1	0.21
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB2	1	0.21
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB3	1	0.21
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE2	1	0.21
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE3	1	0.21
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE2	1	0.21
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE3	1	0.21
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD2	1	0.21
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD3	1	0.21
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD2	1	0.21
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD3	1	0.21
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB2	1	0.21
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB3	1	0.21
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB2	1	0.21
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB3	1	0.21
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB2	1	0.21
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB3	1	0.21
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB2	1	0.21
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB3	1	0.21
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE2	1	0.21
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE3	1	0.21
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE2	1	0.21
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE3	1	0.21
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD2	1	0.21
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD3	1	0.21
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD2	1	0.21
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD3	1	0.21
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG2	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG3	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG2	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG3	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG2	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG3	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB2	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB3	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB2	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB3	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB2	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB3	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG21	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG22	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG23	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG21	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG22	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG23	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG21	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG22	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG23	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB2	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB1	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB3	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB2	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB1	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB3	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB2	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB1	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB3	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG2	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG3	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG2	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG3	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG2	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG3	7	0.21
(1,1078)	1:B:31:THR:HG21	1:B:80:ILE:HB	7	0.21
(1,1078)	1:B:31:THR:HG22	1:B:80:ILE:HB	7	0.21
(1,1078)	1:B:31:THR:HG23	1:B:80:ILE:HB	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG2	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG3	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG2	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG3	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG2	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG3	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB2	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB3	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB2	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB3	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB2	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB3	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG21	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG22	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG23	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG21	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG22	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG23	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG21	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG22	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG23	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB2	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB1	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB3	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB2	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB1	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB3	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB2	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB1	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB3	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG2	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG3	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG2	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG3	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG2	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG3	7	0.21
(1,1077)	1:A:31:THR:HG21	1:A:80:ILE:HB	7	0.21
(1,1077)	1:A:31:THR:HG22	1:A:80:ILE:HB	7	0.21
(1,1077)	1:A:31:THR:HG23	1:A:80:ILE:HB	7	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD22	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD21	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD23	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD12	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD11	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD13	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD22	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD21	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD23	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD12	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD11	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD13	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD22	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD21	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD23	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD12	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD11	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD13	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD22	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD21	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD23	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD12	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD11	1	0.21
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD13	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD22	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD21	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD23	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD12	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD11	1	0.21
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD13	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD22	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD21	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD23	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD12	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD11	1	0.21
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD13	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD22	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD21	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD23	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD12	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD11	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD13	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD22	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD21	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD23	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD12	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD11	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD13	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD22	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD21	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD23	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD12	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD11	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD13	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD22	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD21	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD23	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD12	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD11	1	0.21
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD13	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD22	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD21	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD23	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD12	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD11	1	0.21
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD13	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD22	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD21	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD23	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD12	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD11	1	0.21
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD13	1	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	2	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	2	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	2	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	2	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	2	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	2	0.21
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	2	0.21
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	2	0.21
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	2	0.21
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	2	0.21
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	2	0.21
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	2	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	6	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	6	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	6	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	6	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	6	0.21
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	6	0.21
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	6	0.21
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	6	0.21
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	6	0.21
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	6	0.21
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	6	0.21
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	6	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	2	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	2	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	2	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	2	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	2	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	2	0.21
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	2	0.21
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	2	0.21
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	2	0.21
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	2	0.21
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	2	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	6	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	6	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	6	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	6	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	6	0.21
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	6	0.21
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	6	0.21
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	6	0.21
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	6	0.21
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	6	0.21
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	6	0.21
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	6	0.21
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	10	0.2
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG2	5	0.2
(3,876)	1:B:30:ASP:H	1:B:29:PRO:HG3	5	0.2
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG2	5	0.2
(3,875)	1:A:30:ASP:H	1:A:29:PRO:HG3	5	0.2
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	8	0.2
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	8	0.2
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	8	0.2
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	8	0.2
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	8	0.2
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	8	0.2
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	10	0.2
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	10	0.2
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	10	0.2
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	10	0.2
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	10	0.2
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	10	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	2	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	2	0.2
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	2	0.2
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	2	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	2	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	2	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	8	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	8	0.2
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	8	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	8	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	8	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	10	0.2
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	10	0.2
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	10	0.2
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	10	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	10	0.2
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	10	0.2
(3,500)	1:B:32:LEU:HG	1:B:23:SER:HB2	8	0.2
(3,500)	1:B:32:LEU:HG	1:B:23:SER:HB3	8	0.2
(3,499)	1:A:32:LEU:HG	1:A:23:SER:HB2	8	0.2
(3,499)	1:A:32:LEU:HG	1:A:23:SER:HB3	8	0.2
(3,320)	1:B:51:LYS:HE2	1:B:51:LYS:H	1	0.2
(3,320)	1:B:51:LYS:HE3	1:B:51:LYS:H	1	0.2
(3,319)	1:A:51:LYS:HE2	1:A:51:LYS:H	1	0.2
(3,319)	1:A:51:LYS:HE3	1:A:51:LYS:H	1	0.2
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG2	1	0.2
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG3	1	0.2
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG2	1	0.2
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG3	1	0.2
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG2	1	0.2
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG3	1	0.2
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG2	1	0.2
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG3	1	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD22	5	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD21	5	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD23	5	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD12	5	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD11	5	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD13	5	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD22	7	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD21	7	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD23	7	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD12	7	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD11	7	0.2
(3,1400)	1:B:90:SER:H	1:B:109:LEU:HD13	7	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD22	5	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD21	5	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD23	5	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD12	5	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD11	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD13	5	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD22	7	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD21	7	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD23	7	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD12	7	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD11	7	0.2
(3,1399)	1:A:90:SER:H	1:A:109:LEU:HD13	7	0.2
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	8	0.2
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	8	0.2
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	4	0.2
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	4	0.2
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	4	0.2
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	10	0.2
(1,918)	1:B:87:THR:HA	1:B:92:GLU:HG2	4	0.2
(1,918)	1:B:87:THR:HA	1:B:92:GLU:HG3	4	0.2
(1,918)	1:B:87:THR:HA	1:A:9:GLU:HB2	4	0.2
(1,918)	1:B:87:THR:HA	1:A:9:GLU:HB3	4	0.2
(1,918)	1:B:87:THR:HA	1:A:12:ILE:HB	4	0.2
(1,917)	1:A:87:THR:HA	1:A:92:GLU:HG2	4	0.2
(1,917)	1:A:87:THR:HA	1:A:92:GLU:HG3	4	0.2
(1,917)	1:A:87:THR:HA	1:B:9:GLU:HB2	4	0.2
(1,917)	1:A:87:THR:HA	1:B:9:GLU:HB3	4	0.2
(1,917)	1:A:87:THR:HA	1:B:12:ILE:HB	4	0.2
(1,754)	1:B:92:GLU:HG2	1:B:51:LYS:HE2	2	0.2
(1,754)	1:B:92:GLU:HG2	1:B:51:LYS:HE3	2	0.2
(1,754)	1:B:92:GLU:HG3	1:B:51:LYS:HE2	2	0.2
(1,754)	1:B:92:GLU:HG3	1:B:51:LYS:HE3	2	0.2
(1,754)	1:B:92:GLU:HG2	1:A:30:ASP:HB2	2	0.2
(1,754)	1:B:92:GLU:HG2	1:A:30:ASP:HB3	2	0.2
(1,754)	1:B:92:GLU:HG3	1:A:30:ASP:HB2	2	0.2
(1,754)	1:B:92:GLU:HG3	1:A:30:ASP:HB3	2	0.2
(1,754)	1:B:111:GLU:HG2	1:B:51:LYS:HE2	2	0.2
(1,754)	1:B:111:GLU:HG2	1:B:51:LYS:HE3	2	0.2
(1,754)	1:B:111:GLU:HG3	1:B:51:LYS:HE2	2	0.2
(1,754)	1:B:111:GLU:HG3	1:B:51:LYS:HE3	2	0.2
(1,754)	1:B:111:GLU:HG2	1:A:4:LYS:HE2	2	0.2
(1,754)	1:B:111:GLU:HG2	1:A:4:LYS:HE3	2	0.2
(1,754)	1:B:111:GLU:HG3	1:A:4:LYS:HE2	2	0.2
(1,754)	1:B:111:GLU:HG3	1:A:4:LYS:HE3	2	0.2
(1,754)	1:B:111:GLU:HG2	1:A:17:ASN:HB2	2	0.2
(1,754)	1:B:111:GLU:HG2	1:A:17:ASN:HB3	2	0.2
(1,754)	1:B:111:GLU:HG3	1:A:17:ASN:HB2	2	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,754)	1:B:111:GLU:HG3	1:A:17:ASN:HB3	2	0.2
(1,753)	1:A:92:GLU:HG2	1:A:51:LYS:HE2	2	0.2
(1,753)	1:A:92:GLU:HG2	1:A:51:LYS:HE3	2	0.2
(1,753)	1:A:92:GLU:HG3	1:A:51:LYS:HE2	2	0.2
(1,753)	1:A:92:GLU:HG3	1:A:51:LYS:HE3	2	0.2
(1,753)	1:A:92:GLU:HG2	1:B:30:ASP:HB2	2	0.2
(1,753)	1:A:92:GLU:HG2	1:B:30:ASP:HB3	2	0.2
(1,753)	1:A:92:GLU:HG3	1:B:30:ASP:HB2	2	0.2
(1,753)	1:A:92:GLU:HG3	1:B:30:ASP:HB3	2	0.2
(1,753)	1:A:111:GLU:HG2	1:A:51:LYS:HE2	2	0.2
(1,753)	1:A:111:GLU:HG2	1:A:51:LYS:HE3	2	0.2
(1,753)	1:A:111:GLU:HG3	1:A:51:LYS:HE2	2	0.2
(1,753)	1:A:111:GLU:HG3	1:A:51:LYS:HE3	2	0.2
(1,753)	1:A:111:GLU:HG2	1:B:4:LYS:HE2	2	0.2
(1,753)	1:A:111:GLU:HG2	1:B:4:LYS:HE3	2	0.2
(1,753)	1:A:111:GLU:HG3	1:B:4:LYS:HE2	2	0.2
(1,753)	1:A:111:GLU:HG3	1:B:4:LYS:HE3	2	0.2
(1,753)	1:A:111:GLU:HG2	1:B:17:ASN:HB2	2	0.2
(1,753)	1:A:111:GLU:HG2	1:B:17:ASN:HB3	2	0.2
(1,753)	1:A:111:GLU:HG3	1:B:17:ASN:HB2	2	0.2
(1,753)	1:A:111:GLU:HG3	1:B:17:ASN:HB3	2	0.2
(1,442)	1:B:10:ARG:HG2	1:A:15:ILE:HG12	8	0.2
(1,442)	1:B:10:ARG:HG2	1:A:15:ILE:HG13	8	0.2
(1,442)	1:B:10:ARG:HG3	1:A:15:ILE:HG12	8	0.2
(1,442)	1:B:10:ARG:HG3	1:A:15:ILE:HG13	8	0.2
(1,442)	1:B:10:ARG:HG2	1:A:18:THR:HG21	8	0.2
(1,442)	1:B:10:ARG:HG2	1:A:18:THR:HG22	8	0.2
(1,442)	1:B:10:ARG:HG2	1:A:18:THR:HG23	8	0.2
(1,442)	1:B:10:ARG:HG3	1:A:18:THR:HG21	8	0.2
(1,442)	1:B:10:ARG:HG3	1:A:18:THR:HG22	8	0.2
(1,442)	1:B:10:ARG:HG3	1:A:18:THR:HG23	8	0.2
(1,442)	1:B:10:ARG:HG2	1:B:4:LYS:HG2	8	0.2
(1,442)	1:B:10:ARG:HG2	1:B:4:LYS:HG3	8	0.2
(1,442)	1:B:10:ARG:HG3	1:B:4:LYS:HG2	8	0.2
(1,442)	1:B:10:ARG:HG3	1:B:4:LYS:HG3	8	0.2
(1,442)	1:B:10:ARG:HG2	1:B:15:ILE:HG12	8	0.2
(1,442)	1:B:10:ARG:HG2	1:B:15:ILE:HG13	8	0.2
(1,442)	1:B:10:ARG:HG3	1:B:15:ILE:HG12	8	0.2
(1,442)	1:B:10:ARG:HG3	1:B:15:ILE:HG13	8	0.2
(1,441)	1:A:10:ARG:HG2	1:B:15:ILE:HG12	8	0.2
(1,441)	1:A:10:ARG:HG2	1:B:15:ILE:HG13	8	0.2
(1,441)	1:A:10:ARG:HG3	1:B:15:ILE:HG12	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,441)	1:A:10:ARG:HG3	1:B:15:ILE:HG13	8	0.2
(1,441)	1:A:10:ARG:HG2	1:B:18:THR:HG21	8	0.2
(1,441)	1:A:10:ARG:HG2	1:B:18:THR:HG22	8	0.2
(1,441)	1:A:10:ARG:HG2	1:B:18:THR:HG23	8	0.2
(1,441)	1:A:10:ARG:HG3	1:B:18:THR:HG21	8	0.2
(1,441)	1:A:10:ARG:HG3	1:B:18:THR:HG22	8	0.2
(1,441)	1:A:10:ARG:HG3	1:B:18:THR:HG23	8	0.2
(1,441)	1:A:10:ARG:HG2	1:A:4:LYS:HG2	8	0.2
(1,441)	1:A:10:ARG:HG2	1:A:4:LYS:HG3	8	0.2
(1,441)	1:A:10:ARG:HG3	1:A:4:LYS:HG2	8	0.2
(1,441)	1:A:10:ARG:HG3	1:A:4:LYS:HG3	8	0.2
(1,441)	1:A:10:ARG:HG2	1:A:15:ILE:HG12	8	0.2
(1,441)	1:A:10:ARG:HG2	1:A:15:ILE:HG13	8	0.2
(1,441)	1:A:10:ARG:HG3	1:A:15:ILE:HG12	8	0.2
(1,441)	1:A:10:ARG:HG3	1:A:15:ILE:HG13	8	0.2
(1,358)	1:B:46:GLN:HB2	1:B:39:GLU:HA	8	0.2
(1,358)	1:B:46:GLN:HB3	1:B:39:GLU:HA	8	0.2
(1,358)	1:B:46:GLN:HB2	1:B:40:LEU:HA	8	0.2
(1,358)	1:B:46:GLN:HB3	1:B:40:LEU:HA	8	0.2
(1,358)	1:B:77:GLU:HB2	1:B:31:THR:HB	8	0.2
(1,358)	1:B:77:GLU:HB3	1:B:31:THR:HB	8	0.2
(1,357)	1:A:46:GLN:HB2	1:A:39:GLU:HA	8	0.2
(1,357)	1:A:46:GLN:HB3	1:A:39:GLU:HA	8	0.2
(1,357)	1:A:46:GLN:HB2	1:A:40:LEU:HA	8	0.2
(1,357)	1:A:46:GLN:HB3	1:A:40:LEU:HA	8	0.2
(1,357)	1:A:77:GLU:HB2	1:A:31:THR:HB	8	0.2
(1,357)	1:A:77:GLU:HB3	1:A:31:THR:HB	8	0.2
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	2	0.2
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	2	0.2
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	2	0.2
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	2	0.2
(1,20)	1:B:65:ASP:HA	1:B:74:LEU:HB2	3	0.2
(1,20)	1:B:65:ASP:HA	1:B:74:LEU:HB3	3	0.2
(1,20)	1:B:65:ASP:HA	1:B:82:LEU:HB2	3	0.2
(1,20)	1:B:65:ASP:HA	1:B:82:LEU:HB3	3	0.2
(1,20)	1:B:92:GLU:HA	1:B:86:LEU:HB2	3	0.2
(1,20)	1:B:92:GLU:HA	1:B:86:LEU:HB3	3	0.2
(1,20)	1:B:92:GLU:HA	1:B:109:LEU:HG	3	0.2
(1,20)	1:B:93:LYS:HA	1:B:51:LYS:HG2	3	0.2
(1,20)	1:B:93:LYS:HA	1:B:51:LYS:HG3	3	0.2
(1,20)	1:B:93:LYS:HA	1:B:109:LEU:HG	3	0.2
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB2	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB3	3	0.2
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB2	3	0.2
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB3	3	0.2
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB2	3	0.2
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB3	3	0.2
(1,19)	1:A:92:GLU:HA	1:A:109:LEU:HG	3	0.2
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG2	3	0.2
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG3	3	0.2
(1,19)	1:A:93:LYS:HA	1:A:109:LEU:HG	3	0.2
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	1	0.2
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	1	0.2
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	1	0.2
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	1	0.2
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	1	0.2
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	1	0.2
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	9	0.2
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	9	0.2
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	9	0.2
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	9	0.2
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	9	0.2
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	9	0.2
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	9	0.2
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	9	0.2
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	9	0.2
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	9	0.2
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	9	0.2
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	9	0.2
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	10	0.2
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	10	0.2
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	10	0.2
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	10	0.2
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	10	0.2
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	10	0.2
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	10	0.2
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	10	0.2
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	10	0.2
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	10	0.2
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	10	0.2
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	10	0.2
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD2	10	0.2
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD3	10	0.2
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD2	10	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD3	10	0.2
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG2	10	0.2
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG3	10	0.2
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG2	10	0.2
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG3	10	0.2
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB2	10	0.2
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB3	10	0.2
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB2	10	0.2
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB3	10	0.2
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD2	10	0.2
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD3	10	0.2
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD2	10	0.2
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD3	10	0.2
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD2	10	0.2
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD3	10	0.2
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD2	10	0.2
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD3	10	0.2
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG2	10	0.2
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG3	10	0.2
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG2	10	0.2
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG3	10	0.2
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB2	10	0.2
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB3	10	0.2
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB2	10	0.2
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB3	10	0.2
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD2	10	0.2
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD3	10	0.2
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD2	10	0.2
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD3	10	0.2
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG2	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG3	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG2	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG3	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG2	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG3	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB2	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB3	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB2	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB3	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB2	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB3	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG21	4	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG22	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG23	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG21	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG22	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG23	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG21	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG22	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG23	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB2	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB1	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB3	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB2	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB1	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB3	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB2	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB1	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB3	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG2	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG3	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG2	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG3	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG2	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG3	4	0.2
(1,1078)	1:B:31:THR:HG21	1:B:80:ILE:HB	4	0.2
(1,1078)	1:B:31:THR:HG22	1:B:80:ILE:HB	4	0.2
(1,1078)	1:B:31:THR:HG23	1:B:80:ILE:HB	4	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD22	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD21	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD23	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD12	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD11	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD13	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD22	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD21	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD23	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD12	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD11	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD13	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD22	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD21	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD23	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD12	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD11	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD13	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD22	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD21	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD23	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD12	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD11	3	0.2
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD13	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD22	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD21	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD23	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD12	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD11	3	0.2
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD13	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD22	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD21	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD23	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD12	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD11	3	0.2
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD13	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD22	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD21	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD23	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD12	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD11	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD13	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD22	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD21	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD23	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD12	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD11	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD13	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD22	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD21	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD23	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD12	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD11	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD13	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD22	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD21	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD23	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD12	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD11	3	0.2
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD13	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD22	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD21	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD23	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD12	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD11	3	0.2
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD13	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD22	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD21	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD23	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD12	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD11	3	0.2
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD13	3	0.2
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	4	0.19
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	4	0.19
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	7	0.19
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG21	8	0.19
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG22	8	0.19
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG23	8	0.19
(3,864)	1:B:74:LEU:H	1:B:31:THR:HB	1	0.19
(3,863)	1:A:74:LEU:H	1:A:31:THR:HB	1	0.19
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	2	0.19
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	2	0.19
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	2	0.19
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	2	0.19
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	2	0.19
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	2	0.19
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	4	0.19
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	4	0.19
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	4	0.19
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	4	0.19
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	4	0.19
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	4	0.19
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	4	0.19
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	4	0.19
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	4	0.19
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	4	0.19
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	4	0.19
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	4	0.19
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB2	7	0.19
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB3	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB2	7	0.19
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB3	7	0.19
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB2	7	0.19
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB3	7	0.19
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB2	7	0.19
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB3	7	0.19
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB2	7	0.19
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB3	7	0.19
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB2	7	0.19
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB3	7	0.19
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA2	4	0.19
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA3	4	0.19
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA2	4	0.19
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA3	4	0.19
(3,486)	1:B:96:GLU:HG2	1:B:97:GLY:H	3	0.19
(3,486)	1:B:96:GLU:HG3	1:B:97:GLY:H	3	0.19
(3,485)	1:A:96:GLU:HG2	1:A:97:GLY:H	3	0.19
(3,485)	1:A:96:GLU:HG3	1:A:97:GLY:H	3	0.19
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	3	0.19
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	3	0.19
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	3	0.19
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	3	0.19
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	8	0.19
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	8	0.19
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	8	0.19
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	8	0.19
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	3	0.19
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	3	0.19
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	3	0.19
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	3	0.19
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	8	0.19
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	8	0.19
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	8	0.19
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	8	0.19
(3,260)	1:B:42:ARG:HB2	1:B:43:LYS:HG2	6	0.19
(3,260)	1:B:42:ARG:HB2	1:B:43:LYS:HG3	6	0.19
(3,260)	1:B:42:ARG:HB3	1:B:43:LYS:HG2	6	0.19
(3,260)	1:B:42:ARG:HB3	1:B:43:LYS:HG3	6	0.19
(3,259)	1:A:42:ARG:HB2	1:A:43:LYS:HG2	6	0.19
(3,259)	1:A:42:ARG:HB2	1:A:43:LYS:HG3	6	0.19
(3,259)	1:A:42:ARG:HB3	1:A:43:LYS:HG2	6	0.19
(3,259)	1:A:42:ARG:HB3	1:A:43:LYS:HG3	6	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA2	7	0.19
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA3	7	0.19
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA2	7	0.19
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA3	7	0.19
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG2	7	0.19
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG3	7	0.19
(3,1364)	1:B:69:ASN:H	1:B:68:THR:HB	8	0.19
(3,1363)	1:A:69:ASN:H	1:A:68:THR:HB	8	0.19
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	7	0.19
(1,800)	1:B:111:GLU:HA	1:B:50:LYS:HE2	3	0.19
(1,800)	1:B:111:GLU:HA	1:B:50:LYS:HE3	3	0.19
(1,800)	1:B:111:GLU:HA	1:B:93:LYS:HE2	3	0.19
(1,800)	1:B:111:GLU:HA	1:B:93:LYS:HE3	3	0.19
(1,799)	1:A:111:GLU:HA	1:A:50:LYS:HE2	3	0.19
(1,799)	1:A:111:GLU:HA	1:A:50:LYS:HE3	3	0.19
(1,799)	1:A:111:GLU:HA	1:A:93:LYS:HE2	3	0.19
(1,799)	1:A:111:GLU:HA	1:A:93:LYS:HE3	3	0.19
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA2	4	0.19
(1,756)	1:B:96:GLU:HG2	1:B:97:GLY:HA3	4	0.19
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA2	4	0.19
(1,756)	1:B:96:GLU:HG3	1:B:97:GLY:HA3	4	0.19
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA2	4	0.19
(1,756)	1:B:111:GLU:HG2	1:B:108:GLY:HA3	4	0.19
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA2	4	0.19
(1,756)	1:B:111:GLU:HG3	1:B:108:GLY:HA3	4	0.19
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA2	4	0.19
(1,755)	1:A:96:GLU:HG2	1:A:97:GLY:HA3	4	0.19
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA2	4	0.19
(1,755)	1:A:96:GLU:HG3	1:A:97:GLY:HA3	4	0.19
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA2	4	0.19
(1,755)	1:A:111:GLU:HG2	1:A:108:GLY:HA3	4	0.19
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA2	4	0.19
(1,755)	1:A:111:GLU:HG3	1:A:108:GLY:HA3	4	0.19
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	5	0.19
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	5	0.19
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	5	0.19
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	5	0.19
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	5	0.19
