



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 08:31 PM EST

PDB ID : 8X1G  
BMRB ID : 36611  
Title : Human adenylate kinase 1 (hAK1) mutant-R97W  
Authors : Yu, J.  
Deposited on : 2023-11-07

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.40

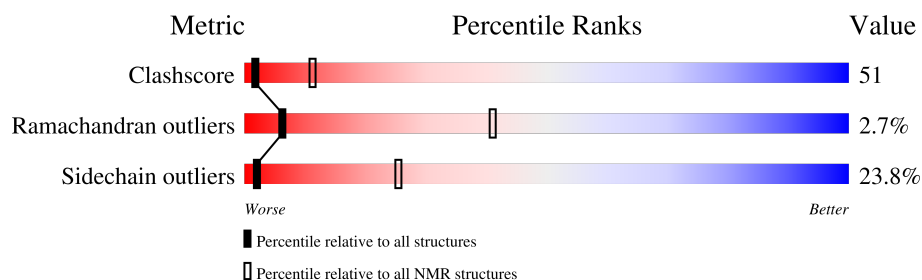
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 78%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	194	<div> <div>26%</div> <div>54%</div> <div>16%</div> <div>• •</div> </div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:1-A:95, A:104-A:194 (186)	0.68	1

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3080 atoms, of which 1560 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adenylate kinase isoenzyme 1.

Mol	Chain	Residues	Atoms						Trace
1	A	194	Total	C	H	N	O	S	0
			3080	956	1560	262	295	7	

There is a discrepancy between the modelled and reference sequences:

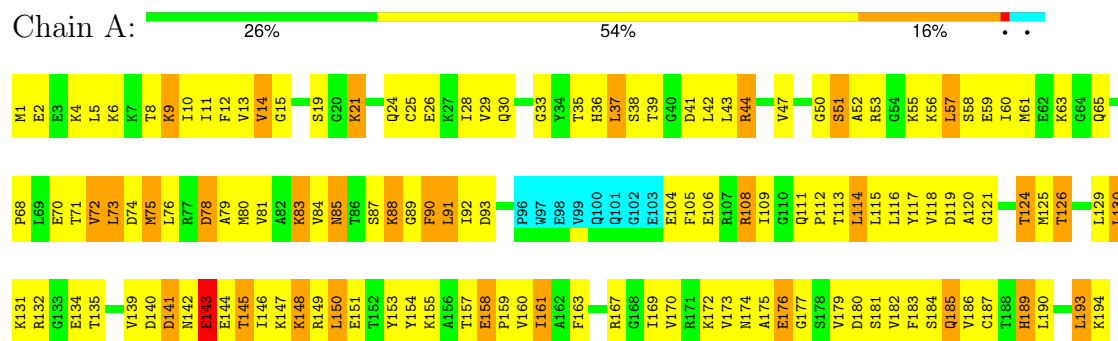
Chain	Residue	Modelled	Actual	Comment	Reference
A	97	TRP	ARG	engineered mutation	UNP P00568