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	5	0.19
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	5	0.19
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	5	0.19
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	4	0.19
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	4	0.19
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	4	0.19
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB2	7	0.19
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB3	7	0.19
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB2	7	0.19
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB3	7	0.19
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB2	7	0.19
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB3	7	0.19
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB2	7	0.19
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB3	7	0.19
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB2	7	0.19
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB3	7	0.19
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB2	7	0.19
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB3	7	0.19
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB2	7	0.19
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB3	7	0.19
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB2	7	0.19
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB3	7	0.19
(1,478)	1:B:37:PHE:HB2	1:B:74:LEU:HG	7	0.19
(1,478)	1:B:37:PHE:HB3	1:B:74:LEU:HG	7	0.19
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB2	7	0.19
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB3	7	0.19
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB2	7	0.19
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB3	7	0.19
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB2	7	0.19
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB3	7	0.19
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB2	7	0.19
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB3	7	0.19
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB2	7	0.19
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB3	7	0.19
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB2	7	0.19
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB3	7	0.19
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB2	7	0.19
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB3	7	0.19
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB2	7	0.19
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB3	7	0.19
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB2	7	0.19
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB3	7	0.19
(1,477)	1:A:37:PHE:HB2	1:A:74:LEU:HG	7	0.19
(1,477)	1:A:37:PHE:HB3	1:A:74:LEU:HG	7	0.19
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB3	7	0.19
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	5	0.19
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	5	0.19
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	5	0.19
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	5	0.19
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	5	0.19
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	5	0.19
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	5	0.19
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	5	0.19
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	5	0.19
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	5	0.19
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	5	0.19
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	5	0.19
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	5	0.19
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	5	0.19
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	5	0.19
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	5	0.19
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	5	0.19
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	5	0.19
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	7	0.19
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	7	0.19
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	7	0.19
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	7	0.19
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	7	0.19
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	7	0.19
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	7	0.19
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	7	0.19
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	7	0.19
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	7	0.19
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	7	0.19
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	7	0.19
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	7	0.19
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	7	0.19
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	7	0.19
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	7	0.19
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	7	0.19
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	7	0.19
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	5	0.19
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	5	0.19
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	5	0.19
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	5	0.19
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	5	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	5	0.19
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	5	0.19
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	5	0.19
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	5	0.19
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	5	0.19
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	5	0.19
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	5	0.19
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	5	0.19
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	5	0.19
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	5	0.19
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	5	0.19
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	5	0.19
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	5	0.19
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	7	0.19
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	7	0.19
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	7	0.19
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	7	0.19
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	7	0.19
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	7	0.19
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	7	0.19
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	7	0.19
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	7	0.19
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	7	0.19
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	7	0.19
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	7	0.19
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	7	0.19
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	7	0.19
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	7	0.19
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	7	0.19
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	7	0.19
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	7	0.19
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	2	0.19
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	2	0.19
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	2	0.19
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	2	0.19
(1,1858)	1:B:108:GLY:H	1:B:111:GLU:HA	7	0.19
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA2	7	0.19
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA3	7	0.19
(1,1858)	1:B:110:GLY:H	1:B:111:GLU:HA	7	0.19
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA2	7	0.19
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA3	7	0.19
(1,1857)	1:A:108:GLY:H	1:A:111:GLU:HA	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA2	7	0.19
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA3	7	0.19
(1,1857)	1:A:110:GLY:H	1:A:111:GLU:HA	7	0.19
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA2	7	0.19
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA3	7	0.19
(1,1706)	1:B:24:VAL:H	1:B:17:ASN:HA	5	0.19
(1,1706)	1:B:78:GLU:H	1:B:67:ASP:HA	5	0.19
(1,1705)	1:A:24:VAL:H	1:A:17:ASN:HA	5	0.19
(1,1705)	1:A:78:GLU:H	1:A:67:ASP:HA	5	0.19
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	1	0.19
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	1	0.19
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	1	0.19
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	1	0.19
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	1	0.19
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	1	0.19
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	1	0.19
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	1	0.19
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	1	0.19
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	1	0.19
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	1	0.19
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	1	0.19
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	1	0.19
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	1	0.19
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	1	0.19
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	1	0.19
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	1	0.19
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	1	0.19
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	1	0.19
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	1	0.19
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	1	0.19
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	1	0.19
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD22	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD21	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD23	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD12	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD11	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD13	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD22	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD21	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD23	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD12	3	0.19
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD11	3	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD13	3	0.19
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD22	3	0.19
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD21	3	0.19
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD23	3	0.19
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD12	3	0.19
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD11	3	0.19
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD13	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD22	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD21	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD23	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD12	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD11	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD13	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD22	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD21	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD23	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD12	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD11	3	0.19
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD13	3	0.19
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD22	3	0.19
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD21	3	0.19
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD23	3	0.19
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD12	3	0.19
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD11	3	0.19
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD13	3	0.19
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE2	1	0.19
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE1	1	0.19
(1,1382)	1:B:18:THR:H	1:B:5:MET:HE3	1	0.19
(1,1382)	1:B:18:THR:H	1:B:10:ARG:HB2	1	0.19
(1,1382)	1:B:18:THR:H	1:B:10:ARG:HB3	1	0.19
(1,1382)	1:B:18:THR:H	1:B:12:ILE:HB	1	0.19
(1,1382)	1:B:18:THR:H	1:A:8:LEU:HB2	1	0.19
(1,1382)	1:B:18:THR:H	1:A:8:LEU:HB3	1	0.19
(1,1382)	1:B:18:THR:H	1:A:83:MET:HB2	1	0.19
(1,1382)	1:B:18:THR:H	1:A:83:MET:HB3	1	0.19
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	7	0.19
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	7	0.19
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	7	0.19
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	7	0.19
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	7	0.19
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	7	0.19
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	7	0.19
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	7	0.19
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	7	0.19
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	7	0.19
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	7	0.19
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG2	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:25:LYS:HG3	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG2	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:25:LYS:HG3	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG2	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:25:LYS:HG3	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB2	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:66:LEU:HB3	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB2	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:66:LEU:HB3	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB2	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:66:LEU:HB3	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG21	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG22	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:68:THR:HG23	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG21	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG22	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:68:THR:HG23	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG21	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG22	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:68:THR:HG23	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB2	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB1	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:70:ALA:HB3	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB2	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB1	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:70:ALA:HB3	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB2	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB1	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:70:ALA:HB3	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG2	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:72:LYS:HG3	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG2	1	0.19
(1,1078)	1:B:31:THR:HG22	1:B:72:LYS:HG3	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG2	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:72:LYS:HG3	1	0.19
(1,1078)	1:B:31:THR:HG21	1:B:80:ILE:HB	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1078)	1:B:31:THR:HG22	1:B:80:ILE:HB	1	0.19
(1,1078)	1:B:31:THR:HG23	1:B:80:ILE:HB	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG2	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG3	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG2	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG3	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG2	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG3	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB2	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB3	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB2	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB3	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB2	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB3	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG21	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG22	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG23	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG21	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG22	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG23	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG21	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG22	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG23	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB2	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB1	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB3	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB2	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB1	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB3	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB2	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB1	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB3	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG2	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG3	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG2	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG3	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG2	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG3	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:80:ILE:HB	1	0.19
(1,1077)	1:A:31:THR:HG22	1:A:80:ILE:HB	1	0.19
(1,1077)	1:A:31:THR:HG23	1:A:80:ILE:HB	1	0.19
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG2	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1077)	1:A:31:THR:HG21	1:A:25:LYS:HG3	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG2	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:25:LYS:HG3	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG2	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:25:LYS:HG3	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB2	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:66:LEU:HB3	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB2	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:66:LEU:HB3	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB2	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:66:LEU:HB3	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG21	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG22	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:68:THR:HG23	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG21	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG22	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:68:THR:HG23	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG21	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG22	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:68:THR:HG23	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB2	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB1	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:70:ALA:HB3	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB2	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB1	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:70:ALA:HB3	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB2	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB1	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:70:ALA:HB3	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG2	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:72:LYS:HG3	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG2	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:72:LYS:HG3	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG2	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:72:LYS:HG3	4	0.19
(1,1077)	1:A:31:THR:HG21	1:A:80:ILE:HB	4	0.19
(1,1077)	1:A:31:THR:HG22	1:A:80:ILE:HB	4	0.19
(1,1077)	1:A:31:THR:HG23	1:A:80:ILE:HB	4	0.19
(1,106)	1:B:7:GLN:HG2	1:B:15:ILE:HD12	7	0.19
(1,106)	1:B:7:GLN:HG2	1:B:15:ILE:HD11	7	0.19
(1,106)	1:B:7:GLN:HG2	1:B:15:ILE:HD13	7	0.19
(1,106)	1:B:7:GLN:HG3	1:B:15:ILE:HD12	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:B:7:GLN:HG3	1:B:15:ILE:HD11	7	0.19
(1,106)	1:B:7:GLN:HG3	1:B:15:ILE:HD13	7	0.19
(1,106)	1:B:7:GLN:HG2	1:A:15:ILE:HD12	7	0.19
(1,106)	1:B:7:GLN:HG2	1:A:15:ILE:HD11	7	0.19
(1,106)	1:B:7:GLN:HG2	1:A:15:ILE:HD13	7	0.19
(1,106)	1:B:7:GLN:HG3	1:A:15:ILE:HD12	7	0.19
(1,106)	1:B:7:GLN:HG3	1:A:15:ILE:HD11	7	0.19
(1,106)	1:B:7:GLN:HG3	1:A:15:ILE:HD13	7	0.19
(1,105)	1:A:7:GLN:HG2	1:A:15:ILE:HD12	7	0.19
(1,105)	1:A:7:GLN:HG2	1:A:15:ILE:HD11	7	0.19
(1,105)	1:A:7:GLN:HG2	1:A:15:ILE:HD13	7	0.19
(1,105)	1:A:7:GLN:HG3	1:A:15:ILE:HD12	7	0.19
(1,105)	1:A:7:GLN:HG3	1:A:15:ILE:HD11	7	0.19
(1,105)	1:A:7:GLN:HG3	1:A:15:ILE:HD13	7	0.19
(1,105)	1:A:7:GLN:HG2	1:B:15:ILE:HD12	7	0.19
(1,105)	1:A:7:GLN:HG2	1:B:15:ILE:HD11	7	0.19
(1,105)	1:A:7:GLN:HG2	1:B:15:ILE:HD13	7	0.19
(1,105)	1:A:7:GLN:HG3	1:B:15:ILE:HD12	7	0.19
(1,105)	1:A:7:GLN:HG3	1:B:15:ILE:HD11	7	0.19
(1,105)	1:A:7:GLN:HG3	1:B:15:ILE:HD13	7	0.19
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	7	0.18
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG21	8	0.18
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG22	8	0.18
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG23	8	0.18
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG21	3	0.18
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG22	3	0.18
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG23	3	0.18
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD12	1	0.18
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD11	1	0.18
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD13	1	0.18
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD12	1	0.18
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD11	1	0.18
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD13	1	0.18
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD12	1	0.18
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD11	1	0.18
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD13	1	0.18
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD12	1	0.18
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD11	1	0.18
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD13	1	0.18
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD12	1	0.18
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD11	1	0.18
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD13	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD12	1	0.18
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD11	1	0.18
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD13	1	0.18
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD12	1	0.18
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD11	1	0.18
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD13	1	0.18
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD12	1	0.18
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD11	1	0.18
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD13	1	0.18
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD12	1	0.18
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD11	1	0.18
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD13	1	0.18
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD12	1	0.18
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD11	1	0.18
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD13	1	0.18
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD12	1	0.18
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD11	1	0.18
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD13	1	0.18
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD12	1	0.18
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD11	1	0.18
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD13	1	0.18
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA2	4	0.18
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA3	4	0.18
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA2	4	0.18
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA3	4	0.18
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA2	9	0.18
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA3	9	0.18
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA2	9	0.18
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA3	9	0.18
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA2	9	0.18
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA3	9	0.18
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA2	9	0.18
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA3	9	0.18
(3,502)	1:B:32:LEU:HA	1:B:32:LEU:HG	9	0.18
(3,500)	1:B:32:LEU:HG	1:B:23:SER:HB2	1	0.18
(3,500)	1:B:32:LEU:HG	1:B:23:SER:HB3	1	0.18
(3,226)	1:B:66:LEU:HD22	1:B:82:LEU:HA	3	0.18
(3,226)	1:B:66:LEU:HD21	1:B:82:LEU:HA	3	0.18
(3,226)	1:B:66:LEU:HD23	1:B:82:LEU:HA	3	0.18
(3,226)	1:B:66:LEU:HD12	1:B:82:LEU:HA	3	0.18
(3,226)	1:B:66:LEU:HD11	1:B:82:LEU:HA	3	0.18
(3,226)	1:B:66:LEU:HD13	1:B:82:LEU:HA	3	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG2	7	0.18
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG3	7	0.18
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG2	9	0.18
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG3	9	0.18
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG2	9	0.18
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG3	9	0.18
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	9	0.18
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	9	0.18
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	9	0.18
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	9	0.18
(3,132)	1:B:78:GLU:HB2	1:B:31:THR:HA	8	0.18
(3,132)	1:B:78:GLU:HB3	1:B:31:THR:HA	8	0.18
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	5	0.18
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	6	0.18
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	8	0.18
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	9	0.18
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	7	0.18
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	9	0.18
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	6	0.18
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	6	0.18
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	10	0.18
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	10	0.18
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	6	0.18
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	6	0.18
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	8	0.18
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	8	0.18
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	5	0.18
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	5	0.18
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	1	0.18
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	5	0.18
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	6	0.18
(2,86)	1:A:94:MET:H	1:A:90:SER:O	8	0.18
(2,79)	1:A:91:HIS:N	1:A:87:THR:O	8	0.18
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	5	0.18
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	9	0.18
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	6	0.18
(2,26)	1:A:22:TYR:H	1:A:18:THR:O	1	0.18
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB2	6	0.18
(1,340)	1:B:41:VAL:HG22	1:A:6:SER:HB3	6	0.18
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB2	6	0.18
(1,340)	1:B:41:VAL:HG21	1:A:6:SER:HB3	6	0.18
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,340)	1:B:41:VAL:HG23	1:A:6:SER:HB3	6	0.18
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB2	6	0.18
(1,340)	1:B:41:VAL:HG12	1:A:6:SER:HB3	6	0.18
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB2	6	0.18
(1,340)	1:B:41:VAL:HG11	1:A:6:SER:HB3	6	0.18
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB2	6	0.18
(1,340)	1:B:41:VAL:HG13	1:A:6:SER:HB3	6	0.18
(1,340)	1:B:66:LEU:HD22	1:B:76:PHE:HA	6	0.18
(1,340)	1:B:66:LEU:HD21	1:B:76:PHE:HA	6	0.18
(1,340)	1:B:66:LEU:HD23	1:B:76:PHE:HA	6	0.18
(1,340)	1:B:66:LEU:HD12	1:B:76:PHE:HA	6	0.18
(1,340)	1:B:66:LEU:HD11	1:B:76:PHE:HA	6	0.18
(1,340)	1:B:66:LEU:HD13	1:B:76:PHE:HA	6	0.18
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB2	6	0.18
(1,339)	1:A:41:VAL:HG22	1:B:6:SER:HB3	6	0.18
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB2	6	0.18
(1,339)	1:A:41:VAL:HG21	1:B:6:SER:HB3	6	0.18
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB2	6	0.18
(1,339)	1:A:41:VAL:HG23	1:B:6:SER:HB3	6	0.18
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB2	6	0.18
(1,339)	1:A:41:VAL:HG12	1:B:6:SER:HB3	6	0.18
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB2	6	0.18
(1,339)	1:A:41:VAL:HG11	1:B:6:SER:HB3	6	0.18
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB2	6	0.18
(1,339)	1:A:41:VAL:HG13	1:B:6:SER:HB3	6	0.18
(1,339)	1:A:66:LEU:HD22	1:A:76:PHE:HA	6	0.18
(1,339)	1:A:66:LEU:HD21	1:A:76:PHE:HA	6	0.18
(1,339)	1:A:66:LEU:HD23	1:A:76:PHE:HA	6	0.18
(1,339)	1:A:66:LEU:HD12	1:A:76:PHE:HA	6	0.18
(1,339)	1:A:66:LEU:HD11	1:A:76:PHE:HA	6	0.18
(1,339)	1:A:66:LEU:HD13	1:A:76:PHE:HA	6	0.18
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD22	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD21	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD23	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD12	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD11	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD13	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD22	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD21	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD23	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD12	10	0.18
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD11	10	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD13	10	0.18
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD12	10	0.18
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD11	10	0.18
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD13	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD22	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD21	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD23	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD12	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD11	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD13	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD22	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD21	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD23	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD12	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD11	10	0.18
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD13	10	0.18
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD12	10	0.18
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD11	10	0.18
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD13	10	0.18
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	4	0.18
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	4	0.18
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	4	0.18
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	4	0.18
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	4	0.18
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	4	0.18
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	4	0.18
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	4	0.18
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	4	0.18
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	4	0.18
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	4	0.18
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	4	0.18
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG22	2	0.18
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG21	2	0.18
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG23	2	0.18
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD12	2	0.18
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD11	2	0.18
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD13	2	0.18
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD12	2	0.18
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD11	2	0.18
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD13	2	0.18
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD12	2	0.18
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD11	2	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD13	2	0.18
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG22	2	0.18
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG21	2	0.18
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG23	2	0.18
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD12	2	0.18
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD11	2	0.18
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD13	2	0.18
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD12	2	0.18
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD11	2	0.18
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD13	2	0.18
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD12	2	0.18
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD11	2	0.18
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD13	2	0.18
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	5	0.18
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	5	0.18
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	5	0.18
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	5	0.18
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	5	0.18
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	5	0.18
(1,1196)	1:B:98:ASP:HA	1:B:95:HIS:HB3	8	0.18
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB2	8	0.18
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB3	8	0.18
(1,1195)	1:A:98:ASP:HA	1:A:95:HIS:HB3	8	0.18
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB2	8	0.18
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB3	8	0.18
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD2	8	0.18
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD3	8	0.18
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD2	8	0.18
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD3	8	0.18
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG2	8	0.18
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG3	8	0.18
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG2	8	0.18
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG3	8	0.18
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB2	8	0.18
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB3	8	0.18
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB2	8	0.18
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB3	8	0.18
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD2	8	0.18
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD3	8	0.18
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD2	8	0.18
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD3	8	0.18
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD2	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD3	8	0.18
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD2	8	0.18
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD3	8	0.18
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG2	8	0.18
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG3	8	0.18
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG2	8	0.18
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG3	8	0.18
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB2	8	0.18
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB3	8	0.18
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB2	8	0.18
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB3	8	0.18
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD2	8	0.18
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD3	8	0.18
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD2	8	0.18
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD3	8	0.18
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	1	0.17
(4,260)	1:B:113:THR:H	1:B:107:PRO:HA	2	0.17
(4,259)	1:A:113:THR:H	1:A:107:PRO:HA	2	0.17
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	2	0.17
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	1	0.17
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	2	0.17
(4,112)	1:B:76:PHE:H	1:B:31:THR:H	1	0.17
(4,111)	1:A:76:PHE:H	1:A:31:THR:H	1	0.17
(3,980)	1:B:9:GLU:H	1:B:5:MET:HG2	1	0.17
(3,980)	1:B:9:GLU:H	1:B:5:MET:HG3	1	0.17
(3,979)	1:A:9:GLU:H	1:A:5:MET:HG2	1	0.17
(3,979)	1:A:9:GLU:H	1:A:5:MET:HG3	1	0.17
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG21	3	0.17
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG22	3	0.17
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG23	3	0.17
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB2	3	0.17
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB3	3	0.17
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB2	3	0.17
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB3	3	0.17
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB2	3	0.17
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB3	3	0.17
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB2	3	0.17
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB3	3	0.17
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB2	3	0.17
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB3	3	0.17
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB2	3	0.17
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB3	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,501)	1:A:32:LEU:HA	1:A:32:LEU:HG	9	0.17
(3,50)	1:B:78:GLU:HG2	1:B:77:GLU:H	8	0.17
(3,50)	1:B:78:GLU:HG3	1:B:77:GLU:H	8	0.17
(3,499)	1:A:32:LEU:HG	1:A:23:SER:HB2	1	0.17
(3,499)	1:A:32:LEU:HG	1:A:23:SER:HB3	1	0.17
(3,49)	1:A:78:GLU:HG2	1:A:77:GLU:H	8	0.17
(3,49)	1:A:78:GLU:HG3	1:A:77:GLU:H	8	0.17
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	5	0.17
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	5	0.17
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	5	0.17
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	5	0.17
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	10	0.17
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	10	0.17
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	10	0.17
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	10	0.17
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	5	0.17
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	5	0.17
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	5	0.17
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	5	0.17
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	10	0.17
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	10	0.17
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	10	0.17
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	10	0.17
(3,225)	1:A:66:LEU:HD22	1:A:82:LEU:HA	3	0.17
(3,225)	1:A:66:LEU:HD21	1:A:82:LEU:HA	3	0.17
(3,225)	1:A:66:LEU:HD23	1:A:82:LEU:HA	3	0.17
(3,225)	1:A:66:LEU:HD12	1:A:82:LEU:HA	3	0.17
(3,225)	1:A:66:LEU:HD11	1:A:82:LEU:HA	3	0.17
(3,225)	1:A:66:LEU:HD13	1:A:82:LEU:HA	3	0.17
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB2	7	0.17
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB3	7	0.17
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB2	10	0.17
(3,1482)	1:B:102:GLY:H	1:B:104:HIS:HB3	10	0.17
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB2	7	0.17
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB3	7	0.17
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB2	10	0.17
(3,1481)	1:A:102:GLY:H	1:A:104:HIS:HB3	10	0.17
(3,131)	1:A:78:GLU:HB2	1:A:31:THR:HA	8	0.17
(3,131)	1:A:78:GLU:HB3	1:A:31:THR:HA	8	0.17
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	1	0.17
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	4	0.17
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	10	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	3	0.17
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	8	0.17
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	10	0.17
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	1	0.17
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	1	0.17
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	1	0.17
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	1	0.17
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	5	0.17
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	5	0.17
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	8	0.17
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	8	0.17
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	5	0.17
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	5	0.17
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	10	0.17
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	10	0.17
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	8	0.17
(2,80)	1:A:91:HIS:H	1:A:87:THR:O	3	0.17
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	2	0.17
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	3	0.17
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	2	0.17
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB2	10	0.17
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB3	10	0.17
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE2	10	0.17
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE3	10	0.17
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB2	10	0.17
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB3	10	0.17
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE2	10	0.17
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE3	10	0.17
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	1	0.17
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	1	0.17
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	1	0.17
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	1	0.17
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	4	0.17
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	4	0.17
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	4	0.17
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	4	0.17
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	4	0.17
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	4	0.17
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	4	0.17
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	4	0.17
(1,646)	1:B:53:ASN:HA	1:B:49:LEU:HA	7	0.17
(1,646)	1:B:86:LEU:HA	1:B:49:LEU:HA	7	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,645)	1:A:53:ASN:HA	1:A:49:LEU:HA	7	0.17
(1,645)	1:A:86:LEU:HA	1:A:49:LEU:HA	7	0.17
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	8	0.17
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	8	0.17
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	8	0.17
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	8	0.17
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	8	0.17
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	8	0.17
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	8	0.17
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	8	0.17
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	8	0.17
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	8	0.17
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	8	0.17
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	8	0.17
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG2	4	0.17
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG3	4	0.17
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG2	4	0.17
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG3	4	0.17
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG2	4	0.17
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG3	4	0.17
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG2	4	0.17
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG3	4	0.17
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG2	4	0.17
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG3	4	0.17
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG2	4	0.17
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG3	4	0.17
(1,358)	1:B:46:GLN:HB2	1:B:39:GLU:HA	6	0.17
(1,358)	1:B:46:GLN:HB3	1:B:39:GLU:HA	6	0.17
(1,358)	1:B:46:GLN:HB2	1:B:40:LEU:HA	6	0.17
(1,358)	1:B:46:GLN:HB3	1:B:40:LEU:HA	6	0.17
(1,358)	1:B:77:GLU:HB2	1:B:31:THR:HB	6	0.17
(1,358)	1:B:77:GLU:HB3	1:B:31:THR:HB	6	0.17
(1,358)	1:B:46:GLN:HB2	1:B:39:GLU:HA	7	0.17
(1,358)	1:B:46:GLN:HB3	1:B:39:GLU:HA	7	0.17
(1,358)	1:B:46:GLN:HB2	1:B:40:LEU:HA	7	0.17
(1,358)	1:B:46:GLN:HB3	1:B:40:LEU:HA	7	0.17
(1,358)	1:B:77:GLU:HB2	1:B:31:THR:HB	7	0.17
(1,358)	1:B:77:GLU:HB3	1:B:31:THR:HB	7	0.17
(1,357)	1:A:46:GLN:HB2	1:A:39:GLU:HA	6	0.17
(1,357)	1:A:46:GLN:HB3	1:A:39:GLU:HA	6	0.17
(1,357)	1:A:46:GLN:HB2	1:A:40:LEU:HA	6	0.17
(1,357)	1:A:46:GLN:HB3	1:A:40:LEU:HA	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,357)	1:A:77:GLU:HB2	1:A:31:THR:HB	6	0.17
(1,357)	1:A:77:GLU:HB3	1:A:31:THR:HB	6	0.17
(1,357)	1:A:46:GLN:HB2	1:A:39:GLU:HA	7	0.17
(1,357)	1:A:46:GLN:HB3	1:A:39:GLU:HA	7	0.17
(1,357)	1:A:46:GLN:HB2	1:A:40:LEU:HA	7	0.17
(1,357)	1:A:46:GLN:HB3	1:A:40:LEU:HA	7	0.17
(1,357)	1:A:77:GLU:HB2	1:A:31:THR:HB	7	0.17
(1,357)	1:A:77:GLU:HB3	1:A:31:THR:HB	7	0.17
(1,354)	1:B:58:VAL:HG22	1:B:54:LYS:HA	7	0.17
(1,354)	1:B:58:VAL:HG21	1:B:54:LYS:HA	7	0.17
(1,354)	1:B:58:VAL:HG23	1:B:54:LYS:HA	7	0.17
(1,354)	1:B:58:VAL:HG12	1:B:54:LYS:HA	7	0.17
(1,354)	1:B:58:VAL:HG11	1:B:54:LYS:HA	7	0.17
(1,354)	1:B:58:VAL:HG13	1:B:54:LYS:HA	7	0.17
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG21	7	0.17
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG22	7	0.17
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG23	7	0.17
(1,353)	1:A:58:VAL:HG22	1:A:54:LYS:HA	7	0.17
(1,353)	1:A:58:VAL:HG21	1:A:54:LYS:HA	7	0.17
(1,353)	1:A:58:VAL:HG23	1:A:54:LYS:HA	7	0.17
(1,353)	1:A:58:VAL:HG12	1:A:54:LYS:HA	7	0.17
(1,353)	1:A:58:VAL:HG11	1:A:54:LYS:HA	7	0.17
(1,353)	1:A:58:VAL:HG13	1:A:54:LYS:HA	7	0.17
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG21	7	0.17
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG22	7	0.17
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG23	7	0.17
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD22	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD21	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD23	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD12	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD11	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD13	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD22	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD21	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD23	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD12	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD11	8	0.17
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD13	8	0.17
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD12	8	0.17
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD11	8	0.17
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD13	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD22	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD21	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD23	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD12	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD11	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD13	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD22	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD21	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD23	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD12	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD11	8	0.17
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD13	8	0.17
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD12	8	0.17
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD11	8	0.17
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD13	8	0.17
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE2	7	0.17
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE1	7	0.17
(1,224)	1:B:12:ILE:HG22	1:A:83:MET:HE3	7	0.17
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE2	7	0.17
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE1	7	0.17
(1,224)	1:B:12:ILE:HG21	1:A:83:MET:HE3	7	0.17
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE2	7	0.17
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE1	7	0.17
(1,224)	1:B:12:ILE:HG23	1:A:83:MET:HE3	7	0.17
(1,224)	1:B:62:ILE:HG22	1:B:66:LEU:HG	7	0.17
(1,224)	1:B:62:ILE:HG21	1:B:66:LEU:HG	7	0.17
(1,224)	1:B:62:ILE:HG23	1:B:66:LEU:HG	7	0.17
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	3	0.17
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	3	0.17
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	3	0.17
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	3	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG22	9	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG21	9	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG23	9	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD12	9	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD11	9	0.17
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD13	9	0.17
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD12	9	0.17
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD11	9	0.17
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD13	9	0.17
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD12	9	0.17
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD11	9	0.17
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD13	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG22	9	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG21	9	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG23	9	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD12	9	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD11	9	0.17
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD13	9	0.17
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD12	9	0.17
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD11	9	0.17
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD13	9	0.17
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD12	9	0.17
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD11	9	0.17
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD13	9	0.17
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	5	0.17
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	5	0.17
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	5	0.17
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	5	0.17
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	5	0.17
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	5	0.17
(1,1196)	1:B:98:ASP:HA	1:B:95:HIS:HB3	7	0.17
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB2	7	0.17
(1,1196)	1:B:98:ASP:HA	1:B:104:HIS:HB3	7	0.17
(1,1195)	1:A:98:ASP:HA	1:A:95:HIS:HB3	7	0.17
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB2	7	0.17
(1,1195)	1:A:98:ASP:HA	1:A:104:HIS:HB3	7	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	3	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	3	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	3	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	3	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	3	0.17
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	3	0.17
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	3	0.17
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	3	0.17
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	3	0.17
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	3	0.17
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	3	0.17
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	3	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	3	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	3	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	3	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	3	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	3	0.17
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	3	0.17
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	3	0.17
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	3	0.17
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	3	0.17
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	3	0.17
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	3	0.17
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	1	0.16
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	1	0.16
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	9	0.16
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG21	7	0.16
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG22	7	0.16
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG23	7	0.16
(3,864)	1:B:74:LEU:H	1:B:31:THR:HB	5	0.16
(3,864)	1:B:74:LEU:H	1:B:31:THR:HB	10	0.16
(3,863)	1:A:74:LEU:H	1:A:31:THR:HB	5	0.16
(3,863)	1:A:74:LEU:H	1:A:31:THR:HB	10	0.16
(3,801)	1:A:29:PRO:HD2	1:A:30:ASP:HB2	9	0.16
(3,801)	1:A:29:PRO:HD2	1:A:30:ASP:HB3	9	0.16
(3,801)	1:A:29:PRO:HD3	1:A:30:ASP:HB2	9	0.16
(3,801)	1:A:29:PRO:HD3	1:A:30:ASP:HB3	9	0.16
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	8	0.16
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	8	0.16
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	8	0.16
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	8	0.16
(3,34)	1:B:87:THR:HG21	1:B:88:TRP:HA	8	0.16
(3,34)	1:B:87:THR:HG22	1:B:88:TRP:HA	8	0.16
(3,34)	1:B:87:THR:HG23	1:B:88:TRP:HA	8	0.16
(3,33)	1:A:87:THR:HG21	1:A:88:TRP:HA	8	0.16
(3,33)	1:A:87:THR:HG22	1:A:88:TRP:HA	8	0.16
(3,33)	1:A:87:THR:HG23	1:A:88:TRP:HA	8	0.16
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	4	0.16
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	4	0.16
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	4	0.16
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	4	0.16
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	7	0.16
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	7	0.16
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	7	0.16
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	7	0.16
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	4	0.16
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	4	0.16
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	4	0.16
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	7	0.16
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	7	0.16
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	7	0.16
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	7	0.16
(3,252)	1:B:33:ASN:HB2	1:B:72:LYS:HA	8	0.16
(3,252)	1:B:33:ASN:HB3	1:B:72:LYS:HA	8	0.16
(3,251)	1:A:33:ASN:HB2	1:A:72:LYS:HA	8	0.16
(3,251)	1:A:33:ASN:HB3	1:A:72:LYS:HA	8	0.16
(3,200)	1:B:46:GLN:HB2	1:B:43:LYS:HA	4	0.16
(3,200)	1:B:46:GLN:HB3	1:B:43:LYS:HA	4	0.16
(3,199)	1:A:46:GLN:HB2	1:A:43:LYS:HA	4	0.16
(3,199)	1:A:46:GLN:HB3	1:A:43:LYS:HA	4	0.16
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG2	8	0.16
(3,186)	1:B:19:PHE:HB2	1:B:83:MET:HG3	8	0.16
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG2	8	0.16
(3,186)	1:B:19:PHE:HB3	1:B:83:MET:HG3	8	0.16
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG2	8	0.16
(3,185)	1:A:19:PHE:HB2	1:A:83:MET:HG3	8	0.16
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG2	8	0.16
(3,185)	1:A:19:PHE:HB3	1:A:83:MET:HG3	8	0.16
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG2	3	0.16
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG3	3	0.16
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG2	3	0.16
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG3	3	0.16
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	8	0.16
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	1	0.16
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	3	0.16
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	1	0.16
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	3	0.16
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	3	0.16
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	3	0.16
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	3	0.16
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	2	0.16
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	2	0.16
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	4	0.16
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	4	0.16
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	2	0.16
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	2	0.16
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	4	0.16
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	4	0.16
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	9	0.16
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	9	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	3	0.16
(3,11)	1:A:98:ASP:H	1:A:98:ASP:HA	4	0.16
(2,64)	1:A:82:LEU:H	1:A:78:GLU:O	2	0.16
(2,62)	1:A:81:MET:H	1:A:77:GLU:O	8	0.16
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	7	0.16
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	9	0.16
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	9	0.16
(2,3)	1:A:74:LEU:H	1:A:32:LEU:O	3	0.16
(2,2)	1:A:32:LEU:N	1:A:74:LEU:O	8	0.16
(1,752)	1:B:111:GLU:HG2	1:A:5:MET:HG2	6	0.16
(1,752)	1:B:111:GLU:HG2	1:A:5:MET:HG3	6	0.16
(1,752)	1:B:111:GLU:HG3	1:A:5:MET:HG2	6	0.16
(1,752)	1:B:111:GLU:HG3	1:A:5:MET:HG3	6	0.16
(1,752)	1:B:99:GLU:HG2	1:B:98:ASP:HB2	6	0.16
(1,752)	1:B:99:GLU:HG2	1:B:98:ASP:HB3	6	0.16
(1,752)	1:B:99:GLU:HG3	1:B:98:ASP:HB2	6	0.16
(1,752)	1:B:99:GLU:HG3	1:B:98:ASP:HB3	6	0.16
(1,751)	1:A:111:GLU:HG2	1:B:5:MET:HG2	6	0.16
(1,751)	1:A:111:GLU:HG2	1:B:5:MET:HG3	6	0.16
(1,751)	1:A:111:GLU:HG3	1:B:5:MET:HG2	6	0.16
(1,751)	1:A:111:GLU:HG3	1:B:5:MET:HG3	6	0.16
(1,751)	1:A:99:GLU:HG2	1:A:98:ASP:HB2	6	0.16
(1,751)	1:A:99:GLU:HG2	1:A:98:ASP:HB3	6	0.16
(1,751)	1:A:99:GLU:HG3	1:A:98:ASP:HB2	6	0.16
(1,751)	1:A:99:GLU:HG3	1:A:98:ASP:HB3	6	0.16
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	3	0.16
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	3	0.16
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	3	0.16
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	3	0.16
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	1	0.16
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	1	0.16
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	1	0.16
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	1	0.16
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	3	0.16
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	3	0.16
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	3	0.16
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	3	0.16
(1,566)	1:B:39:GLU:H	1:B:42:ARG:HA	7	0.16
(1,566)	1:B:42:ARG:HA	1:B:49:LEU:H	7	0.16
(1,565)	1:A:39:GLU:H	1:A:42:ARG:HA	7	0.16
(1,565)	1:A:42:ARG:HA	1:A:49:LEU:H	7	0.16
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB2	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB3	1	0.16
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB2	1	0.16
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB3	1	0.16
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB2	1	0.16
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB3	1	0.16
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB2	1	0.16
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB3	1	0.16
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB2	1	0.16
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB3	1	0.16
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB2	1	0.16
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB3	1	0.16
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB2	1	0.16
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB3	1	0.16
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB2	1	0.16
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB3	1	0.16
(1,478)	1:B:37:PHE:HB2	1:B:74:LEU:HG	1	0.16
(1,478)	1:B:37:PHE:HB3	1:B:74:LEU:HG	1	0.16
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB2	1	0.16
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB3	1	0.16
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB2	1	0.16
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB3	1	0.16
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB2	1	0.16
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB3	1	0.16
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB2	1	0.16
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB3	1	0.16
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB2	1	0.16
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB3	1	0.16
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB2	1	0.16
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB3	1	0.16
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB2	1	0.16
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB3	1	0.16
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB2	1	0.16
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB3	1	0.16
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB2	1	0.16
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB3	1	0.16
(1,477)	1:A:37:PHE:HB2	1:A:74:LEU:HG	1	0.16
(1,477)	1:A:37:PHE:HB3	1:A:74:LEU:HG	1	0.16
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB2	1	0.16
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB3	1	0.16
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG2	4	0.16
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG3	4	0.16
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG3	4	0.16
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG2	4	0.16
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG3	4	0.16
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG2	4	0.16
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG3	4	0.16
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG2	4	0.16
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG3	4	0.16
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG2	4	0.16
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG3	4	0.16
(1,42)	1:B:64:GLU:HG2	1:B:61:HIS:HB2	5	0.16
(1,42)	1:B:64:GLU:HG2	1:B:61:HIS:HB3	5	0.16
(1,42)	1:B:64:GLU:HG3	1:B:61:HIS:HB2	5	0.16
(1,42)	1:B:64:GLU:HG3	1:B:61:HIS:HB3	5	0.16
(1,42)	1:B:78:GLU:HG2	1:B:76:PHE:HA	5	0.16
(1,42)	1:B:78:GLU:HG3	1:B:76:PHE:HA	5	0.16
(1,41)	1:A:64:GLU:HG2	1:A:61:HIS:HB2	5	0.16
(1,41)	1:A:64:GLU:HG2	1:A:61:HIS:HB3	5	0.16
(1,41)	1:A:64:GLU:HG3	1:A:61:HIS:HB2	5	0.16
(1,41)	1:A:64:GLU:HG3	1:A:61:HIS:HB3	5	0.16
(1,41)	1:A:78:GLU:HG2	1:A:76:PHE:HA	5	0.16
(1,41)	1:A:78:GLU:HG3	1:A:76:PHE:HA	5	0.16
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	4	0.16
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	4	0.16
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	4	0.16
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	4	0.16
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	4	0.16
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	4	0.16
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	4	0.16
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	4	0.16
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE2	7	0.16
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE1	7	0.16
(1,223)	1:A:12:ILE:HG22	1:B:83:MET:HE3	7	0.16
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE2	7	0.16
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE1	7	0.16
(1,223)	1:A:12:ILE:HG21	1:B:83:MET:HE3	7	0.16
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE2	7	0.16
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE1	7	0.16
(1,223)	1:A:12:ILE:HG23	1:B:83:MET:HE3	7	0.16
(1,223)	1:A:62:ILE:HG22	1:A:66:LEU:HG	7	0.16
(1,223)	1:A:62:ILE:HG21	1:A:66:LEU:HG	7	0.16
(1,223)	1:A:62:ILE:HG23	1:A:66:LEU:HG	7	0.16
(1,1858)	1:B:108:GLY:H	1:B:111:GLU:HA	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA2	2	0.16
(1,1858)	1:B:108:GLY:H	1:B:112:GLY:HA3	2	0.16
(1,1858)	1:B:110:GLY:H	1:B:111:GLU:HA	2	0.16
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA2	2	0.16
(1,1858)	1:B:110:GLY:H	1:B:112:GLY:HA3	2	0.16
(1,1857)	1:A:108:GLY:H	1:A:111:GLU:HA	2	0.16
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA2	2	0.16
(1,1857)	1:A:108:GLY:H	1:A:112:GLY:HA3	2	0.16
(1,1857)	1:A:110:GLY:H	1:A:111:GLU:HA	2	0.16
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA2	2	0.16
(1,1857)	1:A:110:GLY:H	1:A:112:GLY:HA3	2	0.16
(1,1798)	1:B:5:MET:H	1:B:4:LYS:HE2	10	0.16
(1,1798)	1:B:5:MET:H	1:B:4:LYS:HE3	10	0.16
(1,1798)	1:B:16:ILE:H	1:B:17:ASN:HB2	10	0.16
(1,1798)	1:B:16:ILE:H	1:B:17:ASN:HB3	10	0.16
(1,1798)	1:B:94:MET:H	1:B:93:LYS:HE2	10	0.16
(1,1798)	1:B:94:MET:H	1:B:93:LYS:HE3	10	0.16
(1,1798)	1:B:109:LEU:H	1:B:93:LYS:HE2	10	0.16
(1,1798)	1:B:109:LEU:H	1:B:93:LYS:HE3	10	0.16
(1,1797)	1:A:5:MET:H	1:A:4:LYS:HE2	10	0.16
(1,1797)	1:A:5:MET:H	1:A:4:LYS:HE3	10	0.16
(1,1797)	1:A:16:ILE:H	1:A:17:ASN:HB2	10	0.16
(1,1797)	1:A:16:ILE:H	1:A:17:ASN:HB3	10	0.16
(1,1797)	1:A:94:MET:H	1:A:93:LYS:HE2	10	0.16
(1,1797)	1:A:94:MET:H	1:A:93:LYS:HE3	10	0.16
(1,1797)	1:A:109:LEU:H	1:A:93:LYS:HE2	10	0.16
(1,1797)	1:A:109:LEU:H	1:A:93:LYS:HE3	10	0.16
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	10	0.16
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	10	0.16
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	10	0.16
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	10	0.16
(1,1706)	1:B:24:VAL:H	1:B:17:ASN:HA	2	0.16
(1,1706)	1:B:78:GLU:H	1:B:67:ASP:HA	2	0.16
(1,1705)	1:A:24:VAL:H	1:A:17:ASN:HA	2	0.16
(1,1705)	1:A:78:GLU:H	1:A:67:ASP:HA	2	0.16
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	5	0.16
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	5	0.16
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	5	0.16
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	5	0.16
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	5	0.16
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	5	0.16
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB2	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	1:B:47:ASN:H	1:B:45:LEU:HB3	10	0.16
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB2	10	0.16
(1,1572)	1:B:47:ASN:H	1:B:49:LEU:HB3	10	0.16
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD2	10	0.16
(1,1572)	1:B:47:ASN:H	1:B:50:LYS:HD3	10	0.16
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	5	0.16
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	5	0.16
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	5	0.16
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	5	0.16
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	5	0.16
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	5	0.16
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB2	10	0.16
(1,1571)	1:A:47:ASN:H	1:A:45:LEU:HB3	10	0.16
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB2	10	0.16
(1,1571)	1:A:47:ASN:H	1:A:49:LEU:HB3	10	0.16
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD2	10	0.16
(1,1571)	1:A:47:ASN:H	1:A:50:LYS:HD3	10	0.16
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	8	0.16
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	8	0.16
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	8	0.16
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	8	0.16
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	8	0.16
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	8	0.16
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	8	0.16
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	8	0.16
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	8	0.16
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	8	0.16
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	8	0.16
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	8	0.16
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	8	0.16
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	8	0.16
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	8	0.16
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	8	0.16
(1,143)	1:A:75:SER:HB2	1:A:68:THR:HB	1	0.16
(1,143)	1:A:75:SER:HB3	1:A:68:THR:HB	1	0.16
(1,143)	1:A:75:SER:HB2	1:A:79:PHE:HA	1	0.16
(1,143)	1:A:75:SER:HB3	1:A:79:PHE:HA	1	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG22	1	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG21	1	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG23	1	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG12	1	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG11	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG13	1	0.16
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD12	1	0.16
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD11	1	0.16
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD13	1	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG22	4	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG21	4	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG23	4	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG12	4	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG11	4	0.16
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG13	4	0.16
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD12	4	0.16
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD11	4	0.16
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD13	4	0.16
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG22	4	0.16
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG21	4	0.16
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG23	4	0.16
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG12	4	0.16
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG11	4	0.16
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG13	4	0.16
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD12	4	0.16
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD11	4	0.16
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD13	4	0.16
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE2	1	0.16
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE1	1	0.16
(1,1381)	1:A:18:THR:H	1:A:5:MET:HE3	1	0.16
(1,1381)	1:A:18:THR:H	1:A:10:ARG:HB2	1	0.16
(1,1381)	1:A:18:THR:H	1:A:10:ARG:HB3	1	0.16
(1,1381)	1:A:18:THR:H	1:A:12:ILE:HB	1	0.16
(1,1381)	1:A:18:THR:H	1:B:8:LEU:HB2	1	0.16
(1,1381)	1:A:18:THR:H	1:B:8:LEU:HB3	1	0.16
(1,1381)	1:A:18:THR:H	1:B:83:MET:HB2	1	0.16
(1,1381)	1:A:18:THR:H	1:B:83:MET:HB3	1	0.16
(1,1332)	1:B:12:ILE:H	1:B:14:THR:H	9	0.16
(1,1332)	1:B:12:ILE:H	1:B:15:ILE:H	9	0.16
(1,1331)	1:A:12:ILE:H	1:A:14:THR:H	9	0.16
(1,1331)	1:A:12:ILE:H	1:A:15:ILE:H	9	0.16
(1,1215)	1:A:49:LEU:HB2	1:A:39:GLU:HB2	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:A:39:GLU:HB3	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:A:39:GLU:HB2	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:A:39:GLU:HB3	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:A:56:GLU:HG2	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:A:56:GLU:HG3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:A:49:LEU:HB3	1:A:56:GLU:HG2	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:A:56:GLU:HG3	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:A:62:ILE:HB	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:A:62:ILE:HB	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:B:5:MET:HB2	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:B:5:MET:HB3	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:B:5:MET:HB2	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:B:5:MET:HB3	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:B:9:GLU:HB2	4	0.16
(1,1215)	1:A:49:LEU:HB2	1:B:9:GLU:HB3	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:B:9:GLU:HB2	4	0.16
(1,1215)	1:A:49:LEU:HB3	1:B:9:GLU:HB3	4	0.16
(1,1208)	1:B:39:GLU:HB2	1:B:32:LEU:HA	6	0.16
(1,1208)	1:B:39:GLU:HB3	1:B:32:LEU:HA	6	0.16
(1,1208)	1:B:34:GLN:HB2	1:B:32:LEU:HA	6	0.16
(1,1208)	1:B:34:GLN:HB3	1:B:32:LEU:HA	6	0.16
(1,1208)	1:B:34:GLN:HB2	1:B:71:ASP:HA	6	0.16
(1,1208)	1:B:34:GLN:HB3	1:B:71:ASP:HA	6	0.16
(1,1207)	1:A:39:GLU:HB2	1:A:32:LEU:HA	6	0.16
(1,1207)	1:A:39:GLU:HB3	1:A:32:LEU:HA	6	0.16
(1,1207)	1:A:34:GLN:HB2	1:A:32:LEU:HA	6	0.16
(1,1207)	1:A:34:GLN:HB3	1:A:32:LEU:HA	6	0.16
(1,1207)	1:A:34:GLN:HB2	1:A:71:ASP:HA	6	0.16
(1,1207)	1:A:34:GLN:HB3	1:A:71:ASP:HA	6	0.16
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD2	6	0.16
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD3	6	0.16
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD2	6	0.16
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD3	6	0.16
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG2	6	0.16
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG3	6	0.16
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG2	6	0.16
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG3	6	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB2	6	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB3	6	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB2	6	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB3	6	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD2	6	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD3	6	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD2	6	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD3	6	0.16
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD2	7	0.16
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD2	7	0.16
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD3	7	0.16
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG2	7	0.16
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG3	7	0.16
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG2	7	0.16
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG3	7	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB2	7	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB3	7	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB2	7	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB3	7	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD2	7	0.16
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD3	7	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD2	7	0.16
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD3	7	0.16
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD2	6	0.16
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD3	6	0.16
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD2	6	0.16
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD3	6	0.16
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG2	6	0.16
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG3	6	0.16
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG2	6	0.16
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG3	6	0.16
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB2	6	0.16
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB3	6	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB2	6	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB3	6	0.16
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD2	6	0.16
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD3	6	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD2	6	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD3	6	0.16
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD2	7	0.16
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD3	7	0.16
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD2	7	0.16
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD3	7	0.16
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG2	7	0.16
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG3	7	0.16
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG2	7	0.16
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG3	7	0.16
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB2	7	0.16
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB3	7	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB2	7	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB3	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD2	7	0.16
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD3	7	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD2	7	0.16
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD3	7	0.16
(4,255)	1:A:73:GLN:H	1:A:67:ASP:H	8	0.15
(4,2)	1:B:98:ASP:HA	1:B:95:HIS:HA	10	0.15
(4,1)	1:A:98:ASP:HA	1:A:95:HIS:HA	10	0.15
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB2	7	0.15
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB3	7	0.15
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB2	7	0.15
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB3	7	0.15
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG21	9	0.15
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG22	9	0.15
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG23	9	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG21	7	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG22	7	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG23	7	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG21	9	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG22	9	0.15
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG23	9	0.15
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	5	0.15
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	5	0.15
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	5	0.15
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	5	0.15
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	5	0.15
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	5	0.15
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	7	0.15
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	7	0.15
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	7	0.15
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	7	0.15
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	7	0.15
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	7	0.15
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	5	0.15
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	5	0.15
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	5	0.15
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	5	0.15
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	5	0.15
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	5	0.15
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	7	0.15
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	7	0.15
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	7	0.15
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	7	0.15
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	7	0.15
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD22	6	0.15
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD21	6	0.15
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD23	6	0.15
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD12	6	0.15
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD11	6	0.15
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD13	6	0.15
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD22	6	0.15
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD21	6	0.15
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD23	6	0.15
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD12	6	0.15
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD11	6	0.15
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD13	6	0.15
(3,504)	1:B:111:GLU:HA	1:B:107:PRO:HB2	5	0.15
(3,504)	1:B:111:GLU:HA	1:B:107:PRO:HB3	5	0.15
(3,503)	1:A:111:GLU:HA	1:A:107:PRO:HB2	5	0.15
(3,503)	1:A:111:GLU:HA	1:A:107:PRO:HB3	5	0.15
(3,492)	1:B:59:ILE:HD12	1:B:52:GLU:HG2	7	0.15
(3,492)	1:B:59:ILE:HD12	1:B:52:GLU:HG3	7	0.15
(3,492)	1:B:59:ILE:HD11	1:B:52:GLU:HG2	7	0.15
(3,492)	1:B:59:ILE:HD11	1:B:52:GLU:HG3	7	0.15
(3,492)	1:B:59:ILE:HD13	1:B:52:GLU:HG2	7	0.15
(3,492)	1:B:59:ILE:HD13	1:B:52:GLU:HG3	7	0.15
(3,491)	1:A:59:ILE:HD12	1:A:52:GLU:HG2	7	0.15
(3,491)	1:A:59:ILE:HD12	1:A:52:GLU:HG3	7	0.15
(3,491)	1:A:59:ILE:HD11	1:A:52:GLU:HG2	7	0.15