## 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: Adenylate kinase isoenzyme 1

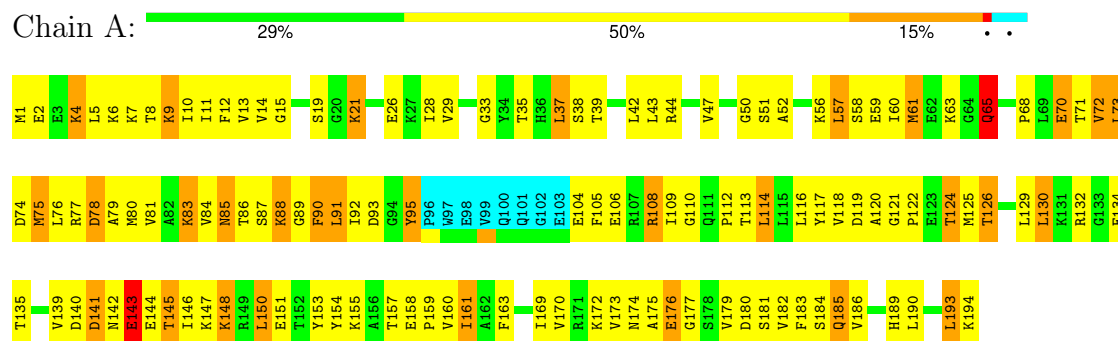


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

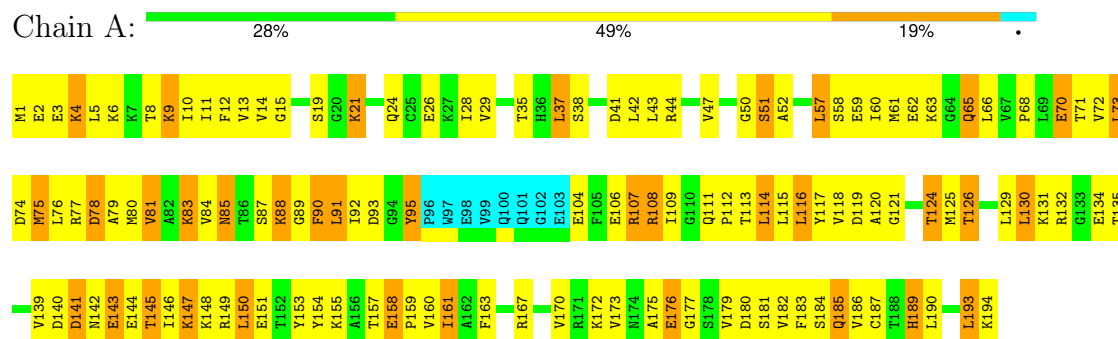
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Adenylate kinase isoenzyme 1



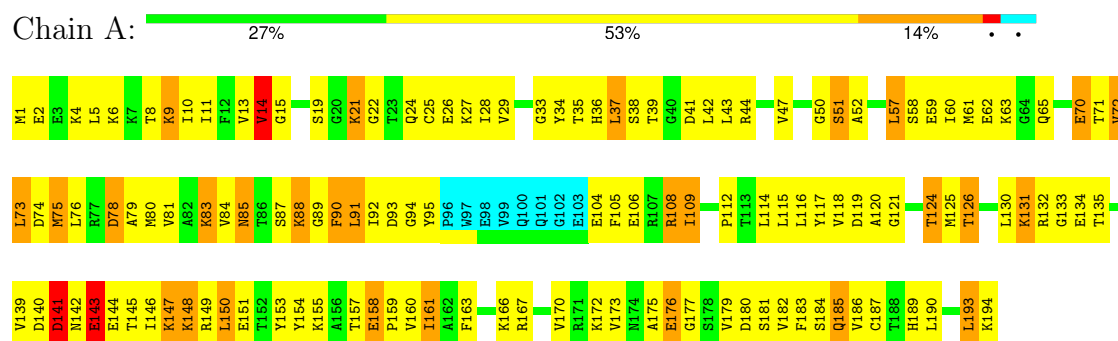
### 4.2.2 Score per residue for model 2

#### • Molecule 1: Adenylate kinase isoenzyme 1



### 4.2.5 Score per residue for model 5

- Molecule 1: Adenylate kinase isoenzyme 1



## 4.2.8 Score per residue for model 8

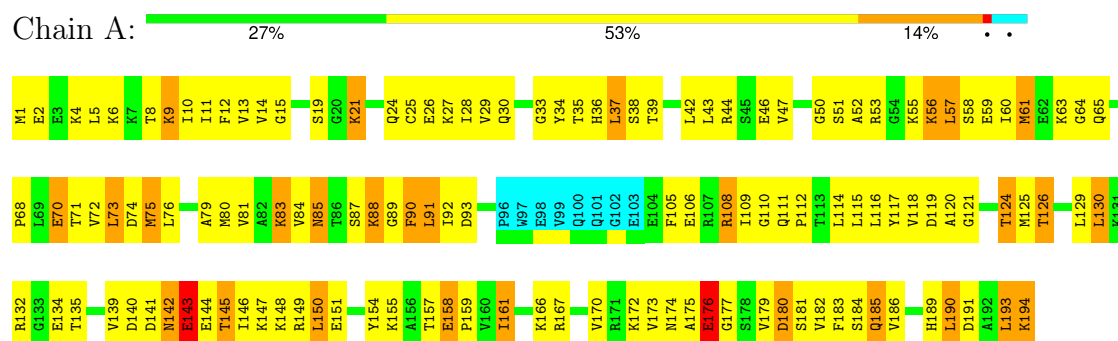
- Molecule 1: Adenylate kinase isoenzyme 1