(3,491)	1:A:59:ILE:HD11	1:A:52:GLU:HG3	7	0.15
(3,491)	1:A:59:ILE:HD13	1:A:52:GLU:HG2	7	0.15
(3,491)	1:A:59:ILE:HD13	1:A:52:GLU:HG3	7	0.15
(3,345)	1:A:5:MET:H	1:A:4:LYS:HG2	6	0.15
(3,345)	1:A:5:MET:H	1:A:4:LYS:HG3	6	0.15
(3,34)	1:B:87:THR:HG21	1:B:88:TRP:HA	10	0.15
(3,34)	1:B:87:THR:HG22	1:B:88:TRP:HA	10	0.15
(3,34)	1:B:87:THR:HG23	1:B:88:TRP:HA	10	0.15
(3,33)	1:A:87:THR:HG21	1:A:88:TRP:HA	10	0.15
(3,33)	1:A:87:THR:HG22	1:A:88:TRP:HA	10	0.15
(3,33)	1:A:87:THR:HG23	1:A:88:TRP:HA	10	0.15
(3,320)	1:B:51:LYS:HE2	1:B:51:LYS:H	5	0.15
(3,320)	1:B:51:LYS:HE3	1:B:51:LYS:H	5	0.15
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	1	0.15
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	1	0.15
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	1	0.15
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	1	0.15
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	1	0.15
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	1	0.15
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	1	0.15
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG2	3	0.15
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG3	3	0.15
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG2	3	0.15
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG3	3	0.15
(3,1381)	1:A:71:ASP:H	1:A:72:LYS:HE2	5	0.15
(3,1381)	1:A:71:ASP:H	1:A:72:LYS:HE3	5	0.15
(3,1353)	1:A:69:ASN:H	1:A:68:THR:HG21	1	0.15
(3,1353)	1:A:69:ASN:H	1:A:68:THR:HG22	1	0.15
(3,1353)	1:A:69:ASN:H	1:A:68:THR:HG23	1	0.15
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	5	0.15
(3,12)	1:B:98:ASP:H	1:B:98:ASP:HA	3	0.15
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	5	0.15
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG2	6	0.15
(3,1152)	1:B:96:GLU:H	1:B:96:GLU:HG3	6	0.15
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG2	6	0.15
(3,1151)	1:A:96:GLU:H	1:A:96:GLU:HG3	6	0.15
(2,86)	1:A:94:MET:H	1:A:90:SER:O	3	0.15
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	6	0.15
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	6	0.15
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	6	0.15
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	6	0.15
(1,710)	1:B:21:GLN:HG2	1:B:23:SER:HA	9	0.15
(1,710)	1:B:21:GLN:HG3	1:B:23:SER:HA	9	0.15
(1,710)	1:B:46:GLN:HG2	1:A:9:GLU:HA	9	0.15
(1,710)	1:B:46:GLN:HG3	1:A:9:GLU:HA	9	0.15
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	6	0.15
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	6	0.15
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	6	0.15
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	6	0.15
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	10	0.15
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	10	0.15
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	10	0.15
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	10	0.15
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	10	0.15
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	10	0.15
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	10	0.15
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	10	0.15
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	10	0.15
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	10	0.15
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	10	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG12	2	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG13	2	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE2	2	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE1	2	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE3	2	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG12	2	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG13	2	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE2	2	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE1	2	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE3	2	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB2	2	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB3	2	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG12	9	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG13	9	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE2	9	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE1	9	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE3	9	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG12	9	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG13	9	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE2	9	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE1	9	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE3	9	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB2	9	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB3	9	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG12	10	0.15
(1,562)	1:B:16:ILE:HB	1:B:12:ILE:HG13	10	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE2	10	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE1	10	0.15
(1,562)	1:B:16:ILE:HB	1:B:83:MET:HE3	10	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG12	10	0.15
(1,562)	1:B:16:ILE:HB	1:A:12:ILE:HG13	10	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE2	10	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE1	10	0.15
(1,562)	1:B:16:ILE:HB	1:A:83:MET:HE3	10	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB2	10	0.15
(1,562)	1:B:16:ILE:HB	1:A:93:LYS:HB3	10	0.15
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG12	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG13	2	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE2	2	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE1	2	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE3	2	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG12	2	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG13	2	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE2	2	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE1	2	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE3	2	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB2	2	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB3	2	0.15
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG12	9	0.15
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG13	9	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE2	9	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE1	9	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE3	9	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG12	9	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG13	9	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE2	9	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE1	9	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE3	9	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB2	9	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB3	9	0.15
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG12	10	0.15
(1,561)	1:A:16:ILE:HB	1:A:12:ILE:HG13	10	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE2	10	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE1	10	0.15
(1,561)	1:A:16:ILE:HB	1:A:83:MET:HE3	10	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG12	10	0.15
(1,561)	1:A:16:ILE:HB	1:B:12:ILE:HG13	10	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE2	10	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE1	10	0.15
(1,561)	1:A:16:ILE:HB	1:B:83:MET:HE3	10	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB2	10	0.15
(1,561)	1:A:16:ILE:HB	1:B:93:LYS:HB3	10	0.15
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB2	4	0.15
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB3	4	0.15
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB2	4	0.15
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB3	4	0.15
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB2	4	0.15
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB3	4	0.15
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB2	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB3	4	0.15
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB2	4	0.15
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB3	4	0.15
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB2	4	0.15
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB3	4	0.15
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB2	4	0.15
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB3	4	0.15
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB2	4	0.15
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB3	4	0.15
(1,478)	1:B:37:PHE:HB2	1:B:74:LEU:HG	4	0.15
(1,478)	1:B:37:PHE:HB3	1:B:74:LEU:HG	4	0.15
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB2	4	0.15
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB3	4	0.15
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB2	4	0.15
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB3	4	0.15
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB2	4	0.15
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB3	4	0.15
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB2	4	0.15
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB3	4	0.15
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB2	4	0.15
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB3	4	0.15
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB2	4	0.15
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB3	4	0.15
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB2	4	0.15
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB3	4	0.15
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB2	4	0.15
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB3	4	0.15
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB2	4	0.15
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB3	4	0.15
(1,477)	1:A:37:PHE:HB2	1:A:74:LEU:HG	4	0.15
(1,477)	1:A:37:PHE:HB3	1:A:74:LEU:HG	4	0.15
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB2	4	0.15
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB3	4	0.15
(1,358)	1:B:46:GLN:HB2	1:B:39:GLU:HA	3	0.15
(1,358)	1:B:46:GLN:HB3	1:B:39:GLU:HA	3	0.15
(1,358)	1:B:46:GLN:HB2	1:B:40:LEU:HA	3	0.15
(1,358)	1:B:46:GLN:HB3	1:B:40:LEU:HA	3	0.15
(1,358)	1:B:77:GLU:HB2	1:B:31:THR:HB	3	0.15
(1,358)	1:B:77:GLU:HB3	1:B:31:THR:HB	3	0.15
(1,358)	1:B:46:GLN:HB2	1:B:39:GLU:HA	9	0.15
(1,358)	1:B:46:GLN:HB3	1:B:39:GLU:HA	9	0.15
(1,358)	1:B:46:GLN:HB2	1:B:40:LEU:HA	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,358)	1:B:46:GLN:HB3	1:B:40:LEU:HA	9	0.15
(1,358)	1:B:77:GLU:HB2	1:B:31:THR:HB	9	0.15
(1,358)	1:B:77:GLU:HB3	1:B:31:THR:HB	9	0.15
(1,357)	1:A:46:GLN:HB2	1:A:39:GLU:HA	3	0.15
(1,357)	1:A:46:GLN:HB3	1:A:39:GLU:HA	3	0.15
(1,357)	1:A:46:GLN:HB2	1:A:40:LEU:HA	3	0.15
(1,357)	1:A:46:GLN:HB3	1:A:40:LEU:HA	3	0.15
(1,357)	1:A:77:GLU:HB2	1:A:31:THR:HB	3	0.15
(1,357)	1:A:77:GLU:HB3	1:A:31:THR:HB	3	0.15
(1,357)	1:A:46:GLN:HB2	1:A:39:GLU:HA	9	0.15
(1,357)	1:A:46:GLN:HB3	1:A:39:GLU:HA	9	0.15
(1,357)	1:A:46:GLN:HB2	1:A:40:LEU:HA	9	0.15
(1,357)	1:A:46:GLN:HB3	1:A:40:LEU:HA	9	0.15
(1,357)	1:A:77:GLU:HB2	1:A:31:THR:HB	9	0.15
(1,357)	1:A:77:GLU:HB3	1:A:31:THR:HB	9	0.15
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD22	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD21	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD23	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD12	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD11	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD13	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD22	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD21	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD23	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD12	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD11	2	0.15
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD13	2	0.15
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD12	2	0.15
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD11	2	0.15
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD13	2	0.15
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	8	0.15
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	8	0.15
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	8	0.15
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	8	0.15
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD2	10	0.15
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD3	10	0.15
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD2	10	0.15
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD3	10	0.15
(1,24)	1:B:65:ASP:HA	1:B:72:LYS:HA	10	0.15
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD2	10	0.15
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD3	10	0.15
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD2	10	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD3	10	0.15
(1,23)	1:A:65:ASP:HA	1:A:72:LYS:HA	10	0.15
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	1	0.15
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	1	0.15
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	4	0.15
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	4	0.15
(1,144)	1:B:75:SER:HB2	1:B:68:THR:HB	1	0.15
(1,144)	1:B:75:SER:HB3	1:B:68:THR:HB	1	0.15
(1,144)	1:B:75:SER:HB2	1:B:79:PHE:HA	1	0.15
(1,144)	1:B:75:SER:HB3	1:B:79:PHE:HA	1	0.15
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG22	1	0.15
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG21	1	0.15
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG23	1	0.15
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG12	1	0.15
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG11	1	0.15
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG13	1	0.15
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD12	1	0.15
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD11	1	0.15
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD13	1	0.15
(1,1216)	1:B:49:LEU:HB2	1:B:39:GLU:HB2	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:B:39:GLU:HB3	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:B:39:GLU:HB2	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:B:39:GLU:HB3	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:B:56:GLU:HG2	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:B:56:GLU:HG3	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:B:56:GLU:HG2	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:B:56:GLU:HG3	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:B:62:ILE:HB	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:B:62:ILE:HB	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:A:5:MET:HB2	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:A:5:MET:HB3	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:A:5:MET:HB2	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:A:5:MET:HB3	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:A:9:GLU:HB2	4	0.15
(1,1216)	1:B:49:LEU:HB2	1:A:9:GLU:HB3	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:A:9:GLU:HB2	4	0.15
(1,1216)	1:B:49:LEU:HB3	1:A:9:GLU:HB3	4	0.15
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD2	3	0.15
(1,1183)	1:A:56:GLU:HB2	1:A:57:LYS:HD3	3	0.15
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD2	3	0.15
(1,1183)	1:A:56:GLU:HB3	1:A:57:LYS:HD3	3	0.15
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG2	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1183)	1:A:81:MET:HB2	1:A:85:ARG:HG3	3	0.15
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG2	3	0.15
(1,1183)	1:A:81:MET:HB3	1:A:85:ARG:HG3	3	0.15
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB2	3	0.15
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HB3	3	0.15
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB2	3	0.15
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HB3	3	0.15
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD2	3	0.15
(1,1183)	1:A:96:GLU:HB2	1:A:93:LYS:HD3	3	0.15
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD2	3	0.15
(1,1183)	1:A:96:GLU:HB3	1:A:93:LYS:HD3	3	0.15
(1,1098)	1:B:59:ILE:HG22	1:B:42:ARG:HD2	9	0.15
(1,1098)	1:B:59:ILE:HG22	1:B:42:ARG:HD3	9	0.15
(1,1098)	1:B:59:ILE:HG21	1:B:42:ARG:HD2	9	0.15
(1,1098)	1:B:59:ILE:HG21	1:B:42:ARG:HD3	9	0.15
(1,1098)	1:B:59:ILE:HG23	1:B:42:ARG:HD2	9	0.15
(1,1098)	1:B:59:ILE:HG23	1:B:42:ARG:HD3	9	0.15
(1,1098)	1:B:59:ILE:HG22	1:B:79:PHE:HB2	9	0.15
(1,1098)	1:B:59:ILE:HG22	1:B:79:PHE:HB3	9	0.15
(1,1098)	1:B:59:ILE:HG21	1:B:79:PHE:HB2	9	0.15
(1,1098)	1:B:59:ILE:HG21	1:B:79:PHE:HB3	9	0.15
(1,1098)	1:B:59:ILE:HG23	1:B:79:PHE:HB2	9	0.15
(1,1098)	1:B:59:ILE:HG23	1:B:79:PHE:HB3	9	0.15
(1,1097)	1:A:59:ILE:HG22	1:A:42:ARG:HD2	9	0.15
(1,1097)	1:A:59:ILE:HG22	1:A:42:ARG:HD3	9	0.15
(1,1097)	1:A:59:ILE:HG21	1:A:42:ARG:HD2	9	0.15
(1,1097)	1:A:59:ILE:HG21	1:A:42:ARG:HD3	9	0.15
(1,1097)	1:A:59:ILE:HG23	1:A:42:ARG:HD2	9	0.15
(1,1097)	1:A:59:ILE:HG23	1:A:42:ARG:HD3	9	0.15
(1,1097)	1:A:59:ILE:HG22	1:A:79:PHE:HB2	9	0.15
(1,1097)	1:A:59:ILE:HG22	1:A:79:PHE:HB3	9	0.15
(1,1097)	1:A:59:ILE:HG21	1:A:79:PHE:HB2	9	0.15
(1,1097)	1:A:59:ILE:HG21	1:A:79:PHE:HB3	9	0.15
(1,1097)	1:A:59:ILE:HG23	1:A:79:PHE:HB2	9	0.15
(1,1097)	1:A:59:ILE:HG23	1:A:79:PHE:HB3	9	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD22	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD21	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD23	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD12	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD11	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:66:LEU:HD13	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD22	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD21	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD23	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD12	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD11	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:66:LEU:HD13	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD22	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD21	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD23	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD12	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD11	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:66:LEU:HD13	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD22	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD21	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD23	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD12	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD11	6	0.15
(1,1038)	1:B:70:ALA:HB2	1:B:74:LEU:HD13	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD22	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD21	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD23	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD12	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD11	6	0.15
(1,1038)	1:B:70:ALA:HB1	1:B:74:LEU:HD13	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD22	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD21	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD23	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD12	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD11	6	0.15
(1,1038)	1:B:70:ALA:HB3	1:B:74:LEU:HD13	6	0.15
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	4	0.15
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	4	0.15
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	4	0.15
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	4	0.15
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	4	0.15
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	4	0.15
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	4	0.15
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	4	0.15
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	4	0.15
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	4	0.15
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	4	0.15
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	4	0.15
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	4	0.15
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	4	0.15
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	4	0.15
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	4	0.15
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	4	0.15
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	4	0.15
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	4	0.15
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	4	0.15
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	4	0.15
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	4	0.15
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	4	0.15
(4,256)	1:B:73:GLN:H	1:B:67:ASP:H	8	0.14
(4,236)	1:B:81:MET:H	1:A:81:MET:H	8	0.14
(4,235)	1:A:81:MET:H	1:B:81:MET:H	8	0.14
(4,118)	1:B:33:ASN:H	1:B:26:LEU:H	5	0.14
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	5	0.14
(4,117)	1:A:33:ASN:H	1:A:26:LEU:H	9	0.14
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG21	1	0.14
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG22	1	0.14
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG23	1	0.14
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG21	6	0.14
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG22	6	0.14
(3,969)	1:A:7:GLN:H	1:B:14:THR:HG23	6	0.14
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	9	0.14
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	9	0.14
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	9	0.14
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	9	0.14
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	9	0.14
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	9	0.14
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	9	0.14
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	9	0.14
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	9	0.14
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	9	0.14
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	9	0.14
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	9	0.14
(3,664)	1:B:63:MET:HE2	1:B:72:LYS:HA	1	0.14
(3,664)	1:B:63:MET:HE1	1:B:72:LYS:HA	1	0.14
(3,664)	1:B:63:MET:HE3	1:B:72:LYS:HA	1	0.14
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD12	2	0.14
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD11	2	0.14
(3,641)	1:A:8:LEU:HD22	1:B:15:ILE:HD13	2	0.14
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD12	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD11	2	0.14
(3,641)	1:A:8:LEU:HD21	1:B:15:ILE:HD13	2	0.14
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD12	2	0.14
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD11	2	0.14
(3,641)	1:A:8:LEU:HD23	1:B:15:ILE:HD13	2	0.14
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD12	2	0.14
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD11	2	0.14
(3,641)	1:A:8:LEU:HD12	1:B:15:ILE:HD13	2	0.14
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD12	2	0.14
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD11	2	0.14
(3,641)	1:A:8:LEU:HD11	1:B:15:ILE:HD13	2	0.14
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD12	2	0.14
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD11	2	0.14
(3,641)	1:A:8:LEU:HD13	1:B:15:ILE:HD13	2	0.14
(3,602)	1:B:46:GLN:HG2	1:A:4:LYS:HE2	7	0.14
(3,602)	1:B:46:GLN:HG2	1:A:4:LYS:HE3	7	0.14
(3,602)	1:B:46:GLN:HG3	1:A:4:LYS:HE2	7	0.14
(3,602)	1:B:46:GLN:HG3	1:A:4:LYS:HE3	7	0.14
(3,462)	1:B:5:MET:HB2	1:B:4:LYS:HE2	1	0.14
(3,462)	1:B:5:MET:HB2	1:B:4:LYS:HE3	1	0.14
(3,462)	1:B:5:MET:HB3	1:B:4:LYS:HE2	1	0.14
(3,462)	1:B:5:MET:HB3	1:B:4:LYS:HE3	1	0.14
(3,461)	1:A:5:MET:HB2	1:A:4:LYS:HE2	1	0.14
(3,461)	1:A:5:MET:HB2	1:A:4:LYS:HE3	1	0.14
(3,461)	1:A:5:MET:HB3	1:A:4:LYS:HE2	1	0.14
(3,461)	1:A:5:MET:HB3	1:A:4:LYS:HE3	1	0.14
(3,346)	1:B:5:MET:H	1:B:4:LYS:HG2	6	0.14
(3,346)	1:B:5:MET:H	1:B:4:LYS:HG3	6	0.14
(3,319)	1:A:51:LYS:HE2	1:A:51:LYS:H	5	0.14
(3,319)	1:A:51:LYS:HE3	1:A:51:LYS:H	5	0.14
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD2	7	0.14
(3,1507)	1:A:113:THR:H	1:A:107:PRO:HD3	7	0.14
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG2	5	0.14
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG3	5	0.14
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG2	5	0.14
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG3	5	0.14
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB2	8	0.14
(3,1374)	1:B:70:ALA:H	1:B:78:GLU:HB3	8	0.14
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB2	8	0.14
(3,1373)	1:A:70:ALA:H	1:A:78:GLU:HB3	8	0.14
(3,1354)	1:B:69:ASN:H	1:B:68:THR:HG21	1	0.14
(3,1354)	1:B:69:ASN:H	1:B:68:THR:HG22	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1354)	1:B:69:ASN:H	1:B:68:THR:HG23	1	0.14
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	2	0.14
(3,1280)	1:B:57:LYS:H	1:B:57:LYS:HD2	3	0.14
(3,1280)	1:B:57:LYS:H	1:B:57:LYS:HD3	3	0.14
(3,1279)	1:A:57:LYS:H	1:A:57:LYS:HD2	3	0.14
(3,1279)	1:A:57:LYS:H	1:A:57:LYS:HD3	3	0.14
(3,1208)	1:B:42:ARG:H	1:B:43:LYS:HG2	8	0.14
(3,1208)	1:B:42:ARG:H	1:B:43:LYS:HG3	8	0.14
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	5	0.14
(2,82)	1:A:92:GLU:H	1:A:88:TRP:O	8	0.14
(2,79)	1:A:91:HIS:N	1:A:87:THR:O	5	0.14
(2,79)	1:A:91:HIS:N	1:A:87:THR:O	10	0.14
(2,61)	1:A:81:MET:N	1:A:77:GLU:O	8	0.14
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	5	0.14
(2,4)	1:A:74:LEU:N	1:A:32:LEU:O	9	0.14
(2,26)	1:A:22:TYR:H	1:A:18:THR:O	2	0.14
(2,26)	1:A:22:TYR:H	1:A:18:THR:O	7	0.14
(2,26)	1:A:22:TYR:H	1:A:18:THR:O	10	0.14
(1,988)	1:B:48:PHE:HB2	1:B:93:LYS:H	2	0.14
(1,988)	1:B:48:PHE:HB3	1:B:93:LYS:H	2	0.14
(1,988)	1:B:48:PHE:HB2	1:B:109:LEU:H	2	0.14
(1,988)	1:B:48:PHE:HB3	1:B:109:LEU:H	2	0.14
(1,988)	1:B:48:PHE:HB2	1:A:5:MET:H	2	0.14
(1,988)	1:B:48:PHE:HB3	1:A:5:MET:H	2	0.14
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB2	2	0.14
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB3	2	0.14
(1,988)	1:B:48:PHE:HB2	1:B:93:LYS:H	10	0.14
(1,988)	1:B:48:PHE:HB3	1:B:93:LYS:H	10	0.14
(1,988)	1:B:48:PHE:HB2	1:B:109:LEU:H	10	0.14
(1,988)	1:B:48:PHE:HB3	1:B:109:LEU:H	10	0.14
(1,988)	1:B:48:PHE:HB2	1:A:5:MET:H	10	0.14
(1,988)	1:B:48:PHE:HB3	1:A:5:MET:H	10	0.14
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB2	10	0.14
(1,988)	1:B:41:VAL:H	1:B:48:PHE:HB3	10	0.14
(1,987)	1:A:48:PHE:HB2	1:A:93:LYS:H	2	0.14
(1,987)	1:A:48:PHE:HB3	1:A:93:LYS:H	2	0.14
(1,987)	1:A:48:PHE:HB2	1:A:109:LEU:H	2	0.14
(1,987)	1:A:48:PHE:HB3	1:A:109:LEU:H	2	0.14
(1,987)	1:A:48:PHE:HB2	1:B:5:MET:H	2	0.14
(1,987)	1:A:48:PHE:HB3	1:B:5:MET:H	2	0.14
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB2	2	0.14
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB3	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,987)	1:A:48:PHE:HB2	1:A:93:LYS:H	10	0.14
(1,987)	1:A:48:PHE:HB3	1:A:93:LYS:H	10	0.14
(1,987)	1:A:48:PHE:HB2	1:A:109:LEU:H	10	0.14
(1,987)	1:A:48:PHE:HB3	1:A:109:LEU:H	10	0.14
(1,987)	1:A:48:PHE:HB2	1:B:5:MET:H	10	0.14
(1,987)	1:A:48:PHE:HB3	1:B:5:MET:H	10	0.14
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB2	10	0.14
(1,987)	1:A:41:VAL:H	1:A:48:PHE:HB3	10	0.14
(1,921)	1:A:87:THR:HA	1:B:13:GLU:HB2	9	0.14
(1,921)	1:A:87:THR:HA	1:B:13:GLU:HB3	9	0.14
(1,921)	1:A:87:THR:HA	1:B:13:GLU:HG2	9	0.14
(1,921)	1:A:87:THR:HA	1:B:13:GLU:HG3	9	0.14
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB2	9	0.14
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB3	9	0.14
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE2	9	0.14
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE3	9	0.14
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB2	9	0.14
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB3	9	0.14
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE2	9	0.14
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE3	9	0.14
(1,709)	1:A:21:GLN:HG2	1:A:23:SER:HA	9	0.14
(1,709)	1:A:21:GLN:HG3	1:A:23:SER:HA	9	0.14
(1,709)	1:A:46:GLN:HG2	1:B:9:GLU:HA	9	0.14
(1,709)	1:A:46:GLN:HG3	1:B:9:GLU:HA	9	0.14
(1,524)	1:B:49:LEU:HB2	1:B:83:MET:HG2	5	0.14
(1,524)	1:B:49:LEU:HB2	1:B:83:MET:HG3	5	0.14
(1,524)	1:B:49:LEU:HB3	1:B:83:MET:HG2	5	0.14
(1,524)	1:B:49:LEU:HB3	1:B:83:MET:HG3	5	0.14
(1,524)	1:B:49:LEU:HB2	1:A:5:MET:HG2	5	0.14
(1,524)	1:B:49:LEU:HB2	1:A:5:MET:HG3	5	0.14
(1,524)	1:B:49:LEU:HB3	1:A:5:MET:HG2	5	0.14
(1,524)	1:B:49:LEU:HB3	1:A:5:MET:HG3	5	0.14
(1,524)	1:B:49:LEU:HB2	1:B:58:VAL:HB	5	0.14
(1,524)	1:B:49:LEU:HB3	1:B:58:VAL:HB	5	0.14
(1,524)	1:B:49:LEU:HB2	1:B:60:GLU:HG2	5	0.14
(1,524)	1:B:49:LEU:HB2	1:B:60:GLU:HG3	5	0.14
(1,524)	1:B:49:LEU:HB3	1:B:60:GLU:HG2	5	0.14
(1,524)	1:B:49:LEU:HB3	1:B:60:GLU:HG3	5	0.14
(1,523)	1:A:49:LEU:HB2	1:A:83:MET:HG2	5	0.14
(1,523)	1:A:49:LEU:HB2	1:A:83:MET:HG3	5	0.14
(1,523)	1:A:49:LEU:HB3	1:A:83:MET:HG2	5	0.14
(1,523)	1:A:49:LEU:HB3	1:A:83:MET:HG3	5	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:A:49:LEU:HB2	1:B:5:MET:HG2	5	0.14
(1,523)	1:A:49:LEU:HB2	1:B:5:MET:HG3	5	0.14
(1,523)	1:A:49:LEU:HB3	1:B:5:MET:HG2	5	0.14
(1,523)	1:A:49:LEU:HB3	1:B:5:MET:HG3	5	0.14
(1,523)	1:A:49:LEU:HB2	1:A:58:VAL:HB	5	0.14
(1,523)	1:A:49:LEU:HB3	1:A:58:VAL:HB	5	0.14
(1,523)	1:A:49:LEU:HB2	1:A:60:GLU:HG2	5	0.14
(1,523)	1:A:49:LEU:HB2	1:A:60:GLU:HG3	5	0.14
(1,523)	1:A:49:LEU:HB3	1:A:60:GLU:HG2	5	0.14
(1,523)	1:A:49:LEU:HB3	1:A:60:GLU:HG3	5	0.14
(1,358)	1:B:46:GLN:HB2	1:B:39:GLU:HA	2	0.14
(1,358)	1:B:46:GLN:HB3	1:B:39:GLU:HA	2	0.14
(1,358)	1:B:46:GLN:HB2	1:B:40:LEU:HA	2	0.14
(1,358)	1:B:46:GLN:HB3	1:B:40:LEU:HA	2	0.14
(1,358)	1:B:77:GLU:HB2	1:B:31:THR:HB	2	0.14
(1,358)	1:B:77:GLU:HB3	1:B:31:THR:HB	2	0.14
(1,357)	1:A:46:GLN:HB2	1:A:39:GLU:HA	2	0.14
(1,357)	1:A:46:GLN:HB3	1:A:39:GLU:HA	2	0.14
(1,357)	1:A:46:GLN:HB2	1:A:40:LEU:HA	2	0.14
(1,357)	1:A:46:GLN:HB3	1:A:40:LEU:HA	2	0.14
(1,357)	1:A:77:GLU:HB2	1:A:31:THR:HB	2	0.14
(1,357)	1:A:77:GLU:HB3	1:A:31:THR:HB	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD22	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD21	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD23	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD12	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD11	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD13	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD22	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD21	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD23	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD12	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD11	2	0.14
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD13	2	0.14
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD12	2	0.14
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD11	2	0.14
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD13	2	0.14
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	8	0.14
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	8	0.14
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	8	0.14
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	8	0.14
(1,1826)	1:B:21:GLN:H	1:B:17:ASN:HB2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1826)	1:B:21:GLN:H	1:B:17:ASN:HB3	3	0.14
(1,1826)	1:B:94:MET:H	1:B:93:LYS:HE2	3	0.14
(1,1826)	1:B:94:MET:H	1:B:93:LYS:HE3	3	0.14
(1,1826)	1:B:94:MET:H	1:B:95:HIS:HB3	3	0.14
(1,1826)	1:B:98:ASP:H	1:B:95:HIS:HB3	3	0.14
(1,1826)	1:B:16:ILE:H	1:B:17:ASN:HB2	3	0.14
(1,1826)	1:B:16:ILE:H	1:B:17:ASN:HB3	3	0.14
(1,1825)	1:A:21:GLN:H	1:A:17:ASN:HB2	3	0.14
(1,1825)	1:A:21:GLN:H	1:A:17:ASN:HB3	3	0.14
(1,1825)	1:A:94:MET:H	1:A:93:LYS:HE2	3	0.14
(1,1825)	1:A:94:MET:H	1:A:93:LYS:HE3	3	0.14
(1,1825)	1:A:94:MET:H	1:A:95:HIS:HB3	3	0.14
(1,1825)	1:A:98:ASP:H	1:A:95:HIS:HB3	3	0.14
(1,1825)	1:A:16:ILE:H	1:A:17:ASN:HB2	3	0.14
(1,1825)	1:A:16:ILE:H	1:A:17:ASN:HB3	3	0.14
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	1	0.14
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	1	0.14
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	4	0.14
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	4	0.14
(1,1706)	1:B:24:VAL:H	1:B:17:ASN:HA	3	0.14
(1,1706)	1:B:78:GLU:H	1:B:67:ASP:HA	3	0.14
(1,1705)	1:A:24:VAL:H	1:A:17:ASN:HA	3	0.14
(1,1705)	1:A:78:GLU:H	1:A:67:ASP:HA	3	0.14
(1,1590)	1:B:10:ARG:H	1:B:12:ILE:HA	5	0.14
(1,1590)	1:B:51:LYS:H	1:B:46:GLN:HA	5	0.14
(1,1589)	1:A:10:ARG:H	1:A:12:ILE:HA	5	0.14
(1,1589)	1:A:51:LYS:H	1:A:46:GLN:HA	5	0.14
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG22	8	0.14
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG21	8	0.14
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HG23	8	0.14
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD12	8	0.14
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD11	8	0.14
(1,1524)	1:B:41:VAL:H	1:B:62:ILE:HD13	8	0.14
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD12	8	0.14
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD11	8	0.14
(1,1524)	1:B:41:VAL:H	1:A:12:ILE:HD13	8	0.14
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD12	8	0.14
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD11	8	0.14
(1,1524)	1:B:57:LYS:H	1:B:62:ILE:HD13	8	0.14
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG22	8	0.14
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG21	8	0.14
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HG23	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD12	8	0.14
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD11	8	0.14
(1,1523)	1:A:41:VAL:H	1:A:62:ILE:HD13	8	0.14
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD12	8	0.14
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD11	8	0.14
(1,1523)	1:A:41:VAL:H	1:B:12:ILE:HD13	8	0.14
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD12	8	0.14
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD11	8	0.14
(1,1523)	1:A:57:LYS:H	1:A:62:ILE:HD13	8	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG22	6	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG21	6	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG23	6	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG12	6	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG11	6	0.14
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG13	6	0.14
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD12	6	0.14
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD11	6	0.14
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD13	6	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG22	6	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG21	6	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG23	6	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG12	6	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG11	6	0.14
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG13	6	0.14
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD12	6	0.14
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD11	6	0.14
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD13	6	0.14
(1,1389)	1:A:5:MET:H	1:B:110:GLY:H	2	0.14
(1,1389)	1:A:12:ILE:H	1:A:19:PHE:H	2	0.14
(1,1389)	1:A:19:PHE:H	1:A:44:ASP:H	2	0.14
(1,1389)	1:A:19:PHE:H	1:B:12:ILE:H	2	0.14
(1,1389)	1:A:10:ARG:H	1:A:5:MET:H	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD22	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD21	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD23	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD12	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD11	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD13	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD22	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD21	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD23	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD12	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD11	2	0.14
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD13	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD22	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD21	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD23	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD12	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD11	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD13	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD22	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD21	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD23	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD12	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD11	2	0.14
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD13	2	0.14
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB2	8	0.14
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB3	8	0.14
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB2	8	0.14
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB3	8	0.14
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB2	8	0.14
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB3	8	0.14
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB2	8	0.14
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB3	8	0.14
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE2	8	0.14
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE3	8	0.14
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE2	8	0.14
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE3	8	0.14
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD2	8	0.14
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD3	8	0.14
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD2	8	0.14
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD3	8	0.14
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB2	8	0.14
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB3	8	0.14
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB2	8	0.14
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB3	8	0.14
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB2	8	0.14
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB3	8	0.14
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB2	8	0.14
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB3	8	0.14
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE2	8	0.14
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE3	8	0.14
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE2	8	0.14
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE3	8	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD2	8	0.14
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD3	8	0.14
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD2	8	0.14
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD3	8	0.14
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD2	3	0.14
(1,1184)	1:B:56:GLU:HB2	1:B:57:LYS:HD3	3	0.14
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD2	3	0.14
(1,1184)	1:B:56:GLU:HB3	1:B:57:LYS:HD3	3	0.14
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG2	3	0.14
(1,1184)	1:B:81:MET:HB2	1:B:85:ARG:HG3	3	0.14
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG2	3	0.14
(1,1184)	1:B:81:MET:HB3	1:B:85:ARG:HG3	3	0.14
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB2	3	0.14
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HB3	3	0.14
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB2	3	0.14
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HB3	3	0.14
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD2	3	0.14
(1,1184)	1:B:96:GLU:HB2	1:B:93:LYS:HD3	3	0.14
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD2	3	0.14
(1,1184)	1:B:96:GLU:HB3	1:B:93:LYS:HD3	3	0.14
(1,1044)	1:B:53:ASN:HA	1:B:58:VAL:HB	2	0.14
(1,1044)	1:B:53:ASN:HA	1:B:60:GLU:HG2	2	0.14
(1,1044)	1:B:53:ASN:HA	1:B:60:GLU:HG3	2	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD22	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD21	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD23	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD12	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD11	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:66:LEU:HD13	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD22	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD21	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD23	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD12	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD11	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:66:LEU:HD13	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD22	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD21	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD23	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD12	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD11	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:66:LEU:HD13	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD22	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD21	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD23	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD12	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD11	6	0.14
(1,1037)	1:A:70:ALA:HB2	1:A:74:LEU:HD13	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD22	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD21	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD23	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD12	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD11	6	0.14
(1,1037)	1:A:70:ALA:HB1	1:A:74:LEU:HD13	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD22	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD21	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD23	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD12	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD11	6	0.14
(1,1037)	1:A:70:ALA:HB3	1:A:74:LEU:HD13	6	0.14
(4,64)	1:B:32:LEU:HG	1:B:31:THR:HB	1	0.13
(4,63)	1:A:32:LEU:HG	1:A:31:THR:HB	1	0.13
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	2	0.13
(4,62)	1:B:25:LYS:HA	1:B:21:GLN:HA	5	0.13
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	2	0.13
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB2	5	0.13
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB3	5	0.13
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB2	5	0.13
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB3	5	0.13
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG21	6	0.13
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG22	6	0.13
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG23	6	0.13
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG21	8	0.13
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG22	8	0.13
(3,882)	1:B:30:ASP:H	1:B:31:THR:HG23	8	0.13
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG21	8	0.13
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG22	8	0.13
(3,881)	1:A:30:ASP:H	1:A:31:THR:HG23	8	0.13
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB2	4	0.13
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB3	4	0.13
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB2	4	0.13
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB3	4	0.13
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB2	4	0.13
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB3	4	0.13
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB2	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB3	4	0.13
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB2	4	0.13
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB3	4	0.13
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB2	4	0.13
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB3	4	0.13
(3,663)	1:A:63:MET:HE2	1:A:72:LYS:HA	1	0.13
(3,663)	1:A:63:MET:HE1	1:A:72:LYS:HA	1	0.13
(3,663)	1:A:63:MET:HE3	1:A:72:LYS:HA	1	0.13
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD12	2	0.13
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD11	2	0.13
(3,642)	1:B:8:LEU:HD22	1:A:15:ILE:HD13	2	0.13
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD12	2	0.13
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD11	2	0.13
(3,642)	1:B:8:LEU:HD21	1:A:15:ILE:HD13	2	0.13
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD12	2	0.13
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD11	2	0.13
(3,642)	1:B:8:LEU:HD23	1:A:15:ILE:HD13	2	0.13
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD12	2	0.13
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD11	2	0.13
(3,642)	1:B:8:LEU:HD12	1:A:15:ILE:HD13	2	0.13
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD12	2	0.13
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD11	2	0.13
(3,642)	1:B:8:LEU:HD11	1:A:15:ILE:HD13	2	0.13
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD12	2	0.13
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD11	2	0.13
(3,642)	1:B:8:LEU:HD13	1:A:15:ILE:HD13	2	0.13
(3,601)	1:A:46:GLN:HG2	1:B:4:LYS:HE2	7	0.13
(3,601)	1:A:46:GLN:HG2	1:B:4:LYS:HE3	7	0.13
(3,601)	1:A:46:GLN:HG3	1:B:4:LYS:HE2	7	0.13
(3,601)	1:A:46:GLN:HG3	1:B:4:LYS:HE3	7	0.13
(3,530)	1:B:67:ASP:HB2	1:B:64:GLU:HG2	3	0.13
(3,530)	1:B:67:ASP:HB2	1:B:64:GLU:HG3	3	0.13
(3,530)	1:B:67:ASP:HB3	1:B:64:GLU:HG2	3	0.13
(3,530)	1:B:67:ASP:HB3	1:B:64:GLU:HG3	3	0.13
(3,529)	1:A:67:ASP:HB2	1:A:64:GLU:HG2	3	0.13
(3,529)	1:A:67:ASP:HB2	1:A:64:GLU:HG3	3	0.13
(3,529)	1:A:67:ASP:HB3	1:A:64:GLU:HG2	3	0.13
(3,529)	1:A:67:ASP:HB3	1:A:64:GLU:HG3	3	0.13
(3,346)	1:B:5:MET:H	1:B:4:LYS:HG2	1	0.13
(3,346)	1:B:5:MET:H	1:B:4:LYS:HG3	1	0.13
(3,340)	1:B:57:LYS:HG2	1:B:56:GLU:HB2	9	0.13
(3,340)	1:B:57:LYS:HG2	1:B:56:GLU:HB3	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,340)	1:B:57:LYS:HG3	1:B:56:GLU:HB2	9	0.13
(3,340)	1:B:57:LYS:HG3	1:B:56:GLU:HB3	9	0.13
(3,339)	1:A:57:LYS:HG2	1:A:56:GLU:HB2	9	0.13
(3,339)	1:A:57:LYS:HG2	1:A:56:GLU:HB3	9	0.13
(3,339)	1:A:57:LYS:HG3	1:A:56:GLU:HB2	9	0.13
(3,339)	1:A:57:LYS:HG3	1:A:56:GLU:HB3	9	0.13
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB2	9	0.13
(3,280)	1:B:72:LYS:HG2	1:B:73:GLN:HB3	9	0.13
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB2	9	0.13
(3,280)	1:B:72:LYS:HG3	1:B:73:GLN:HB3	9	0.13
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB2	9	0.13
(3,279)	1:A:72:LYS:HG2	1:A:73:GLN:HB3	9	0.13
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB2	9	0.13
(3,279)	1:A:72:LYS:HG3	1:A:73:GLN:HB3	9	0.13
(3,196)	1:B:46:GLN:HA	1:B:50:LYS:HG2	9	0.13
(3,196)	1:B:46:GLN:HA	1:B:50:LYS:HG3	9	0.13
(3,195)	1:A:46:GLN:HA	1:A:50:LYS:HG2	9	0.13
(3,195)	1:A:46:GLN:HA	1:A:50:LYS:HG3	9	0.13
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD2	7	0.13
(3,1508)	1:B:113:THR:H	1:B:107:PRO:HD3	7	0.13
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG2	2	0.13
(3,1439)	1:A:87:THR:H	1:B:77:GLU:HG3	2	0.13
(3,1382)	1:B:71:ASP:H	1:B:72:LYS:HE2	5	0.13
(3,1382)	1:B:71:ASP:H	1:B:72:LYS:HE3	5	0.13
(3,1344)	1:B:66:LEU:H	1:B:66:LEU:HG	7	0.13
(3,1343)	1:A:66:LEU:H	1:A:66:LEU:HG	7	0.13
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	2	0.13
(3,132)	1:B:78:GLU:HB2	1:B:31:THR:HA	6	0.13
(3,132)	1:B:78:GLU:HB3	1:B:31:THR:HA	6	0.13
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	5	0.13
(3,131)	1:A:78:GLU:HB2	1:A:31:THR:HA	6	0.13
(3,131)	1:A:78:GLU:HB3	1:A:31:THR:HA	6	0.13
(3,1207)	1:A:42:ARG:H	1:A:43:LYS:HG2	8	0.13
(3,1207)	1:A:42:ARG:H	1:A:43:LYS:HG3	8	0.13
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	1	0.13
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	1	0.13
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB2	3	0.13
(3,1148)	1:B:35:GLY:H	1:B:32:LEU:HB3	3	0.13
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	3	0.13
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	3	0.13
(3,1124)	1:B:31:THR:H	1:B:23:SER:HA	7	0.13
(3,1123)	1:A:31:THR:H	1:A:23:SER:HA	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,76)	1:A:89:ALA:H	1:A:85:ARG:O	5	0.13
(2,62)	1:A:81:MET:H	1:A:77:GLU:O	7	0.13
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	6	0.13
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	8	0.13
(2,4)	1:A:74:LEU:N	1:A:32:LEU:O	6	0.13
(2,21)	1:A:20:HIS:N	1:A:16:ILE:O	5	0.13
(1,937)	1:A:5:MET:HB2	1:A:8:LEU:HD22	1	0.13
(1,937)	1:A:5:MET:HB2	1:A:8:LEU:HD21	1	0.13
(1,937)	1:A:5:MET:HB2	1:A:8:LEU:HD23	1	0.13
(1,937)	1:A:5:MET:HB2	1:A:8:LEU:HD12	1	0.13
(1,937)	1:A:5:MET:HB2	1:A:8:LEU:HD11	1	0.13
(1,937)	1:A:5:MET:HB2	1:A:8:LEU:HD13	1	0.13
(1,937)	1:A:5:MET:HB3	1:A:8:LEU:HD22	1	0.13
(1,937)	1:A:5:MET:HB3	1:A:8:LEU:HD21	1	0.13
(1,937)	1:A:5:MET:HB3	1:A:8:LEU:HD23	1	0.13
(1,937)	1:A:5:MET:HB3	1:A:8:LEU:HD12	1	0.13
(1,937)	1:A:5:MET:HB3	1:A:8:LEU:HD11	1	0.13
(1,937)	1:A:5:MET:HB3	1:A:8:LEU:HD13	1	0.13
(1,937)	1:A:46:GLN:HG2	1:A:59:ILE:HG22	1	0.13
(1,937)	1:A:46:GLN:HG2	1:A:59:ILE:HG21	1	0.13
(1,937)	1:A:46:GLN:HG2	1:A:59:ILE:HG23	1	0.13
(1,937)	1:A:46:GLN:HG3	1:A:59:ILE:HG22	1	0.13
(1,937)	1:A:46:GLN:HG3	1:A:59:ILE:HG21	1	0.13
(1,937)	1:A:46:GLN:HG3	1:A:59:ILE:HG23	1	0.13
(1,937)	1:A:46:GLN:HG2	1:B:8:LEU:HD22	1	0.13
(1,937)	1:A:46:GLN:HG2	1:B:8:LEU:HD21	1	0.13
(1,937)	1:A:46:GLN:HG2	1:B:8:LEU:HD23	1	0.13
(1,937)	1:A:46:GLN:HG2	1:B:8:LEU:HD12	1	0.13
(1,937)	1:A:46:GLN:HG2	1:B:8:LEU:HD11	1	0.13
(1,937)	1:A:46:GLN:HG2	1:B:8:LEU:HD13	1	0.13
(1,937)	1:A:46:GLN:HG3	1:B:8:LEU:HD22	1	0.13
(1,937)	1:A:46:GLN:HG3	1:B:8:LEU:HD21	1	0.13
(1,937)	1:A:46:GLN:HG3	1:B:8:LEU:HD23	1	0.13
(1,937)	1:A:46:GLN:HG3	1:B:8:LEU:HD12	1	0.13
(1,937)	1:A:46:GLN:HG3	1:B:8:LEU:HD11	1	0.13
(1,937)	1:A:46:GLN:HG3	1:B:8:LEU:HD13	1	0.13
(1,922)	1:B:87:THR:HA	1:A:13:GLU:HB2	9	0.13
(1,922)	1:B:87:THR:HA	1:A:13:GLU:HB3	9	0.13
(1,922)	1:B:87:THR:HA	1:A:13:GLU:HG2	9	0.13
(1,922)	1:B:87:THR:HA	1:A:13:GLU:HG3	9	0.13
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB2	4	0.13
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB3	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG2	4	0.13
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG3	4	0.13
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB2	4	0.13
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB3	4	0.13
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG2	4	0.13
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG3	4	0.13
(1,72)	1:B:33:ASN:HB2	1:B:73:GLN:HG2	4	0.13
(1,72)	1:B:33:ASN:HB2	1:B:73:GLN:HG3	4	0.13
(1,72)	1:B:33:ASN:HB3	1:B:73:GLN:HG2	4	0.13
(1,72)	1:B:33:ASN:HB3	1:B:73:GLN:HG3	4	0.13
(1,72)	1:B:48:PHE:HB2	1:A:9:GLU:HB2	4	0.13
(1,72)	1:B:48:PHE:HB2	1:A:9:GLU:HB3	4	0.13
(1,72)	1:B:48:PHE:HB3	1:A:9:GLU:HB2	4	0.13
(1,72)	1:B:48:PHE:HB3	1:A:9:GLU:HB3	4	0.13
(1,652)	1:B:93:LYS:H	1:B:92:GLU:HB2	8	0.13
(1,652)	1:B:93:LYS:H	1:B:92:GLU:HB3	8	0.13
(1,652)	1:B:100:GLY:H	1:B:99:GLU:HB2	8	0.13
(1,652)	1:B:100:GLY:H	1:B:99:GLU:HB3	8	0.13
(1,651)	1:A:93:LYS:H	1:A:92:GLU:HB2	8	0.13
(1,651)	1:A:93:LYS:H	1:A:92:GLU:HB3	8	0.13
(1,651)	1:A:100:GLY:H	1:A:99:GLU:HB2	8	0.13
(1,651)	1:A:100:GLY:H	1:A:99:GLU:HB3	8	0.13
(1,514)	1:B:4:LYS:HE2	1:A:41:VAL:HG22	2	0.13
(1,514)	1:B:4:LYS:HE2	1:A:41:VAL:HG21	2	0.13
(1,514)	1:B:4:LYS:HE2	1:A:41:VAL:HG23	2	0.13
(1,514)	1:B:4:LYS:HE2	1:A:41:VAL:HG12	2	0.13
(1,514)	1:B:4:LYS:HE2	1:A:41:VAL:HG11	2	0.13
(1,514)	1:B:4:LYS:HE2	1:A:41:VAL:HG13	2	0.13
(1,514)	1:B:4:LYS:HE3	1:A:41:VAL:HG22	2	0.13
(1,514)	1:B:4:LYS:HE3	1:A:41:VAL:HG21	2	0.13
(1,514)	1:B:4:LYS:HE3	1:A:41:VAL:HG23	2	0.13
(1,514)	1:B:4:LYS:HE3	1:A:41:VAL:HG12	2	0.13
(1,514)	1:B:4:LYS:HE3	1:A:41:VAL:HG11	2	0.13
(1,514)	1:B:4:LYS:HE3	1:A:41:VAL:HG13	2	0.13
(1,514)	1:B:51:LYS:HE2	1:B:41:VAL:HG22	2	0.13
(1,514)	1:B:51:LYS:HE2	1:B:41:VAL:HG21	2	0.13
(1,514)	1:B:51:LYS:HE2	1:B:41:VAL:HG23	2	0.13
(1,514)	1:B:51:LYS:HE2	1:B:41:VAL:HG12	2	0.13
(1,514)	1:B:51:LYS:HE2	1:B:41:VAL:HG11	2	0.13
(1,514)	1:B:51:LYS:HE2	1:B:41:VAL:HG13	2	0.13
(1,514)	1:B:51:LYS:HE3	1:B:41:VAL:HG22	2	0.13
(1,514)	1:B:51:LYS:HE3	1:B:41:VAL:HG21	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,514)	1:B:51:LYS:HE3	1:B:41:VAL:HG23	2	0.13
(1,514)	1:B:51:LYS:HE3	1:B:41:VAL:HG12	2	0.13
(1,514)	1:B:51:LYS:HE3	1:B:41:VAL:HG11	2	0.13
(1,514)	1:B:51:LYS:HE3	1:B:41:VAL:HG13	2	0.13
(1,513)	1:A:4:LYS:HE2	1:B:41:VAL:HG22	2	0.13
(1,513)	1:A:4:LYS:HE2	1:B:41:VAL:HG21	2	0.13
(1,513)	1:A:4:LYS:HE2	1:B:41:VAL:HG23	2	0.13
(1,513)	1:A:4:LYS:HE2	1:B:41:VAL:HG12	2	0.13
(1,513)	1:A:4:LYS:HE2	1:B:41:VAL:HG11	2	0.13
(1,513)	1:A:4:LYS:HE2	1:B:41:VAL:HG13	2	0.13
(1,513)	1:A:4:LYS:HE3	1:B:41:VAL:HG22	2	0.13
(1,513)	1:A:4:LYS:HE3	1:B:41:VAL:HG21	2	0.13
(1,513)	1:A:4:LYS:HE3	1:B:41:VAL:HG23	2	0.13
(1,513)	1:A:4:LYS:HE3	1:B:41:VAL:HG12	2	0.13
(1,513)	1:A:4:LYS:HE3	1:B:41:VAL:HG11	2	0.13
(1,513)	1:A:4:LYS:HE3	1:B:41:VAL:HG13	2	0.13
(1,513)	1:A:51:LYS:HE2	1:A:41:VAL:HG22	2	0.13
(1,513)	1:A:51:LYS:HE2	1:A:41:VAL:HG21	2	0.13
(1,513)	1:A:51:LYS:HE2	1:A:41:VAL:HG23	2	0.13
(1,513)	1:A:51:LYS:HE2	1:A:41:VAL:HG12	2	0.13
(1,513)	1:A:51:LYS:HE2	1:A:41:VAL:HG11	2	0.13
(1,513)	1:A:51:LYS:HE2	1:A:41:VAL:HG13	2	0.13
(1,513)	1:A:51:LYS:HE3	1:A:41:VAL:HG22	2	0.13
(1,513)	1:A:51:LYS:HE3	1:A:41:VAL:HG21	2	0.13
(1,513)	1:A:51:LYS:HE3	1:A:41:VAL:HG23	2	0.13
(1,513)	1:A:51:LYS:HE3	1:A:41:VAL:HG12	2	0.13
(1,513)	1:A:51:LYS:HE3	1:A:41:VAL:HG11	2	0.13
(1,513)	1:A:51:LYS:HE3	1:A:41:VAL:HG13	2	0.13
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB2	6	0.13
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB3	6	0.13
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB2	6	0.13
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB3	6	0.13
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB2	6	0.13
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB3	6	0.13
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB2	6	0.13
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB3	6	0.13
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB2	6	0.13
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB3	6	0.13
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB2	6	0.13
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB3	6	0.13
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB2	6	0.13
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB3	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB2	6	0.13
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB3	6	0.13
(1,478)	1:B:37:PHE:HB2	1:B:74:LEU:HG	6	0.13
(1,478)	1:B:37:PHE:HB3	1:B:74:LEU:HG	6	0.13
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB2	6	0.13
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB3	6	0.13
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB2	6	0.13
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB3	6	0.13
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB2	6	0.13
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB3	6	0.13
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB2	6	0.13
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB3	6	0.13
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB2	6	0.13
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB3	6	0.13
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB2	6	0.13
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB3	6	0.13
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB2	6	0.13
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB3	6	0.13
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB2	6	0.13
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB3	6	0.13
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB2	6	0.13
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB3	6	0.13
(1,477)	1:A:37:PHE:HB2	1:A:74:LEU:HG	6	0.13
(1,477)	1:A:37:PHE:HB3	1:A:74:LEU:HG	6	0.13
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB2	6	0.13
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB3	6	0.13
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG2	1	0.13
(1,456)	1:B:7:GLN:HB2	1:B:9:GLU:HG3	1	0.13
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG2	1	0.13
(1,456)	1:B:7:GLN:HB3	1:B:9:GLU:HG3	1	0.13
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG2	1	0.13
(1,456)	1:B:7:GLN:HB2	1:A:21:GLN:HG3	1	0.13
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG2	1	0.13
(1,456)	1:B:7:GLN:HB3	1:A:21:GLN:HG3	1	0.13
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG2	1	0.13
(1,456)	1:B:7:GLN:HB2	1:A:46:GLN:HG3	1	0.13
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG2	1	0.13
(1,456)	1:B:7:GLN:HB3	1:A:46:GLN:HG3	1	0.13
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG2	1	0.13
(1,455)	1:A:7:GLN:HB2	1:A:9:GLU:HG3	1	0.13
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG2	1	0.13
(1,455)	1:A:7:GLN:HB3	1:A:9:GLU:HG3	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG2	1	0.13
(1,455)	1:A:7:GLN:HB2	1:B:21:GLN:HG3	1	0.13
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG2	1	0.13
(1,455)	1:A:7:GLN:HB3	1:B:21:GLN:HG3	1	0.13
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG2	1	0.13
(1,455)	1:A:7:GLN:HB2	1:B:46:GLN:HG3	1	0.13
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG2	1	0.13
(1,455)	1:A:7:GLN:HB3	1:B:46:GLN:HG3	1	0.13
(1,402)	1:B:38:LYS:HD2	1:B:57:LYS:HE2	8	0.13
(1,402)	1:B:38:LYS:HD2	1:B:57:LYS:HE3	8	0.13
(1,402)	1:B:38:LYS:HD3	1:B:57:LYS:HE2	8	0.13
(1,402)	1:B:38:LYS:HD3	1:B:57:LYS:HE3	8	0.13
(1,402)	1:B:38:LYS:HD2	1:B:72:LYS:HE2	8	0.13
(1,402)	1:B:38:LYS:HD2	1:B:72:LYS:HE3	8	0.13
(1,402)	1:B:38:LYS:HD3	1:B:72:LYS:HE2	8	0.13
(1,402)	1:B:38:LYS:HD3	1:B:72:LYS:HE3	8	0.13
(1,402)	1:B:42:ARG:HB2	1:B:19:PHE:HB2	8	0.13
(1,402)	1:B:42:ARG:HB2	1:B:19:PHE:HB3	8	0.13
(1,402)	1:B:42:ARG:HB3	1:B:19:PHE:HB2	8	0.13
(1,402)	1:B:42:ARG:HB3	1:B:19:PHE:HB3	8	0.13
(1,402)	1:B:42:ARG:HB2	1:B:51:LYS:HE2	8	0.13
(1,402)	1:B:42:ARG:HB2	1:B:51:LYS:HE3	8	0.13
(1,402)	1:B:42:ARG:HB3	1:B:51:LYS:HE2	8	0.13
(1,402)	1:B:42:ARG:HB3	1:B:51:LYS:HE3	8	0.13
(1,402)	1:B:42:ARG:HB2	1:A:4:LYS:HE2	8	0.13
(1,402)	1:B:42:ARG:HB2	1:A:4:LYS:HE3	8	0.13
(1,402)	1:B:42:ARG:HB3	1:A:4:LYS:HE2	8	0.13
(1,402)	1:B:42:ARG:HB3	1:A:4:LYS:HE3	8	0.13
(1,402)	1:B:85:ARG:HB2	1:B:51:LYS:HE2	8	0.13
(1,402)	1:B:85:ARG:HB2	1:B:51:LYS:HE3	8	0.13
(1,402)	1:B:85:ARG:HB3	1:B:51:LYS:HE2	8	0.13
(1,402)	1:B:85:ARG:HB3	1:B:51:LYS:HE3	8	0.13
(1,402)	1:B:85:ARG:HB2	1:A:30:ASP:HB2	8	0.13
(1,402)	1:B:85:ARG:HB2	1:A:30:ASP:HB3	8	0.13
(1,402)	1:B:85:ARG:HB3	1:A:30:ASP:HB2	8	0.13
(1,402)	1:B:85:ARG:HB3	1:A:30:ASP:HB3	8	0.13
(1,402)	1:B:92:GLU:HB2	1:B:51:LYS:HE2	8	0.13
(1,402)	1:B:92:GLU:HB2	1:B:51:LYS:HE3	8	0.13
(1,402)	1:B:92:GLU:HB3	1:B:51:LYS:HE2	8	0.13
(1,402)	1:B:92:GLU:HB3	1:B:51:LYS:HE3	8	0.13
(1,402)	1:B:92:GLU:HB2	1:A:30:ASP:HB2	8	0.13
(1,402)	1:B:92:GLU:HB2	1:A:30:ASP:HB3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,402)	1:B:92:GLU:HB3	1:A:30:ASP:HB2	8	0.13
(1,402)	1:B:92:GLU:HB3	1:A:30:ASP:HB3	8	0.13
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	5	0.13
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	5	0.13
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	5	0.13
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	5	0.13
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	5	0.13
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	5	0.13
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	5	0.13
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	5	0.13
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	5	0.13
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	5	0.13
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	5	0.13
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	5	0.13
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	5	0.13
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	5	0.13
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	5	0.13
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	5	0.13
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD22	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD21	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD23	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD12	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD11	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD13	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD22	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD21	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD23	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD12	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD11	10	0.13
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD13	10	0.13
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD22	10	0.13
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD21	10	0.13
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD23	10	0.13
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD12	10	0.13
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD11	10	0.13
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD13	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD22	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD21	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD23	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD12	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD11	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD13	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD22	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD21	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD23	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD12	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD11	10	0.13
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD13	10	0.13
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD22	10	0.13
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD21	10	0.13
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD23	10	0.13
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD12	10	0.13
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD11	10	0.13
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD13	10	0.13
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG22	7	0.13
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG21	7	0.13
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG23	7	0.13
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG12	7	0.13
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG11	7	0.13
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG13	7	0.13
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD12	7	0.13
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD11	7	0.13
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD13	7	0.13
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG22	7	0.13
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG21	7	0.13
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG23	7	0.13
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG12	7	0.13
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG11	7	0.13
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG13	7	0.13
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD12	7	0.13
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD11	7	0.13
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD13	7	0.13
(1,1406)	1:B:20:HIS:H	1:A:8:LEU:HB2	7	0.13
(1,1406)	1:B:20:HIS:H	1:A:8:LEU:HB3	7	0.13
(1,1406)	1:B:20:HIS:H	1:B:25:LYS:HB2	7	0.13
(1,1406)	1:B:20:HIS:H	1:B:25:LYS:HB3	7	0.13
(1,1406)	1:B:20:HIS:H	1:B:32:LEU:HG	7	0.13
(1,1406)	1:B:20:HIS:H	1:B:36:GLU:HB2	7	0.13
(1,1406)	1:B:20:HIS:H	1:B:36:GLU:HB3	7	0.13
(1,1405)	1:A:20:HIS:H	1:B:8:LEU:HB2	7	0.13
(1,1405)	1:A:20:HIS:H	1:B:8:LEU:HB3	7	0.13
(1,1405)	1:A:20:HIS:H	1:A:25:LYS:HB2	7	0.13
(1,1405)	1:A:20:HIS:H	1:A:25:LYS:HB3	7	0.13
(1,1405)	1:A:20:HIS:H	1:A:32:LEU:HG	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1405)	1:A:20:HIS:H	1:A:36:GLU:HB2	7	0.13
(1,1405)	1:A:20:HIS:H	1:A:36:GLU:HB3	7	0.13
(1,1390)	1:B:5:MET:H	1:A:110:GLY:H	2	0.13
(1,1390)	1:B:12:ILE:H	1:B:19:PHE:H	2	0.13
(1,1390)	1:B:19:PHE:H	1:B:44:ASP:H	2	0.13
(1,1390)	1:B:19:PHE:H	1:A:12:ILE:H	2	0.13
(1,1390)	1:B:10:ARG:H	1:B:5:MET:H	2	0.13
(1,1389)	1:A:5:MET:H	1:B:110:GLY:H	7	0.13
(1,1389)	1:A:12:ILE:H	1:A:19:PHE:H	7	0.13
(1,1389)	1:A:19:PHE:H	1:A:44:ASP:H	7	0.13
(1,1389)	1:A:19:PHE:H	1:B:12:ILE:H	7	0.13
(1,1389)	1:A:10:ARG:H	1:A:5:MET:H	7	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD22	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD21	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD23	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD12	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD11	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD13	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD22	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD21	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD23	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD12	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD11	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD13	4	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD22	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD21	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD23	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD12	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD11	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD13	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD22	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD21	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD23	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD12	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD11	9	0.13
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD13	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD22	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD21	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD23	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD12	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD11	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD13	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD22	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD21	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD23	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD12	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD11	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD13	4	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD22	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD21	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD23	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD12	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD11	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD13	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD22	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD21	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD23	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD12	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD11	9	0.13
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD13	9	0.13
(1,1158)	1:B:20:HIS:H	1:B:32:LEU:HG	3	0.13
(1,1158)	1:B:21:GLN:H	1:B:32:LEU:HG	3	0.13
(1,1158)	1:B:32:LEU:HG	1:B:41:VAL:H	3	0.13
(1,1158)	1:B:20:HIS:H	1:B:32:LEU:HG	7	0.13
(1,1158)	1:B:21:GLN:H	1:B:32:LEU:HG	7	0.13
(1,1158)	1:B:32:LEU:HG	1:B:41:VAL:H	7	0.13
(1,1157)	1:A:20:HIS:H	1:A:32:LEU:HG	3	0.13
(1,1157)	1:A:21:GLN:H	1:A:32:LEU:HG	3	0.13
(1,1157)	1:A:32:LEU:HG	1:A:41:VAL:H	3	0.13
(1,1098)	1:B:59:ILE:HG22	1:B:42:ARG:HD2	4	0.13
(1,1098)	1:B:59:ILE:HG22	1:B:42:ARG:HD3	4	0.13
(1,1098)	1:B:59:ILE:HG21	1:B:42:ARG:HD2	4	0.13
(1,1098)	1:B:59:ILE:HG21	1:B:42:ARG:HD3	4	0.13
(1,1098)	1:B:59:ILE:HG23	1:B:42:ARG:HD2	4	0.13
(1,1098)	1:B:59:ILE:HG23	1:B:42:ARG:HD3	4	0.13
(1,1098)	1:B:59:ILE:HG22	1:B:79:PHE:HB2	4	0.13
(1,1098)	1:B:59:ILE:HG22	1:B:79:PHE:HB3	4	0.13
(1,1098)	1:B:59:ILE:HG21	1:B:79:PHE:HB2	4	0.13
(1,1098)	1:B:59:ILE:HG21	1:B:79:PHE:HB3	4	0.13
(1,1098)	1:B:59:ILE:HG23	1:B:79:PHE:HB2	4	0.13
(1,1098)	1:B:59:ILE:HG23	1:B:79:PHE:HB3	4	0.13
(1,1043)	1:A:53:ASN:HA	1:A:58:VAL:HB	2	0.13
(1,1043)	1:A:53:ASN:HA	1:A:60:GLU:HG2	2	0.13
(1,1043)	1:A:53:ASN:HA	1:A:60:GLU:HG3	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,61)	1:A:25:LYS:HA	1:A:21:GLN:HA	5	0.12
(4,232)	1:B:79:PHE:H	1:B:80:ILE:HB	7	0.12
(4,231)	1:A:79:PHE:H	1:A:80:ILE:HB	7	0.12
(4,111)	1:A:76:PHE:H	1:A:31:THR:H	4	0.12
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB2	3	0.12
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB3	3	0.12
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB2	8	0.12
(3,974)	1:B:5:MET:H	1:B:4:LYS:HB3	8	0.12
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB2	3	0.12
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB3	3	0.12
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB2	8	0.12
(3,973)	1:A:5:MET:H	1:A:4:LYS:HB3	8	0.12
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG21	1	0.12
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG22	1	0.12
(3,970)	1:B:7:GLN:H	1:A:14:THR:HG23	1	0.12
(3,872)	1:B:6:SER:H	1:B:5:MET:HG2	6	0.12
(3,872)	1:B:6:SER:H	1:B:5:MET:HG3	6	0.12
(3,865)	1:A:52:GLU:H	1:A:51:LYS:HG2	3	0.12
(3,865)	1:A:52:GLU:H	1:A:51:LYS:HG3	3	0.12
(3,864)	1:B:74:LEU:H	1:B:31:THR:HB	4	0.12
(3,863)	1:A:74:LEU:H	1:A:31:THR:HB	4	0.12
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG2	3	0.12
(3,84)	1:B:87:THR:HG21	1:B:92:GLU:HG3	3	0.12
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG2	3	0.12
(3,84)	1:B:87:THR:HG22	1:B:92:GLU:HG3	3	0.12
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG2	3	0.12
(3,84)	1:B:87:THR:HG23	1:B:92:GLU:HG3	3	0.12
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG2	3	0.12
(3,83)	1:A:87:THR:HG21	1:A:92:GLU:HG3	3	0.12
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG2	3	0.12
(3,83)	1:A:87:THR:HG22	1:A:92:GLU:HG3	3	0.12
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG2	3	0.12
(3,83)	1:A:87:THR:HG23	1:A:92:GLU:HG3	3	0.12
(3,794)	1:B:107:PRO:HG2	1:B:93:LYS:HG2	4	0.12
(3,794)	1:B:107:PRO:HG2	1:B:93:LYS:HG3	4	0.12
(3,794)	1:B:107:PRO:HG3	1:B:93:LYS:HG2	4	0.12
(3,794)	1:B:107:PRO:HG3	1:B:93:LYS:HG3	4	0.12
(3,793)	1:A:107:PRO:HG2	1:A:93:LYS:HG2	4	0.12
(3,793)	1:A:107:PRO:HG2	1:A:93:LYS:HG3	4	0.12
(3,793)	1:A:107:PRO:HG3	1:A:93:LYS:HG2	4	0.12
(3,793)	1:A:107:PRO:HG3	1:A:93:LYS:HG3	4	0.12
(3,79)	1:A:59:ILE:HB	1:A:38:LYS:HG2	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,79)	1:A:59:ILE:HB	1:A:38:LYS:HG3	7	0.12
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB2	9	0.12
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB3	9	0.12
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB2	9	0.12
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB3	9	0.12
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB2	9	0.12
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB3	9	0.12
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB2	9	0.12
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB3	9	0.12
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB2	9	0.12
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB3	9	0.12
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB2	9	0.12
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB3	9	0.12
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	7	0.12
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	7	0.12
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	7	0.12
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	7	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD22	10	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD21	10	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD23	10	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD12	10	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD11	10	0.12
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD13	10	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD22	10	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD21	10	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD23	10	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD12	10	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD11	10	0.12
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD13	10	0.12
(3,526)	1:B:76:PHE:HB2	1:B:16:ILE:HA	1	0.12
(3,526)	1:B:76:PHE:HB3	1:B:16:ILE:HA	1	0.12
(3,525)	1:A:76:PHE:HB2	1:A:16:ILE:HA	1	0.12
(3,525)	1:A:76:PHE:HB3	1:A:16:ILE:HA	1	0.12
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD22	4	0.12
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD21	4	0.12
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD23	4	0.12
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD12	4	0.12
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD11	4	0.12
(3,354)	1:B:47:ASN:HA	1:B:109:LEU:HD13	4	0.12
(3,345)	1:A:5:MET:H	1:A:4:LYS:HG2	1	0.12
(3,345)	1:A:5:MET:H	1:A:4:LYS:HG3	1	0.12
(3,34)	1:B:87:THR:HG21	1:B:88:TRP:HA	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,34)	1:B:87:THR:HG22	1:B:88:TRP:HA	6	0.12
(3,34)	1:B:87:THR:HG23	1:B:88:TRP:HA	6	0.12
(3,33)	1:A:87:THR:HG21	1:A:88:TRP:HA	6	0.12
(3,33)	1:A:87:THR:HG22	1:A:88:TRP:HA	6	0.12
(3,33)	1:A:87:THR:HG23	1:A:88:TRP:HA	6	0.12
(3,320)	1:B:51:LYS:HE2	1:B:51:LYS:H	4	0.12
(3,320)	1:B:51:LYS:HE3	1:B:51:LYS:H	4	0.12
(3,320)	1:B:51:LYS:HE2	1:B:51:LYS:H	10	0.12
(3,320)	1:B:51:LYS:HE3	1:B:51:LYS:H	10	0.12
(3,319)	1:A:51:LYS:HE2	1:A:51:LYS:H	4	0.12
(3,319)	1:A:51:LYS:HE3	1:A:51:LYS:H	4	0.12
(3,319)	1:A:51:LYS:HE2	1:A:51:LYS:H	10	0.12
(3,319)	1:A:51:LYS:HE3	1:A:51:LYS:H	10	0.12
(3,252)	1:B:33:ASN:HB2	1:B:72:LYS:HA	4	0.12
(3,252)	1:B:33:ASN:HB3	1:B:72:LYS:HA	4	0.12
(3,252)	1:B:33:ASN:HB2	1:B:72:LYS:HA	7	0.12
(3,252)	1:B:33:ASN:HB3	1:B:72:LYS:HA	7	0.12
(3,251)	1:A:33:ASN:HB2	1:A:72:LYS:HA	7	0.12
(3,251)	1:A:33:ASN:HB3	1:A:72:LYS:HA	7	0.12
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA2	4	0.12
(3,1466)	1:B:110:GLY:H	1:B:108:GLY:HA3	4	0.12
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA2	4	0.12
(3,1465)	1:A:110:GLY:H	1:A:108:GLY:HA3	4	0.12
(3,140)	1:B:41:VAL:HB	1:B:59:ILE:HG22	6	0.12
(3,140)	1:B:41:VAL:HB	1:B:59:ILE:HG21	6	0.12
(3,140)	1:B:41:VAL:HB	1:B:59:ILE:HG23	6	0.12
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG2	10	0.12
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG3	10	0.12
(3,139)	1:A:41:VAL:HB	1:A:59:ILE:HG22	6	0.12
(3,139)	1:A:41:VAL:HB	1:A:59:ILE:HG21	6	0.12
(3,139)	1:A:41:VAL:HB	1:A:59:ILE:HG23	6	0.12
(3,1364)	1:B:69:ASN:H	1:B:68:THR:HB	2	0.12
(3,1363)	1:A:69:ASN:H	1:A:68:THR:HB	2	0.12
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG2	5	0.12
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG3	5	0.12
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG2	10	0.12
(3,13)	1:A:111:GLU:HA	1:A:111:GLU:HG3	10	0.12
(3,1160)	1:B:82:LEU:H	1:B:84:ALA:H	6	0.12
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	6	0.12
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB2	1	0.12
(3,1147)	1:A:35:GLY:H	1:A:32:LEU:HB3	1	0.12
(2,84)	1:A:93:LYS:H	1:A:89:ALA:O	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,63)	1:A:82:LEU:N	1:A:78:GLU:O	1	0.12
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	4	0.12
(2,26)	1:A:22:TYR:H	1:A:18:THR:O	8	0.12
(2,21)	1:A:20:HIS:N	1:A:16:ILE:O	2	0.12
(2,2)	1:A:32:LEU:N	1:A:74:LEU:O	5	0.12
(1,917)	1:A:87:THR:HA	1:A:92:GLU:HG2	3	0.12
(1,917)	1:A:87:THR:HA	1:A:92:GLU:HG3	3	0.12
(1,917)	1:A:87:THR:HA	1:B:9:GLU:HB2	3	0.12
(1,917)	1:A:87:THR:HA	1:B:9:GLU:HB3	3	0.12
(1,917)	1:A:87:THR:HA	1:B:12:ILE:HB	3	0.12
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB2	2	0.12
(1,80)	1:B:59:ILE:HB	1:B:37:PHE:HB3	2	0.12
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE2	2	0.12
(1,80)	1:B:59:ILE:HB	1:B:57:LYS:HE3	2	0.12
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB2	2	0.12
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB3	2	0.12
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG2	2	0.12
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG3	2	0.12
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB2	2	0.12
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB3	2	0.12
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG2	2	0.12
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG3	2	0.12
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB2	2	0.12
(1,79)	1:A:59:ILE:HB	1:A:37:PHE:HB3	2	0.12
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE2	2	0.12
(1,79)	1:A:59:ILE:HB	1:A:57:LYS:HE3	2	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD12	1	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD11	1	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD13	1	0.12
(1,772)	1:B:59:ILE:HD12	1:B:62:ILE:HA	1	0.12
(1,772)	1:B:59:ILE:HD11	1:B:62:ILE:HA	1	0.12
(1,772)	1:B:59:ILE:HD13	1:B:62:ILE:HA	1	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD12	9	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD11	9	0.12
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD13	9	0.12
(1,772)	1:B:59:ILE:HD12	1:B:62:ILE:HA	9	0.12
(1,772)	1:B:59:ILE:HD11	1:B:62:ILE:HA	9	0.12
(1,772)	1:B:59:ILE:HD13	1:B:62:ILE:HA	9	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD12	1	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD11	1	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD13	1	0.12
(1,771)	1:A:59:ILE:HD12	1:A:62:ILE:HA	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,771)	1:A:59:ILE:HD11	1:A:62:ILE:HA	1	0.12
(1,771)	1:A:59:ILE:HD13	1:A:62:ILE:HA	1	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD12	9	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD11	9	0.12
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD13	9	0.12
(1,771)	1:A:59:ILE:HD12	1:A:62:ILE:HA	9	0.12
(1,771)	1:A:59:ILE:HD11	1:A:62:ILE:HA	9	0.12
(1,771)	1:A:59:ILE:HD13	1:A:62:ILE:HA	9	0.12
(1,71)	1:A:33:ASN:HB2	1:A:73:GLN:HG2	4	0.12
(1,71)	1:A:33:ASN:HB2	1:A:73:GLN:HG3	4	0.12
(1,71)	1:A:33:ASN:HB3	1:A:73:GLN:HG2	4	0.12
(1,71)	1:A:33:ASN:HB3	1:A:73:GLN:HG3	4	0.12
(1,71)	1:A:48:PHE:HB2	1:B:9:GLU:HB2	4	0.12
(1,71)	1:A:48:PHE:HB2	1:B:9:GLU:HB3	4	0.12
(1,71)	1:A:48:PHE:HB3	1:B:9:GLU:HB2	4	0.12
(1,71)	1:A:48:PHE:HB3	1:B:9:GLU:HB3	4	0.12
(1,652)	1:B:93:LYS:H	1:B:92:GLU:HB2	5	0.12
(1,652)	1:B:93:LYS:H	1:B:92:GLU:HB3	5	0.12
(1,652)	1:B:100:GLY:H	1:B:99:GLU:HB2	5	0.12
(1,652)	1:B:100:GLY:H	1:B:99:GLU:HB3	5	0.12
(1,651)	1:A:93:LYS:H	1:A:92:GLU:HB2	5	0.12
(1,651)	1:A:93:LYS:H	1:A:92:GLU:HB3	5	0.12
(1,651)	1:A:100:GLY:H	1:A:99:GLU:HB2	5	0.12
(1,651)	1:A:100:GLY:H	1:A:99:GLU:HB3	5	0.12
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	6	0.12
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	6	0.12
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	6	0.12
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	6	0.12
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	6	0.12
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	6	0.12
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	6	0.12
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	6	0.12
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	6	0.12
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	6	0.12
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	6	0.12
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	6	0.12
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG2	10	0.12
(1,590)	1:B:85:ARG:HG2	1:B:78:GLU:HG3	10	0.12
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG2	10	0.12
(1,590)	1:B:85:ARG:HG3	1:B:78:GLU:HG3	10	0.12
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG2	10	0.12
(1,590)	1:B:85:ARG:HG2	1:B:83:MET:HG3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG2	10	0.12
(1,590)	1:B:85:ARG:HG3	1:B:83:MET:HG3	10	0.12
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG2	10	0.12
(1,590)	1:B:85:ARG:HG2	1:A:78:GLU:HG3	10	0.12
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG2	10	0.12
(1,590)	1:B:85:ARG:HG3	1:A:78:GLU:HG3	10	0.12
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG2	10	0.12
(1,589)	1:A:85:ARG:HG2	1:A:78:GLU:HG3	10	0.12
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG2	10	0.12
(1,589)	1:A:85:ARG:HG3	1:A:78:GLU:HG3	10	0.12
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG2	10	0.12
(1,589)	1:A:85:ARG:HG2	1:A:83:MET:HG3	10	0.12
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG2	10	0.12
(1,589)	1:A:85:ARG:HG3	1:A:83:MET:HG3	10	0.12
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG2	10	0.12
(1,589)	1:A:85:ARG:HG2	1:B:78:GLU:HG3	10	0.12
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG2	10	0.12
(1,589)	1:A:85:ARG:HG3	1:B:78:GLU:HG3	10	0.12