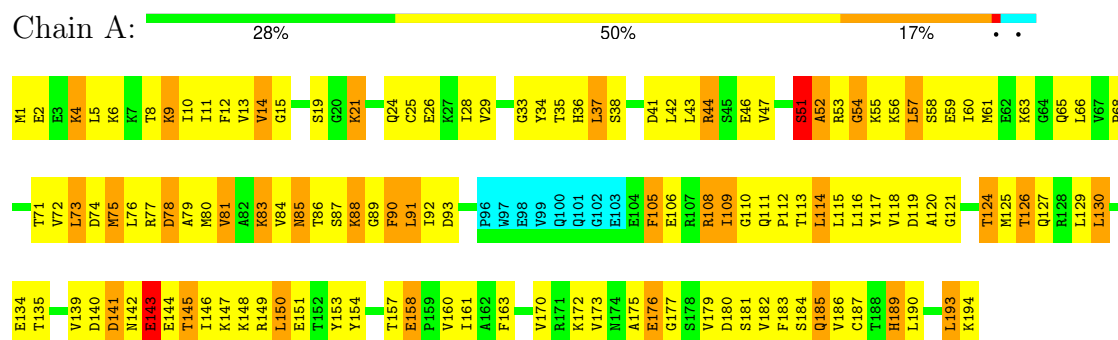
### 4.2.11 Score per residue for model 11

- Molecule 1: Adenylate kinase isoenzyme 1



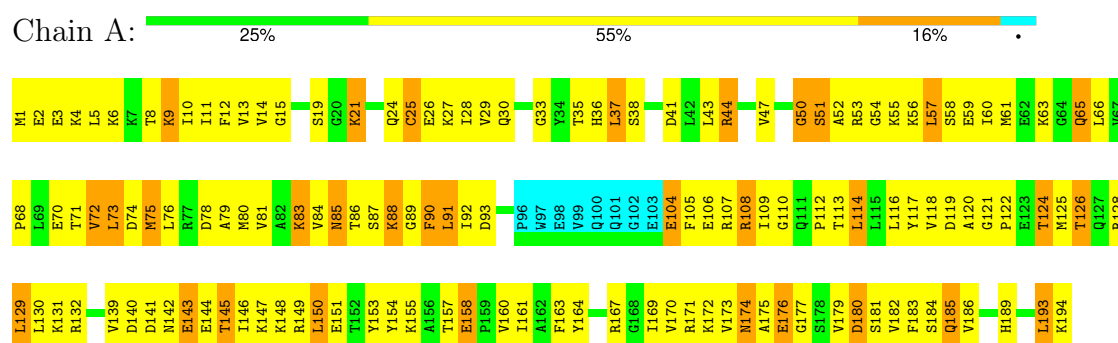
### 4.2.12 Score per residue for model 12

- Molecule 1: Adenylate kinase isoenzyme 1



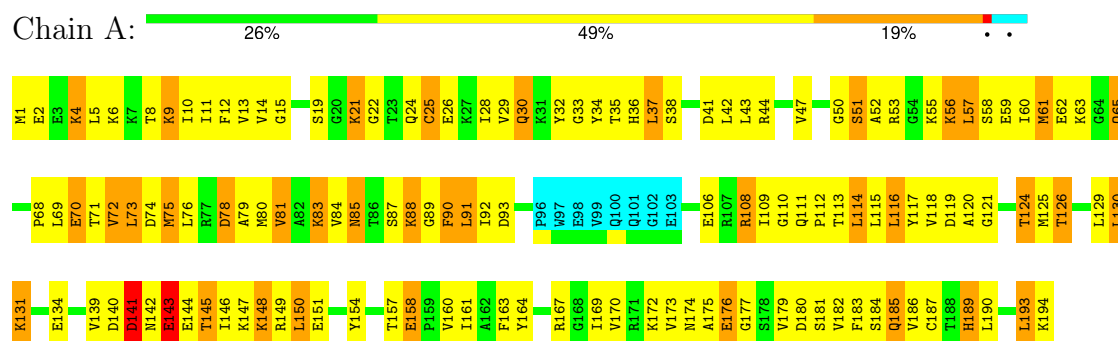
### 4.2.13 Score per residue for model 13