(1,568)	1:B:42:ARG:HA	1:B:43:LYS:HE2	5	0.12
(1,568)	1:B:42:ARG:HA	1:B:43:LYS:HE3	5	0.12
(1,568)	1:B:42:ARG:HA	1:B:50:LYS:HE2	5	0.12
(1,568)	1:B:42:ARG:HA	1:B:50:LYS:HE3	5	0.12
(1,568)	1:B:42:ARG:HA	1:B:54:LYS:HE2	5	0.12
(1,568)	1:B:42:ARG:HA	1:B:54:LYS:HE3	5	0.12
(1,567)	1:A:42:ARG:HA	1:A:43:LYS:HE2	5	0.12
(1,567)	1:A:42:ARG:HA	1:A:43:LYS:HE3	5	0.12
(1,567)	1:A:42:ARG:HA	1:A:50:LYS:HE2	5	0.12
(1,567)	1:A:42:ARG:HA	1:A:50:LYS:HE3	5	0.12
(1,567)	1:A:42:ARG:HA	1:A:54:LYS:HE2	5	0.12
(1,567)	1:A:42:ARG:HA	1:A:54:LYS:HE3	5	0.12
(1,567)	1:A:42:ARG:HA	1:A:43:LYS:HE2	8	0.12
(1,567)	1:A:42:ARG:HA	1:A:43:LYS:HE3	8	0.12
(1,567)	1:A:42:ARG:HA	1:A:50:LYS:HE2	8	0.12
(1,567)	1:A:42:ARG:HA	1:A:50:LYS:HE3	8	0.12
(1,567)	1:A:42:ARG:HA	1:A:54:LYS:HE2	8	0.12
(1,567)	1:A:42:ARG:HA	1:A:54:LYS:HE3	8	0.12
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB2	2	0.12
(1,478)	1:B:11:ASN:HB2	1:B:8:LEU:HB3	2	0.12
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB2	2	0.12
(1,478)	1:B:11:ASN:HB3	1:B:8:LEU:HB3	2	0.12
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB2	2	0.12
(1,478)	1:B:11:ASN:HB2	1:B:10:ARG:HB3	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB2	2	0.12
(1,478)	1:B:11:ASN:HB3	1:B:10:ARG:HB3	2	0.12
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB2	2	0.12
(1,478)	1:B:37:PHE:HB2	1:B:36:GLU:HB3	2	0.12
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB2	2	0.12
(1,478)	1:B:37:PHE:HB3	1:B:36:GLU:HB3	2	0.12
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB2	2	0.12
(1,478)	1:B:63:MET:HB2	1:B:37:PHE:HB3	2	0.12
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB2	2	0.12
(1,478)	1:B:63:MET:HB3	1:B:37:PHE:HB3	2	0.12
(1,478)	1:B:37:PHE:HB2	1:B:74:LEU:HG	2	0.12
(1,478)	1:B:37:PHE:HB3	1:B:74:LEU:HG	2	0.12
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB2	2	0.12
(1,478)	1:B:32:LEU:HG	1:B:79:PHE:HB3	2	0.12
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB2	2	0.12
(1,477)	1:A:11:ASN:HB2	1:A:8:LEU:HB3	2	0.12
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB2	2	0.12
(1,477)	1:A:11:ASN:HB3	1:A:8:LEU:HB3	2	0.12
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB2	2	0.12
(1,477)	1:A:11:ASN:HB2	1:A:10:ARG:HB3	2	0.12
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB2	2	0.12
(1,477)	1:A:11:ASN:HB3	1:A:10:ARG:HB3	2	0.12
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB2	2	0.12
(1,477)	1:A:37:PHE:HB2	1:A:36:GLU:HB3	2	0.12
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB2	2	0.12
(1,477)	1:A:37:PHE:HB3	1:A:36:GLU:HB3	2	0.12
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB2	2	0.12
(1,477)	1:A:63:MET:HB2	1:A:37:PHE:HB3	2	0.12
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB2	2	0.12
(1,477)	1:A:63:MET:HB3	1:A:37:PHE:HB3	2	0.12
(1,477)	1:A:37:PHE:HB2	1:A:74:LEU:HG	2	0.12
(1,477)	1:A:37:PHE:HB3	1:A:74:LEU:HG	2	0.12
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB2	2	0.12
(1,477)	1:A:32:LEU:HG	1:A:79:PHE:HB3	2	0.12
(1,464)	1:B:11:ASN:HB2	1:B:5:MET:HG2	8	0.12
(1,464)	1:B:11:ASN:HB2	1:B:5:MET:HG3	8	0.12
(1,464)	1:B:11:ASN:HB3	1:B:5:MET:HG2	8	0.12
(1,464)	1:B:11:ASN:HB3	1:B:5:MET:HG3	8	0.12
(1,464)	1:B:79:PHE:HB2	1:B:22:TYR:HB2	8	0.12
(1,464)	1:B:79:PHE:HB2	1:B:22:TYR:HB3	8	0.12
(1,464)	1:B:79:PHE:HB3	1:B:22:TYR:HB2	8	0.12
(1,464)	1:B:79:PHE:HB3	1:B:22:TYR:HB3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,464)	1:B:79:PHE:HB2	1:B:67:ASP:HB2	8	0.12
(1,464)	1:B:79:PHE:HB2	1:B:67:ASP:HB3	8	0.12
(1,464)	1:B:79:PHE:HB3	1:B:67:ASP:HB2	8	0.12
(1,464)	1:B:79:PHE:HB3	1:B:67:ASP:HB3	8	0.12
(1,464)	1:B:79:PHE:HB2	1:B:81:MET:HG2	8	0.12
(1,464)	1:B:79:PHE:HB2	1:B:81:MET:HG3	8	0.12
(1,464)	1:B:79:PHE:HB3	1:B:81:MET:HG2	8	0.12
(1,464)	1:B:79:PHE:HB3	1:B:81:MET:HG3	8	0.12
(1,463)	1:A:11:ASN:HB2	1:A:5:MET:HG2	8	0.12
(1,463)	1:A:11:ASN:HB2	1:A:5:MET:HG3	8	0.12
(1,463)	1:A:11:ASN:HB3	1:A:5:MET:HG2	8	0.12
(1,463)	1:A:11:ASN:HB3	1:A:5:MET:HG3	8	0.12
(1,463)	1:A:79:PHE:HB2	1:A:22:TYR:HB2	8	0.12
(1,463)	1:A:79:PHE:HB2	1:A:22:TYR:HB3	8	0.12
(1,463)	1:A:79:PHE:HB3	1:A:22:TYR:HB2	8	0.12
(1,463)	1:A:79:PHE:HB3	1:A:22:TYR:HB3	8	0.12
(1,463)	1:A:79:PHE:HB2	1:A:67:ASP:HB2	8	0.12
(1,463)	1:A:79:PHE:HB2	1:A:67:ASP:HB3	8	0.12
(1,463)	1:A:79:PHE:HB3	1:A:67:ASP:HB2	8	0.12
(1,463)	1:A:79:PHE:HB3	1:A:67:ASP:HB3	8	0.12
(1,463)	1:A:79:PHE:HB2	1:A:81:MET:HG2	8	0.12
(1,463)	1:A:79:PHE:HB2	1:A:81:MET:HG3	8	0.12
(1,463)	1:A:79:PHE:HB3	1:A:81:MET:HG2	8	0.12
(1,463)	1:A:79:PHE:HB3	1:A:81:MET:HG3	8	0.12
(1,414)	1:B:38:LYS:HD2	1:B:59:ILE:HG22	7	0.12
(1,414)	1:B:38:LYS:HD2	1:B:59:ILE:HG21	7	0.12
(1,414)	1:B:38:LYS:HD2	1:B:59:ILE:HG23	7	0.12
(1,414)	1:B:38:LYS:HD3	1:B:59:ILE:HG22	7	0.12
(1,414)	1:B:38:LYS:HD3	1:B:59:ILE:HG21	7	0.12
(1,414)	1:B:38:LYS:HD3	1:B:59:ILE:HG23	7	0.12
(1,414)	1:B:63:MET:HB2	1:B:59:ILE:HG22	7	0.12
(1,414)	1:B:63:MET:HB2	1:B:59:ILE:HG21	7	0.12
(1,414)	1:B:63:MET:HB2	1:B:59:ILE:HG23	7	0.12
(1,414)	1:B:63:MET:HB3	1:B:59:ILE:HG22	7	0.12
(1,414)	1:B:63:MET:HB3	1:B:59:ILE:HG21	7	0.12
(1,414)	1:B:63:MET:HB3	1:B:59:ILE:HG23	7	0.12
(1,414)	1:B:85:ARG:HB2	1:B:62:ILE:HG22	7	0.12
(1,414)	1:B:85:ARG:HB2	1:B:62:ILE:HG21	7	0.12
(1,414)	1:B:85:ARG:HB2	1:B:62:ILE:HG23	7	0.12
(1,414)	1:B:85:ARG:HB3	1:B:62:ILE:HG22	7	0.12
(1,414)	1:B:85:ARG:HB3	1:B:62:ILE:HG21	7	0.12
(1,414)	1:B:85:ARG:HB3	1:B:62:ILE:HG23	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,413)	1:A:38:LYS:HD2	1:A:59:ILE:HG22	7	0.12
(1,413)	1:A:38:LYS:HD2	1:A:59:ILE:HG21	7	0.12
(1,413)	1:A:38:LYS:HD2	1:A:59:ILE:HG23	7	0.12
(1,413)	1:A:38:LYS:HD3	1:A:59:ILE:HG22	7	0.12
(1,413)	1:A:38:LYS:HD3	1:A:59:ILE:HG21	7	0.12
(1,413)	1:A:38:LYS:HD3	1:A:59:ILE:HG23	7	0.12
(1,413)	1:A:63:MET:HB2	1:A:59:ILE:HG22	7	0.12
(1,413)	1:A:63:MET:HB2	1:A:59:ILE:HG21	7	0.12
(1,413)	1:A:63:MET:HB2	1:A:59:ILE:HG23	7	0.12
(1,413)	1:A:63:MET:HB3	1:A:59:ILE:HG22	7	0.12
(1,413)	1:A:63:MET:HB3	1:A:59:ILE:HG21	7	0.12
(1,413)	1:A:63:MET:HB3	1:A:59:ILE:HG23	7	0.12
(1,413)	1:A:85:ARG:HB2	1:A:62:ILE:HG22	7	0.12
(1,413)	1:A:85:ARG:HB2	1:A:62:ILE:HG21	7	0.12
(1,413)	1:A:85:ARG:HB2	1:A:62:ILE:HG23	7	0.12
(1,413)	1:A:85:ARG:HB3	1:A:62:ILE:HG22	7	0.12
(1,413)	1:A:85:ARG:HB3	1:A:62:ILE:HG21	7	0.12
(1,413)	1:A:85:ARG:HB3	1:A:62:ILE:HG23	7	0.12
(1,401)	1:A:38:LYS:HD2	1:A:57:LYS:HE2	8	0.12
(1,401)	1:A:38:LYS:HD2	1:A:57:LYS:HE3	8	0.12
(1,401)	1:A:38:LYS:HD3	1:A:57:LYS:HE2	8	0.12
(1,401)	1:A:38:LYS:HD3	1:A:57:LYS:HE3	8	0.12
(1,401)	1:A:38:LYS:HD2	1:A:72:LYS:HE2	8	0.12
(1,401)	1:A:38:LYS:HD2	1:A:72:LYS:HE3	8	0.12
(1,401)	1:A:38:LYS:HD3	1:A:72:LYS:HE2	8	0.12
(1,401)	1:A:38:LYS:HD3	1:A:72:LYS:HE3	8	0.12
(1,401)	1:A:42:ARG:HB2	1:A:19:PHE:HB2	8	0.12
(1,401)	1:A:42:ARG:HB2	1:A:19:PHE:HB3	8	0.12
(1,401)	1:A:42:ARG:HB3	1:A:19:PHE:HB2	8	0.12
(1,401)	1:A:42:ARG:HB3	1:A:19:PHE:HB3	8	0.12
(1,401)	1:A:42:ARG:HB2	1:A:51:LYS:HE2	8	0.12
(1,401)	1:A:42:ARG:HB2	1:A:51:LYS:HE3	8	0.12
(1,401)	1:A:42:ARG:HB3	1:A:51:LYS:HE2	8	0.12
(1,401)	1:A:42:ARG:HB3	1:A:51:LYS:HE3	8	0.12
(1,401)	1:A:42:ARG:HB2	1:B:4:LYS:HE2	8	0.12
(1,401)	1:A:42:ARG:HB2	1:B:4:LYS:HE3	8	0.12
(1,401)	1:A:42:ARG:HB3	1:B:4:LYS:HE2	8	0.12
(1,401)	1:A:42:ARG:HB3	1:B:4:LYS:HE3	8	0.12
(1,401)	1:A:85:ARG:HB2	1:A:51:LYS:HE2	8	0.12
(1,401)	1:A:85:ARG:HB2	1:A:51:LYS:HE3	8	0.12
(1,401)	1:A:85:ARG:HB3	1:A:51:LYS:HE2	8	0.12
(1,401)	1:A:85:ARG:HB3	1:A:51:LYS:HE3	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:A:85:ARG:HB2	1:B:30:ASP:HB2	8	0.12
(1,401)	1:A:85:ARG:HB2	1:B:30:ASP:HB3	8	0.12
(1,401)	1:A:85:ARG:HB3	1:B:30:ASP:HB2	8	0.12
(1,401)	1:A:85:ARG:HB3	1:B:30:ASP:HB3	8	0.12
(1,401)	1:A:92:GLU:HB2	1:A:51:LYS:HE2	8	0.12
(1,401)	1:A:92:GLU:HB2	1:A:51:LYS:HE3	8	0.12
(1,401)	1:A:92:GLU:HB3	1:A:51:LYS:HE2	8	0.12
(1,401)	1:A:92:GLU:HB3	1:A:51:LYS:HE3	8	0.12
(1,401)	1:A:92:GLU:HB2	1:B:30:ASP:HB2	8	0.12
(1,401)	1:A:92:GLU:HB2	1:B:30:ASP:HB3	8	0.12
(1,401)	1:A:92:GLU:HB3	1:B:30:ASP:HB2	8	0.12
(1,401)	1:A:92:GLU:HB3	1:B:30:ASP:HB3	8	0.12
(1,320)	1:B:41:VAL:HG22	1:B:49:LEU:HD22	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:49:LEU:HD21	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:49:LEU:HD23	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:49:LEU:HD12	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:49:LEU:HD11	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:49:LEU:HD13	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:49:LEU:HD22	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:49:LEU:HD21	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:49:LEU:HD23	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:49:LEU:HD12	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:49:LEU:HD11	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:49:LEU:HD13	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:49:LEU:HD22	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:49:LEU:HD21	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:49:LEU:HD23	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:49:LEU:HD12	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:49:LEU:HD11	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:49:LEU:HD13	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:49:LEU:HD22	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:49:LEU:HD21	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:49:LEU:HD23	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:49:LEU:HD12	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:49:LEU:HD11	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:49:LEU:HD13	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:49:LEU:HD22	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:49:LEU:HD21	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:49:LEU:HD23	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:49:LEU:HD12	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:49:LEU:HD11	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:49:LEU:HD13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:B:41:VAL:HG13	1:B:49:LEU:HD22	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:49:LEU:HD21	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:49:LEU:HD23	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:49:LEU:HD12	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:49:LEU:HD11	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:49:LEU:HD13	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:59:ILE:HD12	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:59:ILE:HD11	6	0.12
(1,320)	1:B:41:VAL:HG22	1:B:59:ILE:HD13	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:59:ILE:HD12	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:59:ILE:HD11	6	0.12
(1,320)	1:B:41:VAL:HG21	1:B:59:ILE:HD13	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:59:ILE:HD12	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:59:ILE:HD11	6	0.12
(1,320)	1:B:41:VAL:HG23	1:B:59:ILE:HD13	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:59:ILE:HD12	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:59:ILE:HD11	6	0.12
(1,320)	1:B:41:VAL:HG12	1:B:59:ILE:HD13	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:59:ILE:HD12	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:59:ILE:HD11	6	0.12
(1,320)	1:B:41:VAL:HG11	1:B:59:ILE:HD13	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:59:ILE:HD12	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:59:ILE:HD11	6	0.12
(1,320)	1:B:41:VAL:HG13	1:B:59:ILE:HD13	6	0.12
(1,320)	1:B:66:LEU:HD22	1:B:82:LEU:HD22	6	0.12
(1,320)	1:B:66:LEU:HD22	1:B:82:LEU:HD21	6	0.12
(1,320)	1:B:66:LEU:HD22	1:B:82:LEU:HD23	6	0.12
(1,320)	1:B:66:LEU:HD22	1:B:82:LEU:HD12	6	0.12
(1,320)	1:B:66:LEU:HD22	1:B:82:LEU:HD11	6	0.12
(1,320)	1:B:66:LEU:HD22	1:B:82:LEU:HD13	6	0.12
(1,320)	1:B:66:LEU:HD21	1:B:82:LEU:HD22	6	0.12
(1,320)	1:B:66:LEU:HD21	1:B:82:LEU:HD21	6	0.12
(1,320)	1:B:66:LEU:HD21	1:B:82:LEU:HD23	6	0.12
(1,320)	1:B:66:LEU:HD21	1:B:82:LEU:HD12	6	0.12
(1,320)	1:B:66:LEU:HD21	1:B:82:LEU:HD11	6	0.12
(1,320)	1:B:66:LEU:HD21	1:B:82:LEU:HD13	6	0.12
(1,320)	1:B:66:LEU:HD23	1:B:82:LEU:HD22	6	0.12
(1,320)	1:B:66:LEU:HD23	1:B:82:LEU:HD21	6	0.12
(1,320)	1:B:66:LEU:HD23	1:B:82:LEU:HD23	6	0.12
(1,320)	1:B:66:LEU:HD23	1:B:82:LEU:HD12	6	0.12
(1,320)	1:B:66:LEU:HD23	1:B:82:LEU:HD11	6	0.12
(1,320)	1:B:66:LEU:HD23	1:B:82:LEU:HD13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,320)	1:B:66:LEU:HD12	1:B:82:LEU:HD22	6	0.12
(1,320)	1:B:66:LEU:HD12	1:B:82:LEU:HD21	6	0.12
(1,320)	1:B:66:LEU:HD12	1:B:82:LEU:HD23	6	0.12
(1,320)	1:B:66:LEU:HD12	1:B:82:LEU:HD12	6	0.12
(1,320)	1:B:66:LEU:HD12	1:B:82:LEU:HD11	6	0.12
(1,320)	1:B:66:LEU:HD12	1:B:82:LEU:HD13	6	0.12
(1,320)	1:B:66:LEU:HD11	1:B:82:LEU:HD22	6	0.12
(1,320)	1:B:66:LEU:HD11	1:B:82:LEU:HD21	6	0.12
(1,320)	1:B:66:LEU:HD11	1:B:82:LEU:HD23	6	0.12
(1,320)	1:B:66:LEU:HD11	1:B:82:LEU:HD12	6	0.12
(1,320)	1:B:66:LEU:HD11	1:B:82:LEU:HD11	6	0.12
(1,320)	1:B:66:LEU:HD11	1:B:82:LEU:HD13	6	0.12
(1,320)	1:B:66:LEU:HD13	1:B:82:LEU:HD22	6	0.12
(1,320)	1:B:66:LEU:HD13	1:B:82:LEU:HD21	6	0.12
(1,320)	1:B:66:LEU:HD13	1:B:82:LEU:HD23	6	0.12
(1,320)	1:B:66:LEU:HD13	1:B:82:LEU:HD12	6	0.12
(1,320)	1:B:66:LEU:HD13	1:B:82:LEU:HD11	6	0.12
(1,320)	1:B:66:LEU:HD13	1:B:82:LEU:HD13	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:49:LEU:HD22	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:49:LEU:HD21	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:49:LEU:HD23	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:49:LEU:HD12	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:49:LEU:HD11	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:49:LEU:HD13	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:49:LEU:HD22	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:49:LEU:HD21	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:49:LEU:HD23	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:49:LEU:HD12	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:49:LEU:HD11	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:49:LEU:HD13	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:49:LEU:HD22	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:49:LEU:HD21	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:49:LEU:HD23	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:49:LEU:HD12	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:49:LEU:HD11	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:49:LEU:HD13	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:49:LEU:HD22	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:49:LEU:HD21	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:49:LEU:HD23	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:49:LEU:HD12	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:49:LEU:HD11	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:49:LEU:HD13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:A:41:VAL:HG11	1:A:49:LEU:HD22	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:49:LEU:HD21	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:49:LEU:HD23	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:49:LEU:HD12	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:49:LEU:HD11	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:49:LEU:HD13	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:49:LEU:HD22	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:49:LEU:HD21	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:49:LEU:HD23	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:49:LEU:HD12	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:49:LEU:HD11	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:49:LEU:HD13	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:59:ILE:HD12	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:59:ILE:HD11	6	0.12
(1,319)	1:A:41:VAL:HG22	1:A:59:ILE:HD13	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:59:ILE:HD12	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:59:ILE:HD11	6	0.12
(1,319)	1:A:41:VAL:HG21	1:A:59:ILE:HD13	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:59:ILE:HD12	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:59:ILE:HD11	6	0.12
(1,319)	1:A:41:VAL:HG23	1:A:59:ILE:HD13	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:59:ILE:HD12	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:59:ILE:HD11	6	0.12
(1,319)	1:A:41:VAL:HG12	1:A:59:ILE:HD13	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:59:ILE:HD12	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:59:ILE:HD11	6	0.12
(1,319)	1:A:41:VAL:HG11	1:A:59:ILE:HD13	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:59:ILE:HD12	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:59:ILE:HD11	6	0.12
(1,319)	1:A:41:VAL:HG13	1:A:59:ILE:HD13	6	0.12
(1,319)	1:A:66:LEU:HD22	1:A:82:LEU:HD22	6	0.12
(1,319)	1:A:66:LEU:HD22	1:A:82:LEU:HD21	6	0.12
(1,319)	1:A:66:LEU:HD22	1:A:82:LEU:HD23	6	0.12
(1,319)	1:A:66:LEU:HD22	1:A:82:LEU:HD12	6	0.12
(1,319)	1:A:66:LEU:HD22	1:A:82:LEU:HD11	6	0.12
(1,319)	1:A:66:LEU:HD22	1:A:82:LEU:HD13	6	0.12
(1,319)	1:A:66:LEU:HD21	1:A:82:LEU:HD22	6	0.12
(1,319)	1:A:66:LEU:HD21	1:A:82:LEU:HD21	6	0.12
(1,319)	1:A:66:LEU:HD21	1:A:82:LEU:HD23	6	0.12
(1,319)	1:A:66:LEU:HD21	1:A:82:LEU:HD12	6	0.12
(1,319)	1:A:66:LEU:HD21	1:A:82:LEU:HD11	6	0.12
(1,319)	1:A:66:LEU:HD21	1:A:82:LEU:HD13	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:A:66:LEU:HD23	1:A:82:LEU:HD22	6	0.12
(1,319)	1:A:66:LEU:HD23	1:A:82:LEU:HD21	6	0.12
(1,319)	1:A:66:LEU:HD23	1:A:82:LEU:HD23	6	0.12
(1,319)	1:A:66:LEU:HD23	1:A:82:LEU:HD12	6	0.12
(1,319)	1:A:66:LEU:HD23	1:A:82:LEU:HD11	6	0.12
(1,319)	1:A:66:LEU:HD23	1:A:82:LEU:HD13	6	0.12
(1,319)	1:A:66:LEU:HD12	1:A:82:LEU:HD22	6	0.12
(1,319)	1:A:66:LEU:HD12	1:A:82:LEU:HD21	6	0.12
(1,319)	1:A:66:LEU:HD12	1:A:82:LEU:HD23	6	0.12
(1,319)	1:A:66:LEU:HD12	1:A:82:LEU:HD12	6	0.12
(1,319)	1:A:66:LEU:HD12	1:A:82:LEU:HD11	6	0.12
(1,319)	1:A:66:LEU:HD12	1:A:82:LEU:HD13	6	0.12
(1,319)	1:A:66:LEU:HD11	1:A:82:LEU:HD22	6	0.12
(1,319)	1:A:66:LEU:HD11	1:A:82:LEU:HD21	6	0.12
(1,319)	1:A:66:LEU:HD11	1:A:82:LEU:HD23	6	0.12
(1,319)	1:A:66:LEU:HD11	1:A:82:LEU:HD12	6	0.12
(1,319)	1:A:66:LEU:HD11	1:A:82:LEU:HD11	6	0.12
(1,319)	1:A:66:LEU:HD11	1:A:82:LEU:HD13	6	0.12
(1,319)	1:A:66:LEU:HD13	1:A:82:LEU:HD22	6	0.12
(1,319)	1:A:66:LEU:HD13	1:A:82:LEU:HD21	6	0.12
(1,319)	1:A:66:LEU:HD13	1:A:82:LEU:HD23	6	0.12
(1,319)	1:A:66:LEU:HD13	1:A:82:LEU:HD12	6	0.12
(1,319)	1:A:66:LEU:HD13	1:A:82:LEU:HD11	6	0.12
(1,319)	1:A:66:LEU:HD13	1:A:82:LEU:HD13	6	0.12
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	1	0.12
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	1	0.12
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	1	0.12
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	1	0.12
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	1	0.12
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	1	0.12
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	1	0.12
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	1	0.12
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD2	6	0.12
(1,24)	1:B:93:LYS:HA	1:B:107:PRO:HD3	6	0.12
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD2	6	0.12
(1,24)	1:B:96:GLU:HA	1:B:107:PRO:HD3	6	0.12
(1,24)	1:B:65:ASP:HA	1:B:72:LYS:HA	6	0.12
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD2	6	0.12
(1,23)	1:A:93:LYS:HA	1:A:107:PRO:HD3	6	0.12
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD2	6	0.12
(1,23)	1:A:96:GLU:HA	1:A:107:PRO:HD3	6	0.12
(1,23)	1:A:65:ASP:HA	1:A:72:LYS:HA	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,20)	1:B:65:ASP:HA	1:B:74:LEU:HB2	6	0.12
(1,20)	1:B:65:ASP:HA	1:B:74:LEU:HB3	6	0.12
(1,20)	1:B:65:ASP:HA	1:B:82:LEU:HB2	6	0.12
(1,20)	1:B:65:ASP:HA	1:B:82:LEU:HB3	6	0.12
(1,20)	1:B:92:GLU:HA	1:B:86:LEU:HB2	6	0.12
(1,20)	1:B:92:GLU:HA	1:B:86:LEU:HB3	6	0.12
(1,20)	1:B:92:GLU:HA	1:B:109:LEU:HG	6	0.12
(1,20)	1:B:93:LYS:HA	1:B:51:LYS:HG2	6	0.12
(1,20)	1:B:93:LYS:HA	1:B:51:LYS:HG3	6	0.12
(1,20)	1:B:93:LYS:HA	1:B:109:LEU:HG	6	0.12
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB2	6	0.12
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB3	6	0.12
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB2	6	0.12
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB3	6	0.12
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB2	6	0.12
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB3	6	0.12
(1,19)	1:A:92:GLU:HA	1:A:109:LEU:HG	6	0.12
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG2	6	0.12
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG3	6	0.12
(1,19)	1:A:93:LYS:HA	1:A:109:LEU:HG	6	0.12
(1,1692)	1:B:62:ILE:H	1:B:59:ILE:H	6	0.12
(1,1692)	1:B:67:ASP:H	1:B:68:THR:H	6	0.12
(1,1691)	1:A:62:ILE:H	1:A:59:ILE:H	6	0.12
(1,1691)	1:A:67:ASP:H	1:A:68:THR:H	6	0.12
(1,1590)	1:B:10:ARG:H	1:B:12:ILE:HA	6	0.12
(1,1590)	1:B:51:LYS:H	1:B:46:GLN:HA	6	0.12
(1,1590)	1:B:10:ARG:H	1:B:12:ILE:HA	8	0.12
(1,1590)	1:B:51:LYS:H	1:B:46:GLN:HA	8	0.12
(1,1589)	1:A:10:ARG:H	1:A:12:ILE:HA	6	0.12
(1,1589)	1:A:51:LYS:H	1:A:46:GLN:HA	6	0.12
(1,1589)	1:A:10:ARG:H	1:A:12:ILE:HA	8	0.12
(1,1589)	1:A:51:LYS:H	1:A:46:GLN:HA	8	0.12
(1,1556)	1:B:46:GLN:H	1:B:45:LEU:HG	3	0.12
(1,1556)	1:B:38:LYS:H	1:B:32:LEU:HB2	3	0.12
(1,1556)	1:B:38:LYS:H	1:B:32:LEU:HB3	3	0.12
(1,1556)	1:B:44:ASP:H	1:B:45:LEU:HG	3	0.12
(1,1556)	1:B:46:GLN:H	1:B:45:LEU:HG	7	0.12
(1,1556)	1:B:38:LYS:H	1:B:32:LEU:HB2	7	0.12
(1,1556)	1:B:38:LYS:H	1:B:32:LEU:HB3	7	0.12
(1,1556)	1:B:44:ASP:H	1:B:45:LEU:HG	7	0.12
(1,1555)	1:A:46:GLN:H	1:A:45:LEU:HG	3	0.12
(1,1555)	1:A:38:LYS:H	1:A:32:LEU:HB2	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1555)	1:A:38:LYS:H	1:A:32:LEU:HB3	3	0.12
(1,1555)	1:A:44:ASP:H	1:A:45:LEU:HG	3	0.12
(1,1555)	1:A:46:GLN:H	1:A:45:LEU:HG	7	0.12
(1,1555)	1:A:38:LYS:H	1:A:32:LEU:HB2	7	0.12
(1,1555)	1:A:38:LYS:H	1:A:32:LEU:HB3	7	0.12
(1,1555)	1:A:44:ASP:H	1:A:45:LEU:HG	7	0.12
(1,1544)	1:B:43:LYS:H	1:B:42:ARG:HG2	3	0.12
(1,1544)	1:B:43:LYS:H	1:B:42:ARG:HG3	3	0.12
(1,1544)	1:B:43:LYS:H	1:B:43:LYS:HD2	3	0.12
(1,1544)	1:B:43:LYS:H	1:B:43:LYS:HD3	3	0.12
(1,1543)	1:A:43:LYS:H	1:A:42:ARG:HG2	3	0.12
(1,1543)	1:A:43:LYS:H	1:A:42:ARG:HG3	3	0.12
(1,1543)	1:A:43:LYS:H	1:A:43:LYS:HD2	3	0.12
(1,1543)	1:A:43:LYS:H	1:A:43:LYS:HD3	3	0.12
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	4	0.12
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	4	0.12
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	4	0.12
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	4	0.12
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	4	0.12
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	4	0.12
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	4	0.12
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	4	0.12
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	10	0.12
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	10	0.12
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	10	0.12
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	10	0.12
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	10	0.12
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	10	0.12
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	10	0.12
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	10	0.12
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	4	0.12
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	4	0.12
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	4	0.12
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	4	0.12
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	4	0.12
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	4	0.12
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	4	0.12
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	4	0.12
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	10	0.12
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	10	0.12
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	10	0.12
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	10	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	10	0.12
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	10	0.12
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	10	0.12
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	10	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD22	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD21	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD23	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD12	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD11	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD13	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD22	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD21	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD23	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD12	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD11	4	0.12
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD13	4	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD22	4	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD21	4	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD23	4	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD12	4	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD11	4	0.12
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD13	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD22	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD21	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD23	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD12	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD11	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD13	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD22	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD21	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD23	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD12	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD11	4	0.12
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD13	4	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD22	4	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD21	4	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD23	4	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD12	4	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD11	4	0.12
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD13	4	0.12
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG22	9	0.12
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG21	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG23	9	0.12
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG12	9	0.12
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG11	9	0.12
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG13	9	0.12
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD12	9	0.12
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD11	9	0.12
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD13	9	0.12
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG22	9	0.12
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG21	9	0.12
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG23	9	0.12
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG12	9	0.12
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG11	9	0.12
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG13	9	0.12
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD12	9	0.12
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD11	9	0.12
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD13	9	0.12
(1,1405)	1:A:20:HIS:H	1:B:8:LEU:HB2	9	0.12
(1,1405)	1:A:20:HIS:H	1:B:8:LEU:HB3	9	0.12
(1,1405)	1:A:20:HIS:H	1:A:25:LYS:HB2	9	0.12
(1,1405)	1:A:20:HIS:H	1:A:25:LYS:HB3	9	0.12
(1,1405)	1:A:20:HIS:H	1:A:32:LEU:HG	9	0.12
(1,1405)	1:A:20:HIS:H	1:A:36:GLU:HB2	9	0.12
(1,1405)	1:A:20:HIS:H	1:A:36:GLU:HB3	9	0.12
(1,1390)	1:B:5:MET:H	1:A:110:GLY:H	7	0.12
(1,1390)	1:B:12:ILE:H	1:B:19:PHE:H	7	0.12
(1,1390)	1:B:19:PHE:H	1:B:44:ASP:H	7	0.12
(1,1390)	1:B:19:PHE:H	1:A:12:ILE:H	7	0.12
(1,1390)	1:B:10:ARG:H	1:B:5:MET:H	7	0.12
(1,1390)	1:B:5:MET:H	1:A:110:GLY:H	9	0.12
(1,1390)	1:B:12:ILE:H	1:B:19:PHE:H	9	0.12
(1,1390)	1:B:19:PHE:H	1:B:44:ASP:H	9	0.12
(1,1390)	1:B:19:PHE:H	1:A:12:ILE:H	9	0.12
(1,1390)	1:B:10:ARG:H	1:B:5:MET:H	9	0.12
(1,1389)	1:A:5:MET:H	1:B:110:GLY:H	9	0.12
(1,1389)	1:A:12:ILE:H	1:A:19:PHE:H	9	0.12
(1,1389)	1:A:19:PHE:H	1:A:44:ASP:H	9	0.12
(1,1389)	1:A:19:PHE:H	1:B:12:ILE:H	9	0.12
(1,1389)	1:A:10:ARG:H	1:A:5:MET:H	9	0.12
(1,1332)	1:B:12:ILE:H	1:B:14:THR:H	4	0.12
(1,1332)	1:B:12:ILE:H	1:B:15:ILE:H	4	0.12
(1,1331)	1:A:12:ILE:H	1:A:14:THR:H	4	0.12
(1,1331)	1:A:12:ILE:H	1:A:15:ILE:H	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB2	2	0.12
(1,1214)	1:B:37:PHE:HB2	1:B:49:LEU:HB3	2	0.12
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB2	2	0.12
(1,1214)	1:B:37:PHE:HB3	1:B:49:LEU:HB3	2	0.12
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB2	2	0.12
(1,1214)	1:B:50:LYS:HE2	1:B:49:LEU:HB3	2	0.12
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB2	2	0.12
(1,1214)	1:B:50:LYS:HE3	1:B:49:LEU:HB3	2	0.12
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE2	2	0.12
(1,1214)	1:B:49:LEU:HB2	1:B:54:LYS:HE3	2	0.12
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE2	2	0.12
(1,1214)	1:B:49:LEU:HB3	1:B:54:LYS:HE3	2	0.12
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD2	2	0.12
(1,1214)	1:B:49:LEU:HB2	1:B:85:ARG:HD3	2	0.12
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD2	2	0.12
(1,1214)	1:B:49:LEU:HB3	1:B:85:ARG:HD3	2	0.12
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB2	2	0.12
(1,1213)	1:A:37:PHE:HB2	1:A:49:LEU:HB3	2	0.12
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB2	2	0.12
(1,1213)	1:A:37:PHE:HB3	1:A:49:LEU:HB3	2	0.12
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB2	2	0.12
(1,1213)	1:A:50:LYS:HE2	1:A:49:LEU:HB3	2	0.12
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB2	2	0.12
(1,1213)	1:A:50:LYS:HE3	1:A:49:LEU:HB3	2	0.12
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE2	2	0.12
(1,1213)	1:A:49:LEU:HB2	1:A:54:LYS:HE3	2	0.12
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE2	2	0.12
(1,1213)	1:A:49:LEU:HB3	1:A:54:LYS:HE3	2	0.12
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD2	2	0.12
(1,1213)	1:A:49:LEU:HB2	1:A:85:ARG:HD3	2	0.12
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD2	2	0.12
(1,1213)	1:A:49:LEU:HB3	1:A:85:ARG:HD3	2	0.12
(1,1158)	1:B:20:HIS:H	1:B:32:LEU:HG	10	0.12
(1,1158)	1:B:21:GLN:H	1:B:32:LEU:HG	10	0.12
(1,1158)	1:B:32:LEU:HG	1:B:41:VAL:H	10	0.12
(1,1157)	1:A:20:HIS:H	1:A:32:LEU:HG	7	0.12
(1,1157)	1:A:21:GLN:H	1:A:32:LEU:HG	7	0.12
(1,1157)	1:A:32:LEU:HG	1:A:41:VAL:H	7	0.12
(1,1157)	1:A:20:HIS:H	1:A:32:LEU:HG	10	0.12
(1,1157)	1:A:21:GLN:H	1:A:32:LEU:HG	10	0.12
(1,1157)	1:A:32:LEU:HG	1:A:41:VAL:H	10	0.12
(1,1097)	1:A:59:ILE:HG22	1:A:42:ARG:HD2	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1097)	1:A:59:ILE:HG22	1:A:42:ARG:HD3	4	0.12
(1,1097)	1:A:59:ILE:HG21	1:A:42:ARG:HD2	4	0.12
(1,1097)	1:A:59:ILE:HG21	1:A:42:ARG:HD3	4	0.12
(1,1097)	1:A:59:ILE:HG23	1:A:42:ARG:HD2	4	0.12
(1,1097)	1:A:59:ILE:HG23	1:A:42:ARG:HD3	4	0.12
(1,1097)	1:A:59:ILE:HG22	1:A:79:PHE:HB2	4	0.12
(1,1097)	1:A:59:ILE:HG22	1:A:79:PHE:HB3	4	0.12
(1,1097)	1:A:59:ILE:HG21	1:A:79:PHE:HB2	4	0.12
(1,1097)	1:A:59:ILE:HG21	1:A:79:PHE:HB3	4	0.12
(1,1097)	1:A:59:ILE:HG23	1:A:79:PHE:HB2	4	0.12
(1,1097)	1:A:59:ILE:HG23	1:A:79:PHE:HB3	4	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	7	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	7	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	7	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	7	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	7	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	7	0.12
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	7	0.12
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	7	0.12
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	7	0.12
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	7	0.12
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	7	0.12
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	7	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	9	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	9	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	9	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	9	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	9	0.12
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	9	0.12
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	9	0.12
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	9	0.12
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	9	0.12
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	9	0.12
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	9	0.12
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	9	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	7	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	7	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	7	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	7	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	7	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	7	0.12
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	7	0.12
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	7	0.12
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	7	0.12
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	7	0.12
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	7	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	9	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	9	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	9	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	9	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	9	0.12
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	9	0.12
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	9	0.12
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	9	0.12
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	9	0.12
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	9	0.12
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	9	0.12
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	9	0.12
(4,9)	1:A:21:GLN:HA	1:A:17:ASN:HA	7	0.11
(4,64)	1:B:32:LEU:HG	1:B:31:THR:HB	2	0.11
(4,64)	1:B:32:LEU:HG	1:B:31:THR:HB	5	0.11
(4,63)	1:A:32:LEU:HG	1:A:31:THR:HB	2	0.11
(4,63)	1:A:32:LEU:HG	1:A:31:THR:HB	5	0.11
(4,236)	1:B:81:MET:H	1:A:81:MET:H	7	0.11
(4,235)	1:A:81:MET:H	1:B:81:MET:H	7	0.11
(4,232)	1:B:79:PHE:H	1:B:80:ILE:HB	8	0.11
(4,231)	1:A:79:PHE:H	1:A:80:ILE:HB	8	0.11
(4,112)	1:B:76:PHE:H	1:B:31:THR:H	4	0.11
(4,10)	1:B:21:GLN:HA	1:B:17:ASN:HA	7	0.11
(3,948)	1:B:75:SER:H	1:B:78:GLU:H	7	0.11
(3,947)	1:A:75:SER:H	1:A:78:GLU:H	7	0.11
(3,942)	1:B:48:PHE:H	1:B:50:LYS:H	9	0.11
(3,941)	1:A:48:PHE:H	1:A:50:LYS:H	9	0.11
(3,916)	1:B:47:ASN:H	1:A:5:MET:HG2	1	0.11
(3,916)	1:B:47:ASN:H	1:A:5:MET:HG3	1	0.11
(3,871)	1:A:6:SER:H	1:A:5:MET:HG2	6	0.11
(3,871)	1:A:6:SER:H	1:A:5:MET:HG3	6	0.11
(3,866)	1:B:52:GLU:H	1:B:51:LYS:HG2	3	0.11
(3,866)	1:B:52:GLU:H	1:B:51:LYS:HG3	3	0.11
(3,80)	1:B:59:ILE:HB	1:B:38:LYS:HG2	7	0.11
(3,80)	1:B:59:ILE:HB	1:B:38:LYS:HG3	7	0.11
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB2	8	0.11
(3,668)	1:B:63:MET:HE2	1:B:32:LEU:HB3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB2	8	0.11
(3,668)	1:B:63:MET:HE1	1:B:32:LEU:HB3	8	0.11
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB2	8	0.11
(3,668)	1:B:63:MET:HE3	1:B:32:LEU:HB3	8	0.11
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB2	8	0.11
(3,667)	1:A:63:MET:HE2	1:A:32:LEU:HB3	8	0.11
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB2	8	0.11
(3,667)	1:A:63:MET:HE1	1:A:32:LEU:HB3	8	0.11
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB2	8	0.11
(3,667)	1:A:63:MET:HE3	1:A:32:LEU:HB3	8	0.11
(3,630)	1:B:48:PHE:HB2	1:B:45:LEU:HA	6	0.11
(3,630)	1:B:48:PHE:HB3	1:B:45:LEU:HA	6	0.11
(3,629)	1:A:48:PHE:HB2	1:A:45:LEU:HA	6	0.11
(3,629)	1:A:48:PHE:HB3	1:A:45:LEU:HA	6	0.11
(3,601)	1:A:46:GLN:HG2	1:B:4:LYS:HE2	10	0.11
(3,601)	1:A:46:GLN:HG2	1:B:4:LYS:HE3	10	0.11
(3,601)	1:A:46:GLN:HG3	1:B:4:LYS:HE2	10	0.11
(3,601)	1:A:46:GLN:HG3	1:B:4:LYS:HE3	10	0.11
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD22	3	0.11
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD21	3	0.11
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD23	3	0.11
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD12	3	0.11
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD11	3	0.11
(3,582)	1:B:66:LEU:H	1:B:66:LEU:HD13	3	0.11
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD22	3	0.11
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD21	3	0.11
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD23	3	0.11
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD12	3	0.11
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD11	3	0.11
(3,581)	1:A:66:LEU:H	1:A:66:LEU:HD13	3	0.11
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA2	7	0.11
(3,566)	1:B:111:GLU:HB2	1:B:108:GLY:HA3	7	0.11
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA2	7	0.11
(3,566)	1:B:111:GLU:HB3	1:B:108:GLY:HA3	7	0.11
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA2	7	0.11
(3,565)	1:A:111:GLU:HB2	1:A:108:GLY:HA3	7	0.11
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA2	7	0.11
(3,565)	1:A:111:GLU:HB3	1:A:108:GLY:HA3	7	0.11
(3,494)	1:B:59:ILE:HD12	1:B:38:LYS:HE2	3	0.11
(3,494)	1:B:59:ILE:HD12	1:B:38:LYS:HE3	3	0.11
(3,494)	1:B:59:ILE:HD11	1:B:38:LYS:HE2	3	0.11
(3,494)	1:B:59:ILE:HD11	1:B:38:LYS:HE3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,494)	1:B:59:ILE:HD13	1:B:38:LYS:HE2	3	0.11
(3,494)	1:B:59:ILE:HD13	1:B:38:LYS:HE3	3	0.11
(3,493)	1:A:59:ILE:HD12	1:A:38:LYS:HE2	3	0.11
(3,493)	1:A:59:ILE:HD12	1:A:38:LYS:HE3	3	0.11
(3,493)	1:A:59:ILE:HD11	1:A:38:LYS:HE2	3	0.11
(3,493)	1:A:59:ILE:HD11	1:A:38:LYS:HE3	3	0.11
(3,493)	1:A:59:ILE:HD13	1:A:38:LYS:HE2	3	0.11
(3,493)	1:A:59:ILE:HD13	1:A:38:LYS:HE3	3	0.11
(3,486)	1:B:96:GLU:HG2	1:B:97:GLY:H	8	0.11
(3,486)	1:B:96:GLU:HG3	1:B:97:GLY:H	8	0.11
(3,42)	1:B:58:VAL:HG22	1:B:57:LYS:HB2	2	0.11
(3,42)	1:B:58:VAL:HG22	1:B:57:LYS:HB3	2	0.11
(3,42)	1:B:58:VAL:HG21	1:B:57:LYS:HB2	2	0.11
(3,42)	1:B:58:VAL:HG21	1:B:57:LYS:HB3	2	0.11
(3,42)	1:B:58:VAL:HG23	1:B:57:LYS:HB2	2	0.11
(3,42)	1:B:58:VAL:HG23	1:B:57:LYS:HB3	2	0.11
(3,42)	1:B:58:VAL:HG12	1:B:57:LYS:HB2	2	0.11
(3,42)	1:B:58:VAL:HG12	1:B:57:LYS:HB3	2	0.11
(3,42)	1:B:58:VAL:HG11	1:B:57:LYS:HB2	2	0.11
(3,42)	1:B:58:VAL:HG11	1:B:57:LYS:HB3	2	0.11
(3,42)	1:B:58:VAL:HG13	1:B:57:LYS:HB2	2	0.11
(3,42)	1:B:58:VAL:HG13	1:B:57:LYS:HB3	2	0.11
(3,41)	1:A:58:VAL:HG22	1:A:57:LYS:HB2	2	0.11
(3,41)	1:A:58:VAL:HG22	1:A:57:LYS:HB3	2	0.11
(3,41)	1:A:58:VAL:HG21	1:A:57:LYS:HB2	2	0.11
(3,41)	1:A:58:VAL:HG21	1:A:57:LYS:HB3	2	0.11
(3,41)	1:A:58:VAL:HG23	1:A:57:LYS:HB2	2	0.11
(3,41)	1:A:58:VAL:HG23	1:A:57:LYS:HB3	2	0.11
(3,41)	1:A:58:VAL:HG12	1:A:57:LYS:HB2	2	0.11
(3,41)	1:A:58:VAL:HG12	1:A:57:LYS:HB3	2	0.11
(3,41)	1:A:58:VAL:HG11	1:A:57:LYS:HB2	2	0.11
(3,41)	1:A:58:VAL:HG11	1:A:57:LYS:HB3	2	0.11
(3,41)	1:A:58:VAL:HG13	1:A:57:LYS:HB2	2	0.11
(3,41)	1:A:58:VAL:HG13	1:A:57:LYS:HB3	2	0.11
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD22	4	0.11
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD21	4	0.11
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD23	4	0.11
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD12	4	0.11
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD11	4	0.11
(3,353)	1:A:47:ASN:HA	1:A:109:LEU:HD13	4	0.11
(3,350)	1:B:71:ASP:HA	1:B:67:ASP:HB2	3	0.11
(3,350)	1:B:71:ASP:HA	1:B:67:ASP:HB3	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,349)	1:A:71:ASP:HA	1:A:67:ASP:HB2	3	0.11
(3,349)	1:A:71:ASP:HA	1:A:67:ASP:HB3	3	0.11
(3,340)	1:B:57:LYS:HG2	1:B:56:GLU:HB2	3	0.11
(3,340)	1:B:57:LYS:HG2	1:B:56:GLU:HB3	3	0.11
(3,340)	1:B:57:LYS:HG3	1:B:56:GLU:HB2	3	0.11
(3,340)	1:B:57:LYS:HG3	1:B:56:GLU:HB3	3	0.11
(3,34)	1:B:87:THR:HG21	1:B:88:TRP:HA	4	0.11
(3,34)	1:B:87:THR:HG22	1:B:88:TRP:HA	4	0.11
(3,34)	1:B:87:THR:HG23	1:B:88:TRP:HA	4	0.11
(3,33)	1:A:87:THR:HG21	1:A:88:TRP:HA	4	0.11
(3,33)	1:A:87:THR:HG22	1:A:88:TRP:HA	4	0.11
(3,33)	1:A:87:THR:HG23	1:A:88:TRP:HA	4	0.11
(3,320)	1:B:51:LYS:HE2	1:B:51:LYS:H	8	0.11
(3,320)	1:B:51:LYS:HE3	1:B:51:LYS:H	8	0.11
(3,319)	1:A:51:LYS:HE2	1:A:51:LYS:H	8	0.11
(3,319)	1:A:51:LYS:HE3	1:A:51:LYS:H	8	0.11
(3,251)	1:A:33:ASN:HB2	1:A:72:LYS:HA	4	0.11
(3,251)	1:A:33:ASN:HB3	1:A:72:LYS:HA	4	0.11
(3,228)	1:B:24:VAL:HB	1:B:32:LEU:HD22	8	0.11
(3,228)	1:B:24:VAL:HB	1:B:32:LEU:HD21	8	0.11
(3,228)	1:B:24:VAL:HB	1:B:32:LEU:HD23	8	0.11
(3,228)	1:B:24:VAL:HB	1:B:32:LEU:HD12	8	0.11
(3,228)	1:B:24:VAL:HB	1:B:32:LEU:HD11	8	0.11
(3,228)	1:B:24:VAL:HB	1:B:32:LEU:HD13	8	0.11
(3,227)	1:A:24:VAL:HB	1:A:32:LEU:HD22	8	0.11
(3,227)	1:A:24:VAL:HB	1:A:32:LEU:HD21	8	0.11
(3,227)	1:A:24:VAL:HB	1:A:32:LEU:HD23	8	0.11
(3,227)	1:A:24:VAL:HB	1:A:32:LEU:HD12	8	0.11
(3,227)	1:A:24:VAL:HB	1:A:32:LEU:HD11	8	0.11
(3,227)	1:A:24:VAL:HB	1:A:32:LEU:HD13	8	0.11
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG2	2	0.11
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG3	2	0.11
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG2	6	0.11
(3,1440)	1:B:87:THR:H	1:A:77:GLU:HG3	6	0.11
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG2	5	0.11
(3,14)	1:B:111:GLU:HA	1:B:111:GLU:HG3	5	0.11
(3,1366)	1:B:69:ASN:H	1:B:73:GLN:HB2	9	0.11
(3,1366)	1:B:69:ASN:H	1:B:73:GLN:HB3	9	0.11
(3,1365)	1:A:69:ASN:H	1:A:73:GLN:HB2	9	0.11
(3,1365)	1:A:69:ASN:H	1:A:73:GLN:HB3	9	0.11
(3,1344)	1:B:66:LEU:H	1:B:66:LEU:HG	1	0.11
(3,1343)	1:A:66:LEU:H	1:A:66:LEU:HG	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1320)	1:B:67:ASP:H	1:B:68:THR:H	1	0.11
(3,132)	1:B:78:GLU:HB2	1:B:31:THR:HA	7	0.11
(3,132)	1:B:78:GLU:HB3	1:B:31:THR:HA	7	0.11
(3,1319)	1:A:67:ASP:H	1:A:68:THR:H	1	0.11
(3,131)	1:A:78:GLU:HB2	1:A:31:THR:HA	7	0.11
(3,131)	1:A:78:GLU:HB3	1:A:31:THR:HA	7	0.11
(3,1159)	1:A:82:LEU:H	1:A:84:ALA:H	2	0.11
(3,1082)	1:B:23:SER:H	1:B:29:PRO:HB2	9	0.11
(3,1082)	1:B:23:SER:H	1:B:29:PRO:HB3	9	0.11
(2,84)	1:A:93:LYS:H	1:A:89:ALA:O	3	0.11
(2,66)	1:A:83:MET:H	1:A:79:PHE:O	4	0.11
(2,58)	1:A:66:LEU:H	1:A:62:ILE:O	10	0.11
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	1	0.11
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	4	0.11
(2,42)	1:A:53:ASN:H	1:A:50:LYS:O	5	0.11
(2,4)	1:A:74:LEU:N	1:A:32:LEU:O	8	0.11
(2,21)	1:A:20:HIS:N	1:A:16:ILE:O	7	0.11
(2,2)	1:A:32:LEU:N	1:A:74:LEU:O	3	0.11
(1,938)	1:B:5:MET:HB2	1:B:8:LEU:HD22	1	0.11
(1,938)	1:B:5:MET:HB2	1:B:8:LEU:HD21	1	0.11
(1,938)	1:B:5:MET:HB2	1:B:8:LEU:HD23	1	0.11
(1,938)	1:B:5:MET:HB2	1:B:8:LEU:HD12	1	0.11
(1,938)	1:B:5:MET:HB2	1:B:8:LEU:HD11	1	0.11
(1,938)	1:B:5:MET:HB2	1:B:8:LEU:HD13	1	0.11
(1,938)	1:B:5:MET:HB3	1:B:8:LEU:HD22	1	0.11
(1,938)	1:B:5:MET:HB3	1:B:8:LEU:HD21	1	0.11
(1,938)	1:B:5:MET:HB3	1:B:8:LEU:HD23	1	0.11
(1,938)	1:B:5:MET:HB3	1:B:8:LEU:HD12	1	0.11
(1,938)	1:B:5:MET:HB3	1:B:8:LEU:HD11	1	0.11
(1,938)	1:B:5:MET:HB3	1:B:8:LEU:HD13	1	0.11
(1,938)	1:B:46:GLN:HG2	1:B:59:ILE:HG22	1	0.11
(1,938)	1:B:46:GLN:HG2	1:B:59:ILE:HG21	1	0.11
(1,938)	1:B:46:GLN:HG2	1:B:59:ILE:HG23	1	0.11
(1,938)	1:B:46:GLN:HG3	1:B:59:ILE:HG22	1	0.11
(1,938)	1:B:46:GLN:HG3	1:B:59:ILE:HG21	1	0.11
(1,938)	1:B:46:GLN:HG3	1:B:59:ILE:HG23	1	0.11
(1,938)	1:B:46:GLN:HG2	1:A:8:LEU:HD22	1	0.11
(1,938)	1:B:46:GLN:HG2	1:A:8:LEU:HD21	1	0.11
(1,938)	1:B:46:GLN:HG2	1:A:8:LEU:HD23	1	0.11
(1,938)	1:B:46:GLN:HG2	1:A:8:LEU:HD12	1	0.11
(1,938)	1:B:46:GLN:HG2	1:A:8:LEU:HD11	1	0.11
(1,938)	1:B:46:GLN:HG2	1:A:8:LEU:HD13	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:B:46:GLN:HG3	1:A:8:LEU:HD22	1	0.11
(1,938)	1:B:46:GLN:HG3	1:A:8:LEU:HD21	1	0.11
(1,938)	1:B:46:GLN:HG3	1:A:8:LEU:HD23	1	0.11
(1,938)	1:B:46:GLN:HG3	1:A:8:LEU:HD12	1	0.11
(1,938)	1:B:46:GLN:HG3	1:A:8:LEU:HD11	1	0.11
(1,938)	1:B:46:GLN:HG3	1:A:8:LEU:HD13	1	0.11
(1,918)	1:B:87:THR:HA	1:B:92:GLU:HG2	3	0.11
(1,918)	1:B:87:THR:HA	1:B:92:GLU:HG3	3	0.11
(1,918)	1:B:87:THR:HA	1:A:9:GLU:HB2	3	0.11
(1,918)	1:B:87:THR:HA	1:A:9:GLU:HB3	3	0.11
(1,918)	1:B:87:THR:HA	1:A:12:ILE:HB	3	0.11
(1,82)	1:B:46:GLN:HG2	1:A:5:MET:H	5	0.11
(1,82)	1:B:46:GLN:HG3	1:A:5:MET:H	5	0.11
(1,82)	1:B:46:GLN:HG2	1:A:8:LEU:H	5	0.11
(1,82)	1:B:46:GLN:HG3	1:A:8:LEU:H	5	0.11
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB2	3	0.11
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB3	3	0.11
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG2	3	0.11
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG3	3	0.11
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB2	10	0.11
(1,796)	1:B:111:GLU:HA	1:B:50:LYS:HB3	10	0.11
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG2	10	0.11
(1,796)	1:B:111:GLU:HA	1:A:10:ARG:HG3	10	0.11
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB2	3	0.11
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB3	3	0.11
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG2	3	0.11
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG3	3	0.11
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB2	10	0.11
(1,795)	1:A:111:GLU:HA	1:A:50:LYS:HB3	10	0.11
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG2	10	0.11
(1,795)	1:A:111:GLU:HA	1:B:10:ARG:HG3	10	0.11
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD12	8	0.11
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD11	8	0.11
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD13	8	0.11
(1,772)	1:B:59:ILE:HD12	1:B:62:ILE:HA	8	0.11
(1,772)	1:B:59:ILE:HD11	1:B:62:ILE:HA	8	0.11
(1,772)	1:B:59:ILE:HD13	1:B:62:ILE:HA	8	0.11
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD12	10	0.11
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD11	10	0.11
(1,772)	1:B:58:VAL:HA	1:B:59:ILE:HD13	10	0.11
(1,772)	1:B:59:ILE:HD12	1:B:62:ILE:HA	10	0.11
(1,772)	1:B:59:ILE:HD11	1:B:62:ILE:HA	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,772)	1:B:59:ILE:HD13	1:B:62:ILE:HA	10	0.11
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD12	8	0.11
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD11	8	0.11
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD13	8	0.11
(1,771)	1:A:59:ILE:HD12	1:A:62:ILE:HA	8	0.11
(1,771)	1:A:59:ILE:HD11	1:A:62:ILE:HA	8	0.11
(1,771)	1:A:59:ILE:HD13	1:A:62:ILE:HA	8	0.11
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD12	10	0.11
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD11	10	0.11
(1,771)	1:A:58:VAL:HA	1:A:59:ILE:HD13	10	0.11
(1,771)	1:A:59:ILE:HD12	1:A:62:ILE:HA	10	0.11
(1,771)	1:A:59:ILE:HD11	1:A:62:ILE:HA	10	0.11
(1,771)	1:A:59:ILE:HD13	1:A:62:ILE:HA	10	0.11
(1,742)	1:B:4:LYS:HA	1:B:4:LYS:HG2	8	0.11
(1,742)	1:B:4:LYS:HA	1:B:4:LYS:HG3	8	0.11
(1,742)	1:B:81:MET:HA	1:B:84:ALA:HB2	8	0.11
(1,742)	1:B:81:MET:HA	1:B:84:ALA:HB1	8	0.11
(1,742)	1:B:81:MET:HA	1:B:84:ALA:HB3	8	0.11
(1,741)	1:A:4:LYS:HA	1:A:4:LYS:HG2	8	0.11
(1,741)	1:A:4:LYS:HA	1:A:4:LYS:HG3	8	0.11
(1,741)	1:A:81:MET:HA	1:A:84:ALA:HB2	8	0.11
(1,741)	1:A:81:MET:HA	1:A:84:ALA:HB1	8	0.11
(1,741)	1:A:81:MET:HA	1:A:84:ALA:HB3	8	0.11
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD2	7	0.11
(1,614)	1:B:36:GLU:HA	1:B:25:LYS:HD3	7	0.11
(1,614)	1:B:50:LYS:HD2	1:B:50:LYS:HA	7	0.11
(1,614)	1:B:50:LYS:HD3	1:B:50:LYS:HA	7	0.11
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD2	7	0.11
(1,614)	1:B:51:LYS:HA	1:B:51:LYS:HD3	7	0.11
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD2	7	0.11
(1,613)	1:A:36:GLU:HA	1:A:25:LYS:HD3	7	0.11
(1,613)	1:A:50:LYS:HD2	1:A:50:LYS:HA	7	0.11
(1,613)	1:A:50:LYS:HD3	1:A:50:LYS:HA	7	0.11
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD2	7	0.11
(1,613)	1:A:51:LYS:HA	1:A:51:LYS:HD3	7	0.11
(1,568)	1:B:42:ARG:HA	1:B:43:LYS:HE2	8	0.11
(1,568)	1:B:42:ARG:HA	1:B:43:LYS:HE3	8	0.11
(1,568)	1:B:42:ARG:HA	1:B:50:LYS:HE2	8	0.11
(1,568)	1:B:42:ARG:HA	1:B:50:LYS:HE3	8	0.11
(1,568)	1:B:42:ARG:HA	1:B:54:LYS:HE2	8	0.11
(1,568)	1:B:42:ARG:HA	1:B:54:LYS:HE3	8	0.11
(1,354)	1:B:58:VAL:HG22	1:B:54:LYS:HA	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:B:58:VAL:HG21	1:B:54:LYS:HA	1	0.11
(1,354)	1:B:58:VAL:HG23	1:B:54:LYS:HA	1	0.11
(1,354)	1:B:58:VAL:HG12	1:B:54:LYS:HA	1	0.11
(1,354)	1:B:58:VAL:HG11	1:B:54:LYS:HA	1	0.11
(1,354)	1:B:58:VAL:HG13	1:B:54:LYS:HA	1	0.11
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG21	1	0.11
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG22	1	0.11
(1,354)	1:B:92:GLU:HA	1:B:87:THR:HG23	1	0.11
(1,353)	1:A:58:VAL:HG22	1:A:54:LYS:HA	1	0.11
(1,353)	1:A:58:VAL:HG21	1:A:54:LYS:HA	1	0.11
(1,353)	1:A:58:VAL:HG23	1:A:54:LYS:HA	1	0.11
(1,353)	1:A:58:VAL:HG12	1:A:54:LYS:HA	1	0.11
(1,353)	1:A:58:VAL:HG11	1:A:54:LYS:HA	1	0.11
(1,353)	1:A:58:VAL:HG13	1:A:54:LYS:HA	1	0.11
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG21	1	0.11
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG22	1	0.11
(1,353)	1:A:92:GLU:HA	1:A:87:THR:HG23	1	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD22	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD21	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD23	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD12	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD11	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD13	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD22	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD21	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD23	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD12	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD11	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD13	3	0.11
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD12	3	0.11
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD11	3	0.11
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD13	3	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD22	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD21	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD23	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD12	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD11	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:49:LEU:HD13	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD22	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD21	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD23	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD12	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD11	4	0.11
(1,308)	1:B:44:ASP:HA	1:B:109:LEU:HD13	4	0.11
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD12	4	0.11
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD11	4	0.11
(1,308)	1:B:44:ASP:HA	1:A:12:ILE:HD13	4	0.11
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD22	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD21	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD23	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD12	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD11	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:49:LEU:HD13	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD22	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD21	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD23	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD12	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD11	3	0.11
(1,307)	1:A:44:ASP:HA	1:A:109:LEU:HD13	3	0.11
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD12	3	0.11
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD11	3	0.11
(1,307)	1:A:44:ASP:HA	1:B:12:ILE:HD13	3	0.11
(1,302)	1:B:44:ASP:HA	1:B:15:ILE:HA	7	0.11
(1,302)	1:B:44:ASP:HA	1:B:18:THR:HA	7	0.11
(1,302)	1:B:44:ASP:HA	1:B:42:ARG:HA	7	0.11
(1,302)	1:B:44:ASP:HA	1:A:7:GLN:HA	7	0.11
(1,301)	1:A:44:ASP:HA	1:A:15:ILE:HA	7	0.11
(1,301)	1:A:44:ASP:HA	1:A:18:THR:HA	7	0.11
(1,301)	1:A:44:ASP:HA	1:A:42:ARG:HA	7	0.11
(1,301)	1:A:44:ASP:HA	1:B:7:GLN:HA	7	0.11
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB2	2	0.11
(1,19)	1:A:65:ASP:HA	1:A:74:LEU:HB3	2	0.11
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB2	2	0.11
(1,19)	1:A:65:ASP:HA	1:A:82:LEU:HB3	2	0.11
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB2	2	0.11
(1,19)	1:A:92:GLU:HA	1:A:86:LEU:HB3	2	0.11
(1,19)	1:A:92:GLU:HA	1:A:109:LEU:HG	2	0.11
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG2	2	0.11
(1,19)	1:A:93:LYS:HA	1:A:51:LYS:HG3	2	0.11
(1,19)	1:A:93:LYS:HA	1:A:109:LEU:HG	2	0.11
(1,1820)	1:B:21:GLN:H	1:B:40:LEU:HG	2	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB2	2	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB1	2	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB3	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1820)	1:B:21:GLN:H	1:B:40:LEU:HG	6	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB2	6	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB1	6	0.11
(1,1820)	1:B:94:MET:H	1:B:89:ALA:HB3	6	0.11
(1,1819)	1:A:21:GLN:H	1:A:40:LEU:HG	2	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB2	2	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB1	2	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB3	2	0.11
(1,1819)	1:A:21:GLN:H	1:A:40:LEU:HG	6	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB2	6	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB1	6	0.11
(1,1819)	1:A:94:MET:H	1:A:89:ALA:HB3	6	0.11
(1,1772)	1:B:87:THR:H	1:B:109:LEU:HG	9	0.11
(1,1772)	1:B:87:THR:H	1:A:80:ILE:HB	9	0.11
(1,1771)	1:A:87:THR:H	1:A:109:LEU:HG	9	0.11
(1,1771)	1:A:87:THR:H	1:B:80:ILE:HB	9	0.11
(1,1728)	1:B:81:MET:H	1:B:80:ILE:HG12	2	0.11
(1,1728)	1:B:81:MET:H	1:B:80:ILE:HG13	2	0.11
(1,1728)	1:B:81:MET:H	1:A:80:ILE:HG12	2	0.11
(1,1728)	1:B:81:MET:H	1:A:80:ILE:HG13	2	0.11
(1,1727)	1:A:81:MET:H	1:A:80:ILE:HG12	2	0.11
(1,1727)	1:A:81:MET:H	1:A:80:ILE:HG13	2	0.11
(1,1727)	1:A:81:MET:H	1:B:80:ILE:HG12	2	0.11
(1,1727)	1:A:81:MET:H	1:B:80:ILE:HG13	2	0.11
(1,152)	1:B:37:PHE:HA	1:B:42:ARG:H	10	0.11
(1,152)	1:B:37:PHE:HA	1:B:63:MET:H	10	0.11
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	2	0.11
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	2	0.11
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	2	0.11
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	2	0.11
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	2	0.11
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	2	0.11
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	2	0.11
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	2	0.11
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD2	9	0.11
(1,1510)	1:B:39:GLU:H	1:B:38:LYS:HD3	9	0.11
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD2	9	0.11
(1,1510)	1:B:39:GLU:H	1:B:43:LYS:HD3	9	0.11
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE2	9	0.11
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE1	9	0.11
(1,1510)	1:B:67:ASP:H	1:B:63:MET:HE3	9	0.11
(1,1510)	1:B:67:ASP:H	1:B:66:LEU:HG	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,151)	1:A:37:PHE:HA	1:A:42:ARG:H	10	0.11
(1,151)	1:A:37:PHE:HA	1:A:63:MET:H	10	0.11
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	2	0.11
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	2	0.11
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	2	0.11
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	2	0.11
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	2	0.11
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	2	0.11
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	2	0.11
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	2	0.11
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD2	9	0.11
(1,1509)	1:A:39:GLU:H	1:A:38:LYS:HD3	9	0.11
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD2	9	0.11
(1,1509)	1:A:39:GLU:H	1:A:43:LYS:HD3	9	0.11
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE2	9	0.11
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE1	9	0.11
(1,1509)	1:A:67:ASP:H	1:A:63:MET:HE3	9	0.11
(1,1509)	1:A:67:ASP:H	1:A:66:LEU:HG	9	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD22	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD21	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD23	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD12	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD11	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD13	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD22	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD21	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD23	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD12	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD11	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD13	2	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD22	2	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD21	2	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD23	2	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD12	2	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD11	2	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD13	2	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD22	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD21	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD23	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD12	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD11	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD13	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD22	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD21	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD23	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD12	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD11	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD13	5	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD22	5	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD21	5	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD23	5	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD12	5	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD11	5	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD13	5	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD22	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD21	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD23	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD12	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD11	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:66:LEU:HD13	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD22	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD21	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD23	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD12	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD11	8	0.11
(1,1444)	1:B:78:GLU:H	1:B:74:LEU:HD13	8	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD22	8	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD21	8	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD23	8	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD12	8	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD11	8	0.11
(1,1444)	1:B:24:VAL:H	1:B:32:LEU:HD13	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD22	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD21	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD23	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD12	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD11	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD13	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD22	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD21	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD23	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD12	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD11	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD13	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD22	2	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD21	2	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD23	2	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD12	2	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD11	2	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD13	2	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD22	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD21	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD23	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD12	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD11	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD13	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD22	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD21	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD23	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD12	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD11	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD13	5	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD22	5	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD21	5	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD23	5	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD12	5	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD11	5	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD13	5	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD22	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD21	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD23	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD12	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD11	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:66:LEU:HD13	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD22	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD21	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD23	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD12	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD11	8	0.11
(1,1443)	1:A:78:GLU:H	1:A:74:LEU:HD13	8	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD22	8	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD21	8	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD23	8	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD12	8	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD11	8	0.11
(1,1443)	1:A:24:VAL:H	1:A:32:LEU:HD13	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG22	10	0.11
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG21	10	0.11
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG23	10	0.11
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG12	10	0.11
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG11	10	0.11
(1,1418)	1:B:21:GLN:H	1:B:24:VAL:HG13	10	0.11
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD12	10	0.11
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD11	10	0.11
(1,1418)	1:B:61:HIS:H	1:B:62:ILE:HD13	10	0.11
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG22	10	0.11
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG21	10	0.11
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG23	10	0.11
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG12	10	0.11
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG11	10	0.11
(1,1417)	1:A:21:GLN:H	1:A:24:VAL:HG13	10	0.11
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD12	10	0.11
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD11	10	0.11
(1,1417)	1:A:61:HIS:H	1:A:62:ILE:HD13	10	0.11
(1,1406)	1:B:20:HIS:H	1:A:8:LEU:HB2	9	0.11
(1,1406)	1:B:20:HIS:H	1:A:8:LEU:HB3	9	0.11
(1,1406)	1:B:20:HIS:H	1:B:25:LYS:HB2	9	0.11
(1,1406)	1:B:20:HIS:H	1:B:25:LYS:HB3	9	0.11
(1,1406)	1:B:20:HIS:H	1:B:32:LEU:HG	9	0.11
(1,1406)	1:B:20:HIS:H	1:B:36:GLU:HB2	9	0.11
(1,1406)	1:B:20:HIS:H	1:B:36:GLU:HB3	9	0.11
(1,1390)	1:B:5:MET:H	1:A:110:GLY:H	6	0.11
(1,1390)	1:B:12:ILE:H	1:B:19:PHE:H	6	0.11
(1,1390)	1:B:19:PHE:H	1:B:44:ASP:H	6	0.11
(1,1390)	1:B:19:PHE:H	1:A:12:ILE:H	6	0.11
(1,1390)	1:B:10:ARG:H	1:B:5:MET:H	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD22	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD21	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD23	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD12	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD11	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD13	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD22	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD21	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD23	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD12	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD11	3	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD13	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD22	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD21	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD23	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD12	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD11	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:45:LEU:HD13	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD22	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD21	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD23	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD12	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD11	6	0.11
(1,1278)	1:B:48:PHE:H	1:B:86:LEU:HD13	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD22	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD21	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD23	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD12	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD11	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD13	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD22	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD21	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD23	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD12	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD11	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD13	3	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD22	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD21	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD23	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD12	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD11	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:45:LEU:HD13	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD22	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD21	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD23	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD12	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD11	6	0.11
(1,1277)	1:A:48:PHE:H	1:A:86:LEU:HD13	6	0.11
(1,1248)	1:B:6:SER:H	1:B:12:ILE:HD12	1	0.11
(1,1248)	1:B:6:SER:H	1:B:12:ILE:HD11	1	0.11
(1,1248)	1:B:6:SER:H	1:B:12:ILE:HD13	1	0.11
(1,1248)	1:B:6:SER:H	1:A:49:LEU:HD22	1	0.11
(1,1248)	1:B:6:SER:H	1:A:49:LEU:HD21	1	0.11
(1,1248)	1:B:6:SER:H	1:A:49:LEU:HD23	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1248)	1:B:6:SER:H	1:A:49:LEU:HD12	1	0.11
(1,1248)	1:B:6:SER:H	1:A:49:LEU:HD11	1	0.11
(1,1248)	1:B:6:SER:H	1:A:49:LEU:HD13	1	0.11
(1,1248)	1:B:6:SER:H	1:A:109:LEU:HD22	1	0.11
(1,1248)	1:B:6:SER:H	1:A:109:LEU:HD21	1	0.11
(1,1248)	1:B:6:SER:H	1:A:109:LEU:HD23	1	0.11
(1,1248)	1:B:6:SER:H	1:A:109:LEU:HD12	1	0.11
(1,1248)	1:B:6:SER:H	1:A:109:LEU:HD11	1	0.11
(1,1248)	1:B:6:SER:H	1:A:109:LEU:HD13	1	0.11
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD22	1	0.11
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD21	1	0.11
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD23	1	0.11
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD12	1	0.11
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD11	1	0.11
(1,1004)	1:B:49:LEU:H	1:B:49:LEU:HD13	1	0.11
(1,1004)	1:B:109:LEU:HD22	1:B:49:LEU:H	1	0.11
(1,1004)	1:B:109:LEU:HD21	1:B:49:LEU:H	1	0.11
(1,1004)	1:B:109:LEU:HD23	1:B:49:LEU:H	1	0.11
(1,1004)	1:B:109:LEU:HD12	1:B:49:LEU:H	1	0.11
(1,1004)	1:B:109:LEU:HD11	1:B:49:LEU:H	1	0.11
(1,1004)	1:B:109:LEU:HD13	1:B:49:LEU:H	1	0.11
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD22	1	0.11
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD21	1	0.11
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD23	1	0.11
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD12	1	0.11
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD11	1	0.11
(1,1003)	1:A:49:LEU:H	1:A:49:LEU:HD13	1	0.11
(1,1003)	1:A:109:LEU:HD22	1:A:49:LEU:H	1	0.11
(1,1003)	1:A:109:LEU:HD21	1:A:49:LEU:H	1	0.11
(1,1003)	1:A:109:LEU:HD23	1:A:49:LEU:H	1	0.11
(1,1003)	1:A:109:LEU:HD12	1:A:49:LEU:H	1	0.11
(1,1003)	1:A:109:LEU:HD11	1:A:49:LEU:H	1	0.11
(1,1003)	1:A:109:LEU:HD13	1:A:49:LEU:H	1	0.11

## 10 Dihedral-angle violation analysis [i](#)

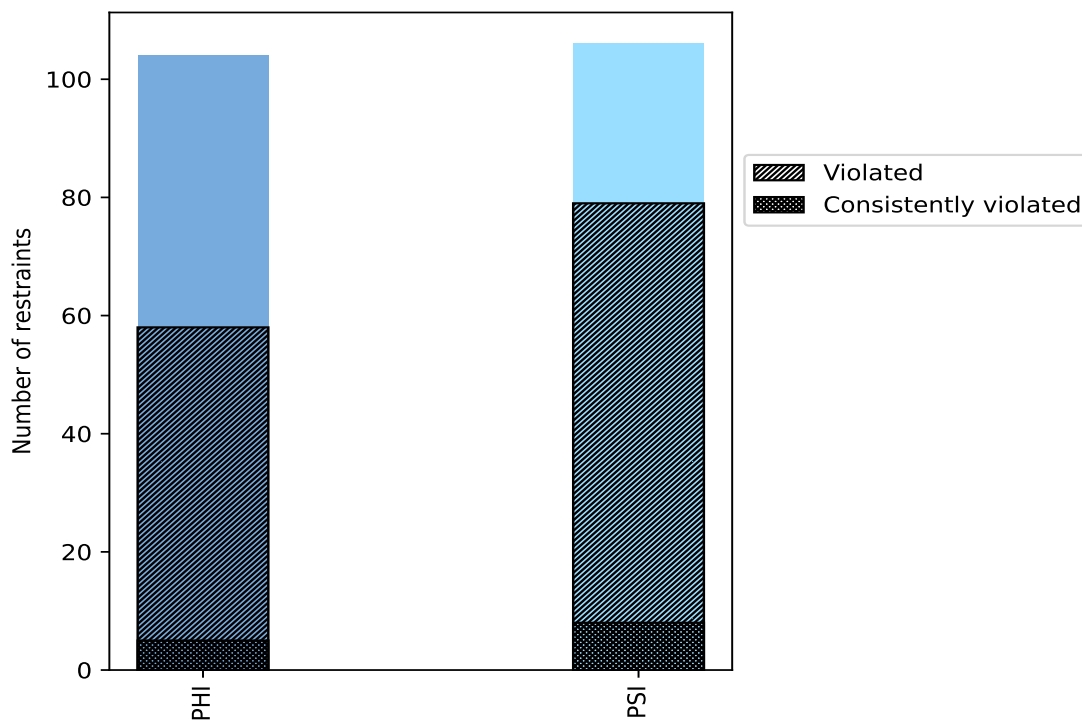
### 10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% <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>
PHI	104	49.5	58	55.8	27.6	5	4.8	2.4
PSI	106	50.5	79	74.5	37.6	8	7.5	3.8
Total	210	100.0	137	65.2	65.2	13	6.2	6.2

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

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



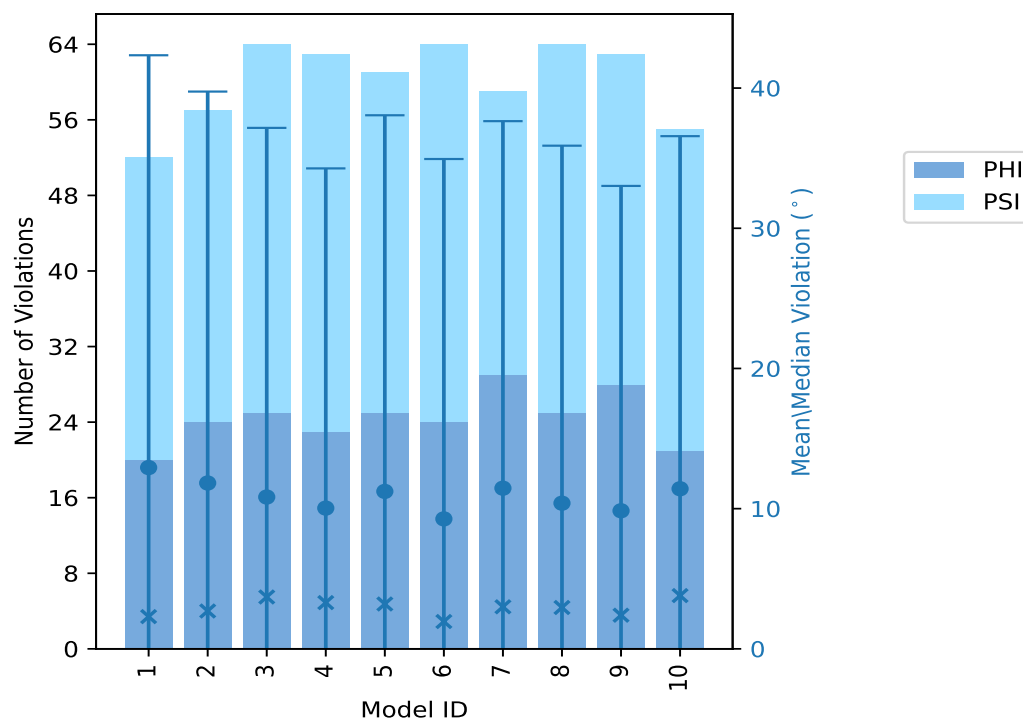
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	20	32	52	12.93	146.9	29.41	2.3
2	24	33	57	11.83	141.7	27.92	2.7
3	25	39	64	10.83	158.8	26.33	3.7
4	23	40	63	10.04	129.0	24.23	3.3
5	25	36	61	11.23	145.8	26.83	3.2
6	24	40	64	9.27	153.9	25.67	1.95
7	29	30	59	11.46	124.7	26.18	3.0
8	25	39	64	10.39	129.2	25.5	2.95
9	28	35	63	9.85	124.0	23.17	2.4
10	21	34	55	11.42	123.3	25.15	3.8

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



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

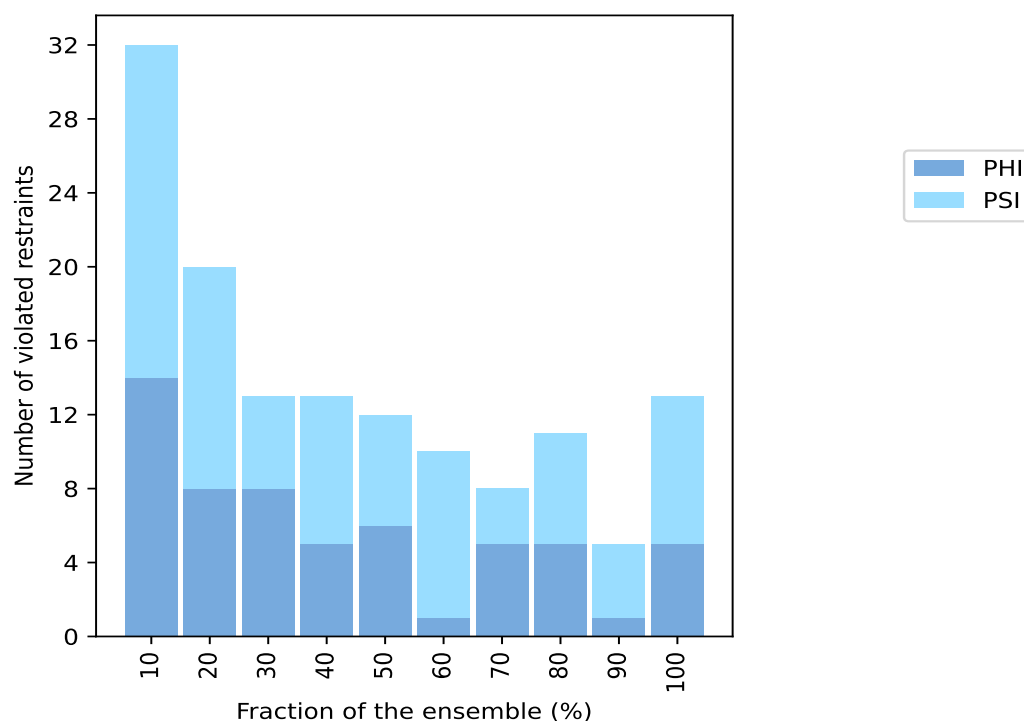
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
14	18	32	1	10.0
8	12	20	2	20.0
8	5	13	3	30.0
5	8	13	4	40.0
6	6	12	5	50.0
1	9	10	6	60.0
5	3	8	7	70.0
5	6	11	8	80.0
1	4	5	9	90.0
5	8	13	10	100.0

<sup>1</sup> Number of models with violations

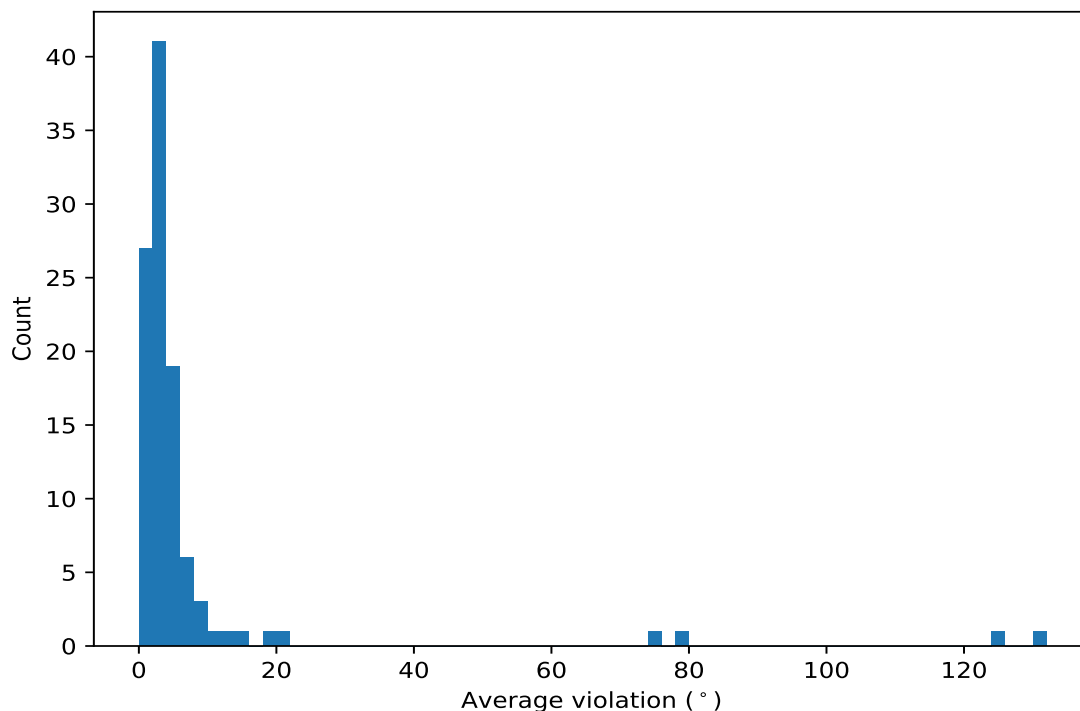
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	10	131.99	18.58	134.65
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	10	125.31	3.29	125.4
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	10	74.64	15.88	66.35
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	10	10.38	1.03	10.5
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	10	9.91	7.01	7.45
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	10	8.39	4.93	8.6
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	10	8.31	1.45	7.8
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	10	7.63	5.42	5.65
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	10	5.18	2.46	5.4
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	10	4.52	1.91	5.05
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	10	4.48	1.0	4.9
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	10	3.48	0.95	3.4
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	10	2.95	1.65	2.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	9	79.66	25.3	88.1
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	9	4.08	2.06	4.0
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	9	3.99	1.76	4.3
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	9	3.61	1.48	3.3
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	9	2.51	0.7	2.5
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	8	15.69	1.26	15.65
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	8	12.74	0.61	12.7
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	8	7.51	6.03	5.6
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	8	6.41	1.11	6.25
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	8	4.8	1.97	4.2
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	8	4.08	1.98	4.65
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	8	3.44	1.13	3.55
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	8	3.32	0.92	3.4
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	8	2.12	0.46	2.1
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	8	1.98	0.46	1.85
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	8	1.72	0.44	1.6
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	7	6.01	3.39	5.5
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	7	5.09	2.82	5.4
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	7	4.96	3.98	3.6
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	7	4.64	2.69	6.1
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	7	2.91	1.09	2.4
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	7	2.73	1.11	2.5
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	7	2.44	0.81	2.4
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	7	2.06	0.9	1.7
(1,200)	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1:A:109:LEU:N	6	20.92	15.3	21.2
(1,180)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	6	7.55	5.5	6.6
(1,176)	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	1:A:97:GLY:N	6	5.33	2.63	4.2
(1,185)	1:A:100:GLY:C	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	6	4.58	2.92	3.4
(1,204)	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1:A:111:GLU:N	6	3.75	3.43	2.4
(1,6)	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	1:A:8:LEU:N	6	2.92	0.96	3.25
(1,52)	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	1:A:33:ASN:N	6	2.88	1.01	2.6
(1,4)	1:A:6:SER:N	1:A:6:SER:CA	1:A:6:SER:C	1:A:7:GLN:N	6	2.87	1.22	3.05
(1,160)	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	1:A:89:ALA:N	6	2.23	0.75	2.05
(1,105)	1:A:60:GLU:N	1:A:60:GLU:CA	1:A:60:GLU:C	1:A:61:HIS:N	6	2.03	0.44	1.95
(1,201)	1:A:108:GLY:C	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	5	19.5	12.49	27.1
(1,184)	1:A:100:GLY:N	1:A:100:GLY:CA	1:A:100:GLY:C	1:A:101:PRO:N	5	6.04	3.46	6.2
(1,181)	1:A:98:ASP:C	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	5	5.76	2.66	4.1
(1,136)	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	1:A:77:GLU:N	5	3.18	1.9	2.3
(1,132)	1:A:74:LEU:N	1:A:74:LEU:CA	1:A:74:LEU:C	1:A:75:SER:N	5	2.98	0.67	3.2
(1,194)	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	1:A:106:LYS:N	5	2.92	1.5	2.0
(1,170)	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	1:A:94:MET:N	5	2.64	1.29	2.2
(1,121)	1:A:68:THR:C	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	5	2.5	0.84	2.3
(1,43)	1:A:25:LYS:C	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	5	2.36	0.91	2.3
(1,89)	1:A:51:LYS:C	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	5	2.32	0.78	2.3
(1,92)	1:A:53:ASN:N	1:A:53:ASN:CA	1:A:53:ASN:C	1:A:54:LYS:N	5	1.74	0.76	1.4
(1,5)	1:A:6:SER:C	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	5	1.72	0.6	1.6
(1,192)	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	1:A:105:HIS:N	4	5.6	3.29	4.75
(1,193)	1:A:104:HIS:C	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	4	5.1	3.17	3.95
(1,75)	1:A:44:ASP:C	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	4	3.38	0.4	3.4
(1,169)	1:A:92:GLU:C	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	4	3.08	2.22	2.0
(1,188)	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	1:A:103:HIS:N	4	2.62	0.68	2.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,142)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:ILE:N	4	2.47	0.51	2.45
(1,74)	1:A:44:ASP:N	1:A:44:ASP:CA	1:A:44:ASP:C	1:A:45:LEU:N	4	2.32	0.53	2.35
(1,35)	1:A:21:GLN:C	1:A:22:TYR:N	1:A:22:TYR:CA	1:A:22:TYR:C	4	1.65	0.41	1.5
(1,109)	1:A:62:ILE:N	1:A:62:ILE:CA	1:A:62:ILE:C	1:A:63:MET:N	4	1.6	0.35	1.45
(1,34)	1:A:21:GLN:N	1:A:21:GLN:CA	1:A:21:GLN:C	1:A:22:TYR:N	4	1.58	0.33	1.5
(1,40)	1:A:24:VAL:N	1:A:24:VAL:CA	1:A:24:VAL:C	1:A:25:LYS:N	4	1.4	0.35	1.25
(1,90)	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	1:A:53:ASN:N	4	1.4	0.46	1.15
(1,57)	1:A:34:GLN:C	1:A:35:GLY:N	1:A:35:GLY:CA	1:A:35:GLY:C	4	1.27	0.13	1.3
(1,48)	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	1:A:31:THR:N	3	4.5	2.36	3.3
(1,173)	1:A:94:MET:C	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	3	4.13	2.26	2.9
(1,177)	1:A:96:GLU:C	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	3	4.07	3.13	2.7
(1,182)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:GLY:N	3	3.8	1.85	3.2
(1,162)	1:A:89:ALA:N	1:A:89:ALA:CA	1:A:89:ALA:C	1:A:90:SER:N	3	3.33	2.13	2.7
(1,135)	1:A:75:SER:C	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	3	3.03	1.77	2.2
(1,18)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:THR:N	3	2.8	1.15	3.0
(1,195)	1:A:105:HIS:C	1:A:106:LYS:N	1:A:106:LYS:CA	1:A:106:LYS:C	3	2.5	0.5	2.2
(1,157)	1:A:86:LEU:C	1:A:87:THR:N	1:A:87:THR:CA	1:A:87:THR:C	3	1.7	0.43	1.9
(1,159)	1:A:87:THR:C	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	3	1.7	0.14	1.6
(1,10)	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	1:A:10:ARG:N	3	1.57	0.34	1.7
(1,127)	1:A:71:ASP:C	1:A:72:LYS:N	1:A:72:LYS:CA	1:A:72:LYS:C	3	1.5	0.22	1.4
(1,31)	1:A:19:PHE:C	1:A:20:HIS:N	1:A:20:HIS:CA	1:A:20:HIS:C	3	1.47	0.17	1.4
(1,164)	1:A:90:SER:N	1:A:90:SER:CA	1:A:90:SER:C	1:A:91:HIS:N	2	5.15	3.25	5.15
(1,205)	1:A:110:GLY:C	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	2	5.05	3.95	5.05
(1,117)	1:A:66:LEU:C	1:A:67:ASP:N	1:A:67:ASP:CA	1:A:67:ASP:C	2	3.4	1.5	3.4
(1,8)	1:A:8:LEU:N	1:A:8:LEU:CA	1:A:8:LEU:C	1:A:9:GLU:N	2	2.95	1.85	2.95
(1,32)	1:A:20:HIS:N	1:A:20:HIS:CA	1:A:20:HIS:C	1:A:21:GLN:N	2	2.7	0.5	2.7
(1,119)	1:A:67:ASP:C	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	2	2.35	0.55	2.35
(1,171)	1:A:93:LYS:C	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	2	2.2	1.1	2.2
(1,16)	1:A:12:ILE:N	1:A:12:ILE:CA	1:A:12:ILE:C	1:A:13:GLU:N	2	2.05	0.45	2.05
(1,129)	1:A:72:LYS:C	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	2	1.85	0.25	1.85
(1,209)	1:A:112:GLY:C	1:A:113:THR:N	1:A:113:THR:CA	1:A:113:THR:C	2	1.85	0.05	1.85
(1,124)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ASP:N	2	1.8	0.7	1.8
(1,51)	1:A:31:THR:C	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	2	1.75	0.65	1.75
(1,116)	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	1:A:67:ASP:N	2	1.7	0.2	1.7
(1,210)	1:A:113:THR:N	1:A:113:THR:CA	1:A:113:THR:C	1:A:114:PRO:N	2	1.7	0.3	1.7
(1,80)	1:A:47:ASN:N	1:A:47:ASN:CA	1:A:47:ASN:C	1:A:48:PHE:N	2	1.65	0.45	1.65
(1,42)	1:A:25:LYS:N	1:A:25:LYS:CA	1:A:25:LYS:C	1:A:26:LEU:N	2	1.5	0.2	1.5
(1,61)	1:A:36:GLU:C	1:A:37:PHE:N	1:A:37:PHE:CA	1:A:37:PHE:C	2	1.4	0.3	1.4
(1,120)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:ASN:N	2	1.4	0.1	1.4
(1,44)	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	1:A:27:GLY:N	2	1.25	0.05	1.25
(1,111)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:GLU:N	2	1.2	0.0	1.2

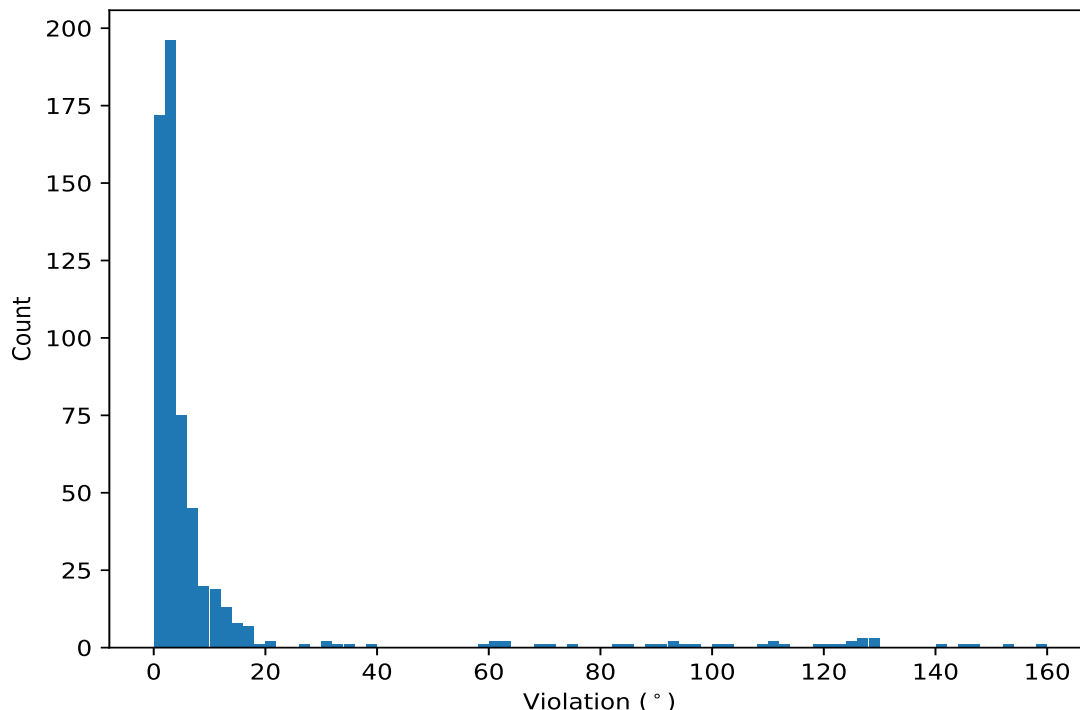
<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)



## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	3	158.8
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	6	153.9
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	1	146.9
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	5	145.8
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	2	141.7
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	6	129.8
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	8	129.2
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	4	129.0
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	4	127.6
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	1	126.3
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	2	126.1
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	7	124.7
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	9	124.0
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	10	123.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	5	121.4
(1,166)	1:A:91:HIS:N	1:A:91:HIS:CA	1:A:91:HIS:C	1:A:92:GLU:N	3	119.3
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	7	113.4
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	8	111.9
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	10	111.4
(1,172)	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	1:A:95:HIS:N	9	108.5
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	7	102.8
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	5	100.6
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	8	97.5
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	2	94.2