- Molecule 1: Adenylate kinase isoenzyme 1



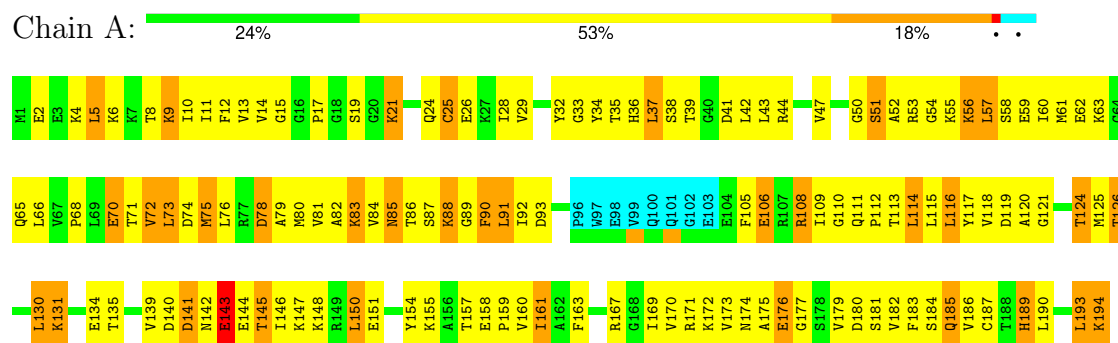
### 4.2.14 Score per residue for model 14

- Molecule 1: Adenylate kinase isoenzyme 1



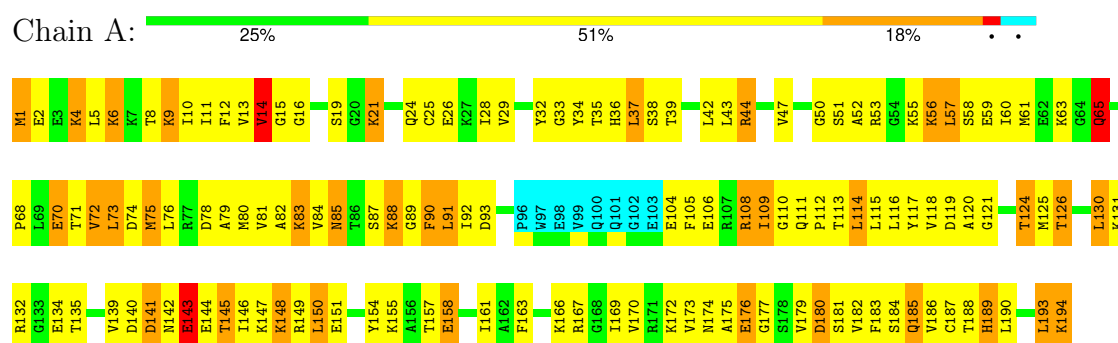
### 4.2.15 Score per residue for model 15

- Molecule 1: Adenylate kinase isoenzyme 1



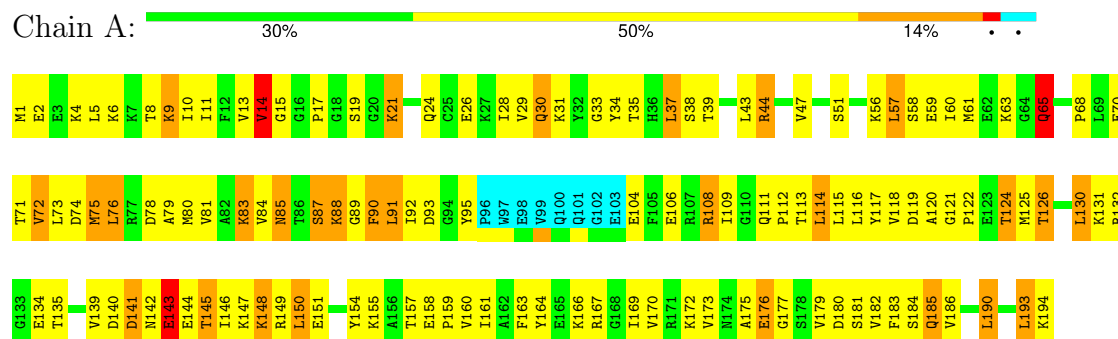
### 4.2.16 Score per residue for model 16

- Molecule 1: Adenylate kinase isoenzyme 1



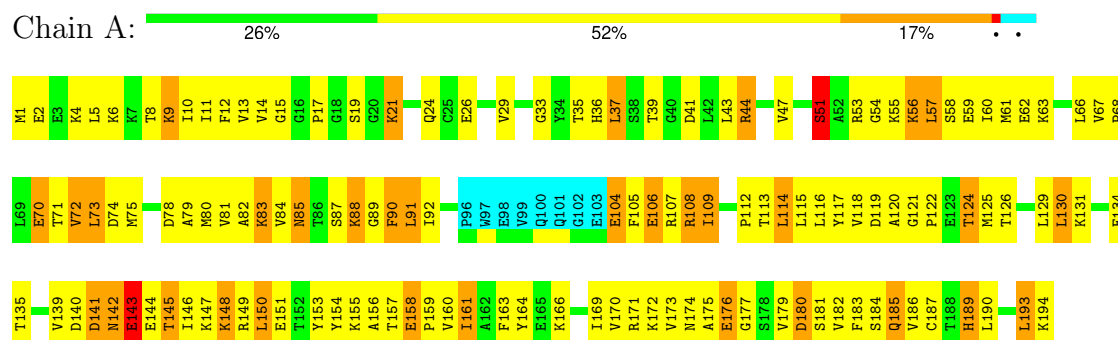
## 4.2.17 Score per residue for model 17

- Molecule 1: Adenylate kinase isoenzyme 1



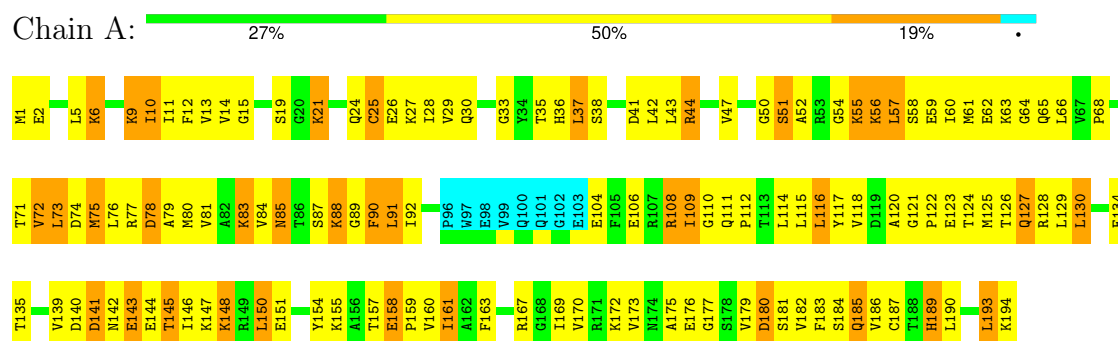
## 4.2.18 Score per residue for model 18

- Molecule 1: Adenylate kinase isoenzyme 1



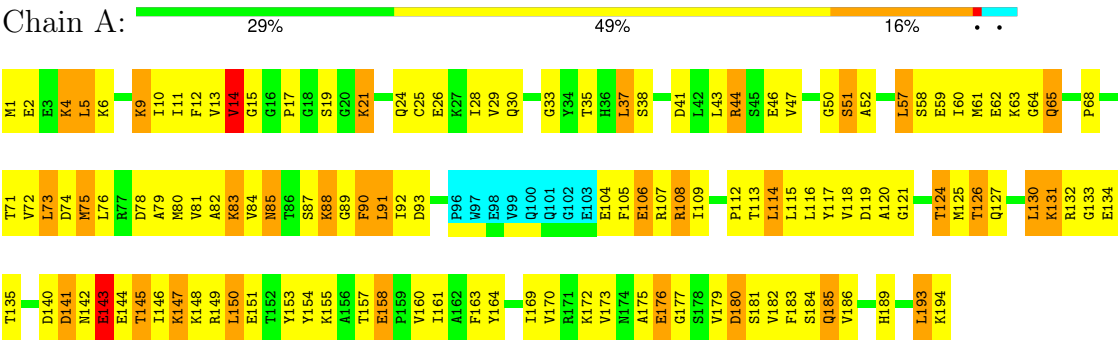
## 4.2.19 Score per residue for model 19

- Molecule 1: Adenylate kinase isoenzyme 1



4.2.20 Score per residue for model 20

● Molecule 1: Adenylate kinase isoenzyme 1



## 5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA2alpha	structure calculation	CNS
ARIA2alpha	refinement	CNS

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	2008
Number of shifts mapped to atoms	2008
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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	1452	1503	1501	150±8
All	All	29040	30060	30020	3002

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 51.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HD11	1:A:193:LEU:HD13	0.94	1.38	7	20
1:A:36:HIS:HA	1:A:91:LEU:HD12	0.93	1.37	3	2
1:A:4:LYS:HG3	1:A:84:VAL:HG21	0.86	1.45	10	5
1:A:13:VAL:HB	1:A:91:LEU:HD13	0.84	1.47	10	17
1:A:5:LEU:HD13	1:A:5:LEU:H	0.83	1.33	15	1
1:A:91:LEU:HD22	1:A:92:ILE:N	0.83	1.88	3	2
1:A:11:ILE:HD11	1:A:193:LEU:CD1	0.80	2.06	7	20
1:A:72:VAL:HG23	1:A:73:LEU:HD12	0.79	1.53	17	11
1:A:182:VAL:O	1:A:186:VAL:HG13	0.77	1.79	17	20
1:A:73:LEU:HD12	1:A:73:LEU:H	0.75	1.40	18	20
1:A:130:LEU:HD22	1:A:141:ASP:HA	0.74	1.59	20	1
1:A:91:LEU:HD12	1:A:92:ILE:N	0.73	1.98	11	16
1:A:43:LEU:HD11	1:A:71:THR:HG21	0.72	1.61	2	20
1:A:130:LEU:HD11	1:A:143:GLU:HB2	0.72	1.60	19	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HD22	1:A:84:VAL:HG11	0.72	1.61	14	18
1:A:5:LEU:HD11	1:A:80:MET:HG3	0.70	1.62	18	1
1:A:143:GLU:HA	1:A:146:ILE:HD12	0.69	1.64	15	20
1:A:37:LEU:HD22	1:A:79:ALA:HB1	0.69	1.65	2	18
1:A:120:ALA:HB2	1:A:175:ALA:HB3	0.69	1.65	15	18
1:A:91:LEU:O	1:A:91:LEU:HD13	0.68	1.88	3	2
1:A:37:LEU:HD12	1:A:91:LEU:O	0.67	1.89	20	18
1:A:35:THR:HG21	1:A:83:LYS:HE3	0.67	1.67	3	10
1:A:44:ARG:O	1:A:47:VAL:HG12	0.67	1.89	4	17
1:A:65:GLN:HG2	1:A:66:LEU:N	0.67	2.05	7	2
1:A:157:THR:HG22	1:A:161:ILE:HD13	0.67	1.67	3	5
1:A:1:MET:O	1:A:5:LEU:HD23	0.67	1.90	14	19
1:A:117:TYR:CE2	1:A:157:THR:HG21	0.67	2.25	12	19
1:A:65:GLN:HG3	1:A:66:LEU:N	0.66	2.04	19	6
1:A:118:VAL:HG13	1:A:175:ALA:HB2	0.66	1.67	5	17
1:A:4:LYS:HB3	1:A:84:VAL:HG11	0.66	1.67	11	1
1:A:68:PRO:O	1:A:72:VAL:HG23	0.65	1.91	8	9
1:A:13:VAL:HB	1:A:91:LEU:HD23	0.65	1.67	3	2
1:A:8:THR:OG1	1:A:84:VAL:HG23	0.65	1.92	11	1
1:A:130:LEU:HD21	1:A:143:GLU:HB3	0.65	1.69	20	1
1:A:121:GLY:HA2	1:A:125:MET:HB2	0.65	1.69	10	19
1:A:14:VAL:HG22	1:A:21:LYS:HD3	0.64	1.68	6	2
1:A:73:LEU:HD12	1:A:73:LEU:N	0.64	2.07	19	20
1:A:106:GLU:O	1:A:110:GLY:N	0.64	2.31	19	5
1:A:37:LEU:HG	1:A:91:LEU:O	0.64	1.93	16	1
1:A:28:ILE:HG23	1:A:190:LEU:HD13	0.64	1.69	2	7
1:A:2:GLU:HA	1:A:5:LEU:HD21	0.63	1.71	15	1
1:A:140:ASP:O	1:A:146:ILE:HD11	0.62	1.94	6	18
1:A:19:SER:OG	1:A:120:ALA:HB3	0.62	1.93	10	12
1:A:72:VAL:HG23	1:A:73:LEU:CD1	0.62	2.24	17	11
1:A:9:LYS:HE3	1:A:193:LEU:HD12	0.62	1.72	7	2
1:A:189:HIS:ND1	1:A:190:LEU:HD22	0.62	2.09	16	1
1:A:167:ARG:CG	1:A:169:ILE:HG23	0.62	2.23	17	1
1:A:5:LEU:HD13	1:A:5:LEU:N	0.62	2.09	15	1
1:A:10:ILE:HG22	1:A:112:PRO:HA	0.62	1.71	6	19
1:A:126:THR:HA	1:A:146:ILE:HG21	0.62	1.72	4	18
1:A:41:ASP:HA	1:A:44:ARG:HB2	0.62	1.70	7	16
1:A:9:LYS:HG2	1:A:89:GLY:HA3	0.62	1.72	19	9
1:A:24:GLN:HB2	1:A:186:VAL:HG11	0.61	1.71	16	8
1:A:60:ILE:HG21	1:A:66:LEU:O	0.61	1.95	19	2
1:A:10:ILE:C	1:A:11:ILE:HD12	0.61	2.15	7	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG13	1:A:15:GLY:N	0.61	2.11	6	8
1:A:10:ILE:CG2	1:A:112:PRO:HA	0.61	2.26	9	20
1:A:175:ALA:HA	1:A:182:VAL:HB	0.61	1.72	18	20
1:A:114:LEU:HD12	1:A:189:HIS:CD2	0.61	2.30	1	2
1:A:193:LEU:HG	1:A:194:LYS:N	0.61	2.10	12	19
1:A:116:LEU:HD11	1:A:186:VAL:HA	0.60	1.72	17	18
1:A:91:LEU:HD13	1:A:91:LEU:C	0.60	2.17	18	2
1:A:21:LYS:HA	1:A:118:VAL:HG21	0.60	1.74	5	20
1:A:148:LYS:HD2	1:A:148:LYS:N	0.60	2.11	2	19
1:A:84:VAL:HG12	1:A:90:PHE:CE2	0.60	2.32	14	19
1:A:2:GLU:O	1:A:5:LEU:HD22	0.60	1.96	15	1
1:A:57:LEU:HD13	1:A:57:LEU:N	0.60	2.12	12	20
1:A:154:TYR:O	1:A:158:GLU:HB2	0.60	1.97	3	20
1:A:158:GLU:HA	1:A:161:ILE:HD11	0.60	1.72	3	20
1:A:33:GLY:C	1:A:88:LYS:HZ1	0.60	1.99	6	10
1:A:2:GLU:HB3	1:A:6:LYS:HE3	0.60	1.74	20	4
1:A:60:ILE:HA	1:A:63:LYS:HB3	0.60	1.74	7	20
1:A:26:GLU:HA	1:A:29:VAL:HG23	0.60	1.74	19	20
1:A:73:LEU:HD23	1:A:105:PHE:HA	0.59	1.74	1	13
1:A:74:ASP:HA	1:A:108:ARG:HD2	0.59	1.74	2	7
1:A:13:VAL:CB	1:A:91:LEU:HD13	0.59	2.28	11	16
1:A:34:TYR:N	1:A:88:LYS:HZ1	0.59	1.96	16	10
1:A:2:GLU:HA	1:A:5:LEU:HB2	0.59	1.74	20	18
1:A:81:VAL:O	1:A:84:VAL:HG22	0.58	1.97	17	18
1:A:150:LEU:C	1:A:150:LEU:HD13	0.58	2.19	13	20
1:A:173:VAL:CG2	1:A:182:VAL:HG23	0.58	2.29	14	20
1:A:9:LYS:HD3	1:A:88:LYS:O	0.58	1.99	2	13
1:A:57:LEU:H	1:A:57:LEU:HD13	0.58	1.57	4	3
1:A:80:MET:C	1:A:84:VAL:HG13	0.57	2.20	2	19
1:A:80:MET:O	1:A:84:VAL:HG13	0.57	2.00	6	19
1:A:125:MET:O	1:A:129:LEU:HB2	0.57	1.99	13	10
1:A:59:GLU:O	1:A:63:LYS:N	0.57	2.37	18	20
1:A:5:LEU:HA	1:A:8:THR:HB	0.57	1.76	15	1
1:A:113:THR:O	1:A:114:LEU:HD22	0.57	2.00	20	15
1:A:184:SER:HB2	1:A:185:GLN:NE2	0.57	2.15	17	8
1:A:118:VAL:CG1	1:A:175:ALA:HB2	0.57	2.30	10	20
1:A:13:VAL:CB	1:A:91:LEU:HD23	0.57	2.30	3	2
1:A:47:VAL:HA	1:A:50:GLY:HA