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	9	93.0
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	1	92.4
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	8	91.7
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	10	88.1
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	3	84.0
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	7	83.9
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	2	75.1
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	4	70.2
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	10	69.4
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	6	63.3
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	4	62.6
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	1	61.8
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	5	61.1
(1,174)	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	1:A:96:GLU:N	3	59.8
(1,200)	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1:A:109:LEU:N	1	39.3
(1,200)	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1:A:109:LEU:N	9	35.4
(1,200)	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1:A:109:LEU:N	6	33.2
(1,201)	1:A:108:GLY:C	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1	31.2
(1,201)	1:A:108:GLY:C	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	9	30.5
(1,201)	1:A:108:GLY:C	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	6	27.1
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	9	21.4
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	7	20.0
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	6	19.4
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	1	17.6
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	10	17.1
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	5	16.5
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	6	16.5
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	2	16.4
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	9	16.2
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	2	16.1
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	9	15.9
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	7	15.7
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	4	15.2
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	7	14.8
(1,180)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	7	14.7
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	8	14.3
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	4	14.1
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1	14.1
(1,49)	1:A:30:ASP:C	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	3	13.9
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	2	13.5
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	10	13.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,180)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	10	13.4
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	9	13.2
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	5	12.9
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	10	12.9
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	2	12.9
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	3	12.8
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	7	12.6
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	2	12.4
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	8	12.3
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	9	12.2
(1,47)	1:A:29:PRO:C	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	1	11.9
(1,46)	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1:A:30:ASP:N	6	11.8
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	3	11.8
(1,204)	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1:A:111:GLU:N	7	11.4
(1,184)	1:A:100:GLY:N	1:A:100:GLY:CA	1:A:100:GLY:C	1:A:101:PRO:N	4	11.4
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	6	11.4
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	2	11.1
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	5	10.8
(1,192)	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	1:A:105:HIS:N	5	10.7
(1,180)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	9	10.6
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	8	10.6
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	1	10.5
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	4	10.5
(1,193)	1:A:104:HIS:C	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	5	10.4
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	1	10.4
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	7	10.3
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	9	10.1
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	2	10.0
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	7	10.0
(1,185)	1:A:100:GLY:C	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	3	9.9
(1,181)	1:A:98:ASP:C	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	10	9.9
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	2	9.9
(1,176)	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	1:A:97:GLY:N	8	9.7
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	3	9.5
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	3	9.5
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	5	9.4
(1,200)	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1:A:109:LEU:N	5	9.2
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	4	9.2
(1,205)	1:A:110:GLY:C	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	7	9.0
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	10	9.0
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	5	8.9
(1,112)	1:A:64:GLU:N	1:A:64:GLU:CA	1:A:64:GLU:C	1:A:65:ASP:N	10	8.6
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	7	8.5
(1,177)	1:A:96:GLU:C	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	10	8.4
(1,164)	1:A:90:SER:N	1:A:90:SER:CA	1:A:90:SER:C	1:A:91:HIS:N	3	8.4
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	2	8.3
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	3	8.1
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	8	8.0
(1,176)	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	1:A:97:GLY:N	10	8.0
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	8	7.9
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	4	7.9

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:A:100:GLY:N	1:A:100:GLY:CA	1:A:100:GLY:C	1:A:101:PRO:N	3	7.9
(1,181)	1:A:98:ASP:C	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	7	7.9
(1,48)	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	1:A:31:THR:N	9	7.8
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	3	7.8
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	4	7.6
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	5	7.6
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	2	7.6
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	4	7.5
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	10	7.5
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	3	7.3
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	8	7.3
(1,173)	1:A:94:MET:C	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	3	7.3
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	10	7.2
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	8	7.2
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	4	7.1
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	2	7.1
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	4	7.0
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	5	6.9
(1,185)	1:A:100:GLY:C	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	4	6.9
(1,169)	1:A:92:GLU:C	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	3	6.9
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1	6.8
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	4	6.8
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	10	6.6
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	3	6.6
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	8	6.6
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	5	6.6
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	1	6.5
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	4	6.5
(1,200)	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1:A:109:LEU:N	3	6.4
(1,76)	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	1:A:46:GLN:N	6	6.3
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	8	6.3
(1,182)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:GLY:N	10	6.3
(1,136)	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	1:A:77:GLU:N	8	6.3
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	3	6.3
(1,192)	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	1:A:105:HIS:N	10	6.2
(1,184)	1:A:100:GLY:N	1:A:100:GLY:CA	1:A:100:GLY:C	1:A:101:PRO:N	8	6.2
(1,162)	1:A:89:ALA:N	1:A:89:ALA:CA	1:A:89:ALA:C	1:A:90:SER:N	3	6.2
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	10	6.1
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	8	6.1
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	5	6.0
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	5	6.0
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	5	6.0
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	2	6.0
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	6	5.9
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	6	5.9
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	2	5.9
(1,201)	1:A:108:GLY:C	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	5	5.9
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	7	5.7
(1,194)	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	1:A:106:LYS:N	9	5.7
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	5	5.7
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	1	5.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	3	5.6
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	5	5.6
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	5	5.6
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	3	5.6
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	6	5.6
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	1	5.5
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	3	5.5
(1,158)	1:A:87:THR:N	1:A:87:THR:CA	1:A:87:THR:C	1:A:88:TRP:N	3	5.5
(1,135)	1:A:75:SER:C	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	8	5.5
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	3	5.5
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	4	5.5
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	7	5.4
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	5	5.4
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	2	5.4
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	8	5.4
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	7	5.3
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	4	5.2
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	7	5.2
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	5	5.2
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1	5.2
(1,45)	1:A:28:HIS:C	1:A:29:PRO:N	1:A:29:PRO:CA	1:A:29:PRO:C	8	5.1
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	2	5.0
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	9	5.0
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	8	5.0
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	5	4.9
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	2	4.9
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	8	4.9
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	8	4.9
(1,117)	1:A:66:LEU:C	1:A:67:ASP:N	1:A:67:ASP:CA	1:A:67:ASP:C	3	4.9
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	5	4.8
(1,8)	1:A:8:LEU:N	1:A:8:LEU:CA	1:A:8:LEU:C	1:A:9:GLU:N	10	4.8
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	8	4.8
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	5	4.8
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	2	4.8
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	4	4.8
(1,52)	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	1:A:33:ASN:N	4	4.7
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	4	4.7
(1,176)	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	1:A:97:GLY:N	9	4.7
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	9	4.6
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	10	4.6
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	10	4.6
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	9	4.5
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	9	4.5
(1,4)	1:A:6:SER:N	1:A:6:SER:CA	1:A:6:SER:C	1:A:7:GLN:N	10	4.4
(1,193)	1:A:104:HIS:C	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	10	4.4
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	7	4.4
(1,170)	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	1:A:94:MET:N	3	4.4
(1,136)	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	1:A:77:GLU:N	3	4.4
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	5	4.4
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	2	4.3
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	9	4.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	8	4.3
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	10	4.2
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1	4.2
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	3	4.1
(1,4)	1:A:6:SER:N	1:A:6:SER:CA	1:A:6:SER:C	1:A:7:GLN:N	4	4.1
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	4	4.1
(1,181)	1:A:98:ASP:C	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	9	4.1
(1,18)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:THR:N	8	4.1
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	1	4.1
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	2	4.0
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	4	4.0
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	1	4.0
(1,6)	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	1:A:8:LEU:N	6	4.0
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	10	4.0
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	4	4.0
(1,175)	1:A:95:HIS:C	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	3	4.0
(1,75)	1:A:44:ASP:C	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	9	3.9
(1,185)	1:A:100:GLY:C	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	5	3.9
(1,170)	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	1:A:94:MET:N	9	3.9
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	10	3.8
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	10	3.8
(1,43)	1:A:25:LYS:C	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	9	3.8
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	4	3.8
(1,160)	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	1:A:89:ALA:N	9	3.8
(1,132)	1:A:74:LEU:N	1:A:74:LEU:CA	1:A:74:LEU:C	1:A:75:SER:N	4	3.8
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	7	3.7
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	3	3.7
(1,181)	1:A:98:ASP:C	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	3	3.7
(1,176)	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	1:A:97:GLY:N	3	3.7
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	6	3.7
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	8	3.7
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	2	3.6
(1,6)	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	1:A:8:LEU:N	1	3.6
(1,6)	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	1:A:8:LEU:N	4	3.6
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	7	3.6
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	3	3.6
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	3	3.6
(1,176)	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	1:A:97:GLY:N	7	3.6
(1,167)	1:A:91:HIS:C	1:A:92:GLU:N	1:A:92:GLU:CA	1:A:92:GLU:C	3	3.6
(1,121)	1:A:68:THR:C	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	4	3.6
(1,89)	1:A:51:LYS:C	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	4	3.5
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	10	3.5
(1,75)	1:A:44:ASP:C	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	3	3.5
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	3	3.5
(1,52)	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	1:A:33:ASN:N	1	3.5
(1,193)	1:A:104:HIS:C	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	7	3.5
(1,132)	1:A:74:LEU:N	1:A:74:LEU:CA	1:A:74:LEU:C	1:A:75:SER:N	1	3.5
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	8	3.5
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	6	3.5
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	3	3.4
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	8	3.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	7	3.4
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	4	3.3
(1,75)	1:A:44:ASP:C	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	2	3.3
(1,48)	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	1:A:31:THR:N	6	3.3
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	4	3.3
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	7	3.3
(1,194)	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	1:A:106:LYS:N	6	3.3
(1,192)	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	1:A:105:HIS:N	2	3.3
(1,188)	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	1:A:103:HIS:N	8	3.3
(1,171)	1:A:93:LYS:C	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	5	3.3
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	1	3.2
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	7	3.2
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	7	3.2
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	4	3.2
(1,32)	1:A:20:HIS:N	1:A:20:HIS:CA	1:A:20:HIS:C	1:A:21:GLN:N	4	3.2
(1,195)	1:A:105:HIS:C	1:A:106:LYS:N	1:A:106:LYS:CA	1:A:106:LYS:C	6	3.2
(1,182)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:GLY:N	2	3.2
(1,181)	1:A:98:ASP:C	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	5	3.2
(1,142)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:ILE:N	10	3.2
(1,132)	1:A:74:LEU:N	1:A:74:LEU:CA	1:A:74:LEU:C	1:A:75:SER:N	5	3.2
(1,121)	1:A:68:THR:C	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	9	3.2
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	8	3.2
(1,92)	1:A:53:ASN:N	1:A:53:ASN:CA	1:A:53:ASN:C	1:A:54:LYS:N	6	3.1
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	6	3.1
(1,52)	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	1:A:33:ASN:N	6	3.1
(1,4)	1:A:6:SER:N	1:A:6:SER:CA	1:A:6:SER:C	1:A:7:GLN:N	8	3.1
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	10	3.1
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	7	3.1
(1,4)	1:A:6:SER:N	1:A:6:SER:CA	1:A:6:SER:C	1:A:7:GLN:N	5	3.0
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	7	3.0
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	7	3.0
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	1	3.0
(1,18)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:THR:N	7	3.0
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	9	3.0
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	6	2.9
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1	2.9
(1,74)	1:A:44:ASP:N	1:A:44:ASP:CA	1:A:44:ASP:C	1:A:45:LEU:N	5	2.9
(1,6)	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	1:A:8:LEU:N	7	2.9
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	9	2.9
(1,188)	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	1:A:103:HIS:N	5	2.9
(1,185)	1:A:100:GLY:C	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	6	2.9
(1,183)	1:A:99:GLU:C	1:A:100:GLY:N	1:A:100:GLY:CA	1:A:100:GLY:C	10	2.9
(1,173)	1:A:94:MET:C	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	7	2.9
(1,119)	1:A:67:ASP:C	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	4	2.9
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	2	2.9
(1,107)	1:A:61:HIS:N	1:A:61:HIS:CA	1:A:61:HIS:C	1:A:62:ILE:N	4	2.9
(1,89)	1:A:51:LYS:C	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	7	2.8
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	5	2.8
(1,75)	1:A:44:ASP:C	1:A:45:LEU:N	1:A:45:LEU:CA	1:A:45:LEU:C	7	2.8
(1,74)	1:A:44:ASP:N	1:A:44:ASP:CA	1:A:44:ASP:C	1:A:45:LEU:N	8	2.8
(1,43)	1:A:25:LYS:C	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	8	2.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,201)	1:A:108:GLY:C	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	3	2.8
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	4	2.8
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	4	2.8
(1,188)	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	1:A:103:HIS:N	4	2.8
(1,78)	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	1:A:47:ASN:N	5	2.7
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	10	2.7
(1,184)	1:A:100:GLY:N	1:A:100:GLY:CA	1:A:100:GLY:C	1:A:101:PRO:N	5	2.7
(1,177)	1:A:96:GLU:C	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	2	2.7
(1,162)	1:A:89:ALA:N	1:A:89:ALA:CA	1:A:89:ALA:C	1:A:90:SER:N	7	2.7
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	9	2.7
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	2	2.6
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	9	2.6
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	8	2.6
(1,5)	1:A:6:SER:C	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	5	2.6
(1,204)	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1:A:111:GLU:N	3	2.6
(1,204)	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1:A:111:GLU:N	5	2.6
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	2	2.6
(1,180)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	3	2.6
(1,142)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:ILE:N	6	2.6
(1,105)	1:A:60:GLU:N	1:A:60:GLU:CA	1:A:60:GLU:C	1:A:61:HIS:N	4	2.6
(1,105)	1:A:60:GLU:N	1:A:60:GLU:CA	1:A:60:GLU:C	1:A:61:HIS:N	8	2.6
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	10	2.5
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	9	2.5
(1,180)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	5	2.5
(1,16)	1:A:12:ILE:N	1:A:12:ILE:CA	1:A:12:ILE:C	1:A:13:GLU:N	6	2.5
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	2	2.5
(1,124)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ASP:N	8	2.5
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	5	2.5
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	10	2.5
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	7	2.4
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	8	2.4
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	5	2.4
(1,51)	1:A:31:THR:C	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	9	2.4
(1,48)	1:A:30:ASP:N	1:A:30:ASP:CA	1:A:30:ASP:C	1:A:31:THR:N	8	2.4
(1,207)	1:A:111:GLU:C	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	7	2.4
(1,199)	1:A:107:PRO:C	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	6	2.4
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	10	2.4
(1,185)	1:A:100:GLY:C	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	8	2.4
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	10	2.4
(1,89)	1:A:51:LYS:C	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	1	2.3
(1,43)	1:A:25:LYS:C	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	5	2.3
(1,35)	1:A:21:GLN:C	1:A:22:TYR:N	1:A:22:TYR:CA	1:A:22:TYR:C	2	2.3
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	6	2.3
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	5	2.3
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	7	2.3
(1,176)	1:A:96:GLU:N	1:A:96:GLU:CA	1:A:96:GLU:C	1:A:97:GLY:N	4	2.3
(1,160)	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	1:A:89:ALA:N	1	2.3
(1,142)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:ILE:N	2	2.3
(1,136)	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	1:A:77:GLU:N	4	2.3
(1,132)	1:A:74:LEU:N	1:A:74:LEU:CA	1:A:74:LEU:C	1:A:75:SER:N	2	2.3
(1,121)	1:A:68:THR:C	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1	2.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	9	2.2
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	2	2.2
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	3	2.2
(1,90)	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	1:A:53:ASN:N	2	2.2
(1,9)	1:A:8:LEU:C	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	10	2.2
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	9	2.2
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	1	2.2
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	2	2.2
(1,6)	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	1:A:8:LEU:N	2	2.2
(1,5)	1:A:6:SER:C	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	8	2.2
(1,32)	1:A:20:HIS:N	1:A:20:HIS:CA	1:A:20:HIS:C	1:A:21:GLN:N	1	2.2
(1,204)	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1:A:111:GLU:N	2	2.2
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	10	2.2
(1,195)	1:A:105:HIS:C	1:A:106:LYS:N	1:A:106:LYS:CA	1:A:106:LYS:C	5	2.2
(1,192)	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	1:A:105:HIS:N	7	2.2
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	9	2.2
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	5	2.2
(1,173)	1:A:94:MET:C	1:A:95:HIS:N	1:A:95:HIS:CA	1:A:95:HIS:C	9	2.2
(1,170)	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	1:A:94:MET:N	1	2.2
(1,160)	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	1:A:89:ALA:N	3	2.2
(1,140)	1:A:78:GLU:N	1:A:78:GLU:CA	1:A:78:GLU:C	1:A:79:PHE:N	3	2.2
(1,135)	1:A:75:SER:C	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	7	2.2
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	6	2.2
(1,121)	1:A:68:THR:C	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	2	2.2
(1,109)	1:A:62:ILE:N	1:A:62:ILE:CA	1:A:62:ILE:C	1:A:63:MET:N	4	2.2
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	1	2.1
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	5	2.1
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	10	2.1
(1,88)	1:A:51:LYS:N	1:A:51:LYS:CA	1:A:51:LYS:C	1:A:52:GLU:N	2	2.1
(1,80)	1:A:47:ASN:N	1:A:47:ASN:CA	1:A:47:ASN:C	1:A:48:PHE:N	8	2.1
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	8	2.1
(1,54)	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	1:A:34:GLN:N	3	2.1
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	10	2.1
(1,52)	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	1:A:33:ASN:N	7	2.1
(1,50)	1:A:31:THR:N	1:A:31:THR:CA	1:A:31:THR:C	1:A:32:LEU:N	1	2.1
(1,34)	1:A:21:GLN:N	1:A:21:GLN:CA	1:A:21:GLN:C	1:A:22:TYR:N	1	2.1
(1,28)	1:A:18:THR:N	1:A:18:THR:CA	1:A:18:THR:C	1:A:19:PHE:N	6	2.1
(1,195)	1:A:105:HIS:C	1:A:106:LYS:N	1:A:106:LYS:CA	1:A:106:LYS:C	9	2.1
(1,193)	1:A:104:HIS:C	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	6	2.1
(1,157)	1:A:86:LEU:C	1:A:87:THR:N	1:A:87:THR:CA	1:A:87:THR:C	3	2.1
(1,137)	1:A:76:PHE:C	1:A:77:GLU:N	1:A:77:GLU:CA	1:A:77:GLU:C	8	2.1
(1,132)	1:A:74:LEU:N	1:A:74:LEU:CA	1:A:74:LEU:C	1:A:75:SER:N	10	2.1
(1,129)	1:A:72:LYS:C	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	8	2.1
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	1	2.1
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	7	2.1
(1,92)	1:A:53:ASN:N	1:A:53:ASN:CA	1:A:53:ASN:C	1:A:54:LYS:N	5	2.0
(1,52)	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	1:A:33:ASN:N	10	2.0
(1,40)	1:A:24:VAL:N	1:A:24:VAL:CA	1:A:24:VAL:C	1:A:25:LYS:N	8	2.0
(1,210)	1:A:113:THR:N	1:A:113:THR:CA	1:A:113:THR:C	1:A:114:PRO:N	9	2.0
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	1	2.0
(1,200)	1:A:108:GLY:N	1:A:108:GLY:CA	1:A:108:GLY:C	1:A:109:LEU:N	8	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,197)	1:A:106:LYS:C	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	9	2.0
(1,194)	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	1:A:106:LYS:N	5	2.0
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	9	2.0
(1,184)	1:A:100:GLY:N	1:A:100:GLY:CA	1:A:100:GLY:C	1:A:101:PRO:N	6	2.0
(1,169)	1:A:92:GLU:C	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	1	2.0
(1,169)	1:A:92:GLU:C	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	2	2.0
(1,14)	1:A:11:ASN:N	1:A:11:ASN:CA	1:A:11:ASN:C	1:A:12:ILE:N	7	2.0
(1,105)	1:A:60:GLU:N	1:A:60:GLU:CA	1:A:60:GLU:C	1:A:61:HIS:N	3	2.0
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	4	1.9
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	3	1.9
(1,74)	1:A:44:ASP:N	1:A:44:ASP:CA	1:A:44:ASP:C	1:A:45:LEU:N	4	1.9
(1,72)	1:A:42:ARG:N	1:A:42:ARG:CA	1:A:42:ARG:C	1:A:43:LYS:N	3	1.9
(1,52)	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	1:A:33:ASN:N	9	1.9
(1,26)	1:A:17:ASN:N	1:A:17:ASN:CA	1:A:17:ASN:C	1:A:18:THR:N	6	1.9
(1,24)	1:A:16:ILE:N	1:A:16:ILE:CA	1:A:16:ILE:C	1:A:17:ASN:N	5	1.9
(1,209)	1:A:112:GLY:C	1:A:113:THR:N	1:A:113:THR:CA	1:A:113:THR:C	2	1.9
(1,204)	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1:A:111:GLU:N	4	1.9
(1,194)	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	1:A:106:LYS:N	4	1.9
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	2	1.9
(1,182)	1:A:99:GLU:N	1:A:99:GLU:CA	1:A:99:GLU:C	1:A:100:GLY:N	5	1.9
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	5	1.9
(1,178)	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	1:A:98:ASP:N	6	1.9
(1,164)	1:A:90:SER:N	1:A:90:SER:CA	1:A:90:SER:C	1:A:91:HIS:N	9	1.9
(1,163)	1:A:89:ALA:C	1:A:90:SER:N	1:A:90:SER:CA	1:A:90:SER:C	9	1.9
(1,160)	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	1:A:89:ALA:N	4	1.9
(1,159)	1:A:87:THR:C	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	6	1.9
(1,157)	1:A:86:LEU:C	1:A:87:THR:N	1:A:87:THR:CA	1:A:87:THR:C	7	1.9
(1,141)	1:A:78:GLU:C	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	7	1.9
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	10	1.9
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	1	1.9
(1,117)	1:A:66:LEU:C	1:A:67:ASP:N	1:A:67:ASP:CA	1:A:67:ASP:C	8	1.9
(1,116)	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	1:A:67:ASP:N	6	1.9
(1,105)	1:A:60:GLU:N	1:A:60:GLU:CA	1:A:60:GLU:C	1:A:61:HIS:N	2	1.9
(1,10)	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	1:A:10:ARG:N	9	1.9
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	6	1.8
(1,77)	1:A:45:LEU:C	1:A:46:GLN:N	1:A:46:GLN:CA	1:A:46:GLN:C	6	1.8
(1,66)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:LEU:N	6	1.8
(1,43)	1:A:25:LYS:C	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	1	1.8
(1,38)	1:A:23:SER:N	1:A:23:SER:CA	1:A:23:SER:C	1:A:24:VAL:N	8	1.8
(1,30)	1:A:19:PHE:N	1:A:19:PHE:CA	1:A:19:PHE:C	1:A:20:HIS:N	4	1.8
(1,209)	1:A:112:GLY:C	1:A:113:THR:N	1:A:113:THR:CA	1:A:113:THR:C	10	1.8
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	1	1.8
(1,204)	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	1:A:111:GLU:N	8	1.8
(1,203)	1:A:109:LEU:C	1:A:110:GLY:N	1:A:110:GLY:CA	1:A:110:GLY:C	3	1.8
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	6	1.8
(1,189)	1:A:102:GLY:C	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	4	1.8
(1,142)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:ILE:N	1	1.8
(1,131)	1:A:73:GLN:C	1:A:74:LEU:N	1:A:74:LEU:CA	1:A:74:LEU:C	1	1.8
(1,130)	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	1:A:74:LEU:N	5	1.8
(1,127)	1:A:71:ASP:C	1:A:72:LYS:N	1:A:72:LYS:CA	1:A:72:LYS:C	8	1.8
(1,119)	1:A:67:ASP:C	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	9	1.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	6	1.7
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	10	1.7
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	6	1.7
(1,89)	1:A:51:LYS:C	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	10	1.7
(1,84)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:LYS:N	3	1.7
(1,74)	1:A:44:ASP:N	1:A:44:ASP:CA	1:A:44:ASP:C	1:A:45:LEU:N	10	1.7
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	4	1.7
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	6	1.7
(1,61)	1:A:36:GLU:C	1:A:37:PHE:N	1:A:37:PHE:CA	1:A:37:PHE:C	3	1.7
(1,42)	1:A:25:LYS:N	1:A:25:LYS:CA	1:A:25:LYS:C	1:A:26:LEU:N	5	1.7
(1,35)	1:A:21:GLN:C	1:A:22:TYR:N	1:A:22:TYR:CA	1:A:22:TYR:C	6	1.7
(1,31)	1:A:19:PHE:C	1:A:20:HIS:N	1:A:20:HIS:CA	1:A:20:HIS:C	4	1.7
(1,206)	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	1:A:112:GLY:N	8	1.7
(1,194)	1:A:105:HIS:N	1:A:105:HIS:CA	1:A:105:HIS:C	1:A:106:LYS:N	10	1.7
(1,190)	1:A:103:HIS:N	1:A:103:HIS:CA	1:A:103:HIS:C	1:A:104:HIS:N	8	1.7
(1,160)	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	1:A:89:ALA:N	8	1.7
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	3	1.7
(1,105)	1:A:60:GLU:N	1:A:60:GLU:CA	1:A:60:GLU:C	1:A:61:HIS:N	1	1.7
(1,10)	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	1:A:10:ARG:N	5	1.7
(1,93)	1:A:53:ASN:C	1:A:54:LYS:N	1:A:54:LYS:CA	1:A:54:LYS:C	8	1.6
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	2	1.6
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	5	1.6
(1,55)	1:A:33:ASN:C	1:A:34:GLN:N	1:A:34:GLN:CA	1:A:34:GLN:C	9	1.6
(1,5)	1:A:6:SER:C	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	3	1.6
(1,34)	1:A:21:GLN:N	1:A:21:GLN:CA	1:A:21:GLN:C	1:A:22:TYR:N	6	1.6
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	7	1.6
(1,196)	1:A:106:LYS:N	1:A:106:LYS:CA	1:A:106:LYS:C	1:A:107:PRO:N	8	1.6
(1,170)	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	1:A:94:MET:N	6	1.6
(1,16)	1:A:12:ILE:N	1:A:12:ILE:CA	1:A:12:ILE:C	1:A:13:GLU:N	10	1.6
(1,159)	1:A:87:THR:C	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	2	1.6
(1,159)	1:A:87:THR:C	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	9	1.6
(1,136)	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	1:A:77:GLU:N	6	1.6
(1,129)	1:A:72:LYS:C	1:A:73:GLN:N	1:A:73:GLN:CA	1:A:73:GLN:C	7	1.6
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	8	1.5
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	4	1.5
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	10	1.5
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	9	1.5
(1,4)	1:A:6:SER:N	1:A:6:SER:CA	1:A:6:SER:C	1:A:7:GLN:N	6	1.5
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	9	1.5
(1,188)	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	1:A:103:HIS:N	3	1.5
(1,185)	1:A:100:GLY:C	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	2	1.5
(1,180)	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	1:A:99:GLU:N	2	1.5
(1,160)	1:A:88:TRP:N	1:A:88:TRP:CA	1:A:88:TRP:C	1:A:89:ALA:N	6	1.5
(1,122)	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	1:A:70:ALA:N	6	1.5
(1,120)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:ASN:N	6	1.5
(1,116)	1:A:66:LEU:N	1:A:66:LEU:CA	1:A:66:LEU:C	1:A:67:ASP:N	8	1.5
(1,109)	1:A:62:ILE:N	1:A:62:ILE:CA	1:A:62:ILE:C	1:A:63:MET:N	6	1.5
(1,103)	1:A:59:ILE:N	1:A:59:ILE:CA	1:A:59:ILE:C	1:A:60:GLU:N	8	1.5
(1,92)	1:A:53:ASN:N	1:A:53:ASN:CA	1:A:53:ASN:C	1:A:54:LYS:N	4	1.4
(1,85)	1:A:49:LEU:C	1:A:50:LYS:N	1:A:50:LYS:CA	1:A:50:LYS:C	4	1.4
(1,82)	1:A:48:PHE:N	1:A:48:PHE:CA	1:A:48:PHE:C	1:A:49:LEU:N	1	1.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,73)	1:A:43:LYS:C	1:A:44:ASP:N	1:A:44:ASP:CA	1:A:44:ASP:C	9	1.4
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	5	1.4
(1,60)	1:A:36:GLU:N	1:A:36:GLU:CA	1:A:36:GLU:C	1:A:37:PHE:N	9	1.4
(1,57)	1:A:34:GLN:C	1:A:35:GLY:N	1:A:35:GLY:CA	1:A:35:GLY:C	4	1.4
(1,57)	1:A:34:GLN:C	1:A:35:GLY:N	1:A:35:GLY:CA	1:A:35:GLY:C	6	1.4
(1,53)	1:A:32:LEU:C	1:A:33:ASN:N	1:A:33:ASN:CA	1:A:33:ASN:C	2	1.4
(1,34)	1:A:21:GLN:N	1:A:21:GLN:CA	1:A:21:GLN:C	1:A:22:TYR:N	4	1.4
(1,31)	1:A:19:PHE:C	1:A:20:HIS:N	1:A:20:HIS:CA	1:A:20:HIS:C	9	1.4
(1,210)	1:A:113:THR:N	1:A:113:THR:CA	1:A:113:THR:C	1:A:114:PRO:N	2	1.4
(1,198)	1:A:107:PRO:N	1:A:107:PRO:CA	1:A:107:PRO:C	1:A:108:GLY:N	9	1.4
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	1	1.4
(1,187)	1:A:101:PRO:C	1:A:102:GLY:N	1:A:102:GLY:CA	1:A:102:GLY:C	7	1.4
(1,179)	1:A:97:GLY:C	1:A:98:ASP:N	1:A:98:ASP:CA	1:A:98:ASP:C	6	1.4
(1,169)	1:A:92:GLU:C	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	6	1.4
(1,135)	1:A:75:SER:C	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	1	1.4
(1,127)	1:A:71:ASP:C	1:A:72:LYS:N	1:A:72:LYS:CA	1:A:72:LYS:C	7	1.4
(1,109)	1:A:62:ILE:N	1:A:62:ILE:CA	1:A:62:ILE:C	1:A:63:MET:N	5	1.4
(1,105)	1:A:60:GLU:N	1:A:60:GLU:CA	1:A:60:GLU:C	1:A:61:HIS:N	10	1.4
(1,89)	1:A:51:LYS:C	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	8	1.3
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	1	1.3
(1,70)	1:A:41:VAL:N	1:A:41:VAL:CA	1:A:41:VAL:C	1:A:42:ARG:N	3	1.3
(1,44)	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	1:A:27:GLY:N	7	1.3
(1,42)	1:A:25:LYS:N	1:A:25:LYS:CA	1:A:25:LYS:C	1:A:26:LEU:N	3	1.3
(1,40)	1:A:24:VAL:N	1:A:24:VAL:CA	1:A:24:VAL:C	1:A:25:LYS:N	1	1.3
(1,35)	1:A:21:GLN:C	1:A:22:TYR:N	1:A:22:TYR:CA	1:A:22:TYR:C	8	1.3
(1,35)	1:A:21:GLN:C	1:A:22:TYR:N	1:A:22:TYR:CA	1:A:22:TYR:C	9	1.3
(1,31)	1:A:19:PHE:C	1:A:20:HIS:N	1:A:20:HIS:CA	1:A:20:HIS:C	6	1.3
(1,25)	1:A:16:ILE:C	1:A:17:ASN:N	1:A:17:ASN:CA	1:A:17:ASN:C	1	1.3
(1,18)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:THR:N	9	1.3
(1,136)	1:A:76:PHE:N	1:A:76:PHE:CA	1:A:76:PHE:C	1:A:77:GLU:N	2	1.3
(1,127)	1:A:71:ASP:C	1:A:72:LYS:N	1:A:72:LYS:CA	1:A:72:LYS:C	6	1.3
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	3	1.3
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	7	1.3
(1,120)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:ASN:N	2	1.3
(1,109)	1:A:62:ILE:N	1:A:62:ILE:CA	1:A:62:ILE:C	1:A:63:MET:N	8	1.3
(1,90)	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	1:A:53:ASN:N	8	1.2
(1,80)	1:A:47:ASN:N	1:A:47:ASN:CA	1:A:47:ASN:C	1:A:48:PHE:N	1	1.2
(1,6)	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	1:A:8:LEU:N	9	1.2
(1,57)	1:A:34:GLN:C	1:A:35:GLY:N	1:A:35:GLY:CA	1:A:35:GLY:C	7	1.2
(1,44)	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	1:A:27:GLY:N	9	1.2
(1,40)	1:A:24:VAL:N	1:A:24:VAL:CA	1:A:24:VAL:C	1:A:25:LYS:N	10	1.2
(1,34)	1:A:21:GLN:N	1:A:21:GLN:CA	1:A:21:GLN:C	1:A:22:TYR:N	7	1.2
(1,208)	1:A:112:GLY:N	1:A:112:GLY:CA	1:A:112:GLY:C	1:A:113:THR:N	6	1.2
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	6	1.2
(1,186)	1:A:101:PRO:N	1:A:101:PRO:CA	1:A:101:PRO:C	1:A:102:GLY:N	9	1.2
(1,121)	1:A:68:THR:C	1:A:69:ASN:N	1:A:69:ASN:CA	1:A:69:ASN:C	5	1.2
(1,114)	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	1:A:66:LEU:N	3	1.2
(1,113)	1:A:64:GLU:C	1:A:65:ASP:N	1:A:65:ASP:CA	1:A:65:ASP:C	4	1.2
(1,111)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:GLU:N	9	1.2
(1,111)	1:A:63:MET:N	1:A:63:MET:CA	1:A:63:MET:C	1:A:64:GLU:N	10	1.2
(1,96)	1:A:55:ASN:N	1:A:55:ASN:CA	1:A:55:ASN:C	1:A:56:GLU:N	4	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,92)	1:A:53:ASN:N	1:A:53:ASN:CA	1:A:53:ASN:C	1:A:54:LYS:N	3	1.1
(1,92)	1:A:53:ASN:N	1:A:53:ASN:CA	1:A:53:ASN:C	1:A:54:LYS:N	9	1.1
(1,90)	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	1:A:53:ASN:N	1	1.1
(1,90)	1:A:52:GLU:N	1:A:52:GLU:CA	1:A:52:GLU:C	1:A:53:ASN:N	7	1.1
(1,8)	1:A:8:LEU:N	1:A:8:LEU:CA	1:A:8:LEU:C	1:A:9:GLU:N	3	1.1
(1,61)	1:A:36:GLU:C	1:A:37:PHE:N	1:A:37:PHE:CA	1:A:37:PHE:C	1	1.1
(1,57)	1:A:34:GLN:C	1:A:35:GLY:N	1:A:35:GLY:CA	1:A:35:GLY:C	2	1.1
(1,51)	1:A:31:THR:C	1:A:32:LEU:N	1:A:32:LEU:CA	1:A:32:LEU:C	6	1.1
(1,5)	1:A:6:SER:C	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	4	1.1
(1,5)	1:A:6:SER:C	1:A:7:GLN:N	1:A:7:GLN:CA	1:A:7:GLN:C	9	1.1
(1,43)	1:A:25:LYS:C	1:A:26:LEU:N	1:A:26:LEU:CA	1:A:26:LEU:C	7	1.1
(1,40)	1:A:24:VAL:N	1:A:24:VAL:CA	1:A:24:VAL:C	1:A:25:LYS:N	6	1.1
(1,4)	1:A:6:SER:N	1:A:6:SER:CA	1:A:6:SER:C	1:A:7:GLN:N	9	1.1
(1,205)	1:A:110:GLY:C	1:A:111:GLU:N	1:A:111:GLU:CA	1:A:111:GLU:C	6	1.1
(1,202)	1:A:109:LEU:N	1:A:109:LEU:CA	1:A:109:LEU:C	1:A:110:GLY:N	2	1.1
(1,191)	1:A:103:HIS:C	1:A:104:HIS:N	1:A:104:HIS:CA	1:A:104:HIS:C	10	1.1
(1,19)	1:A:13:GLU:C	1:A:14:THR:N	1:A:14:THR:CA	1:A:14:THR:C	7	1.1
(1,177)	1:A:96:GLU:C	1:A:97:GLY:N	1:A:97:GLY:CA	1:A:97:GLY:C	8	1.1
(1,171)	1:A:93:LYS:C	1:A:94:MET:N	1:A:94:MET:CA	1:A:94:MET:C	6	1.1
(1,170)	1:A:93:LYS:N	1:A:93:LYS:CA	1:A:93:LYS:C	1:A:94:MET:N	7	1.1
(1,162)	1:A:89:ALA:N	1:A:89:ALA:CA	1:A:89:ALA:C	1:A:90:SER:N	5	1.1
(1,157)	1:A:86:LEU:C	1:A:87:THR:N	1:A:87:THR:CA	1:A:87:THR:C	4	1.1
(1,152)	1:A:84:ALA:N	1:A:84:ALA:CA	1:A:84:ALA:C	1:A:85:ARG:N	3	1.1
(1,125)	1:A:70:ALA:C	1:A:71:ASP:N	1:A:71:ASP:CA	1:A:71:ASP:C	9	1.1
(1,124)	1:A:70:ALA:N	1:A:70:ALA:CA	1:A:70:ALA:C	1:A:71:ASP:N	2	1.1
(1,10)	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	1:A:10:ARG:N	4	1.1
(1,1)	1:A:4:LYS:C	1:A:5:MET:N	1:A:5:MET:CA	1:A:5:MET:C	6	1.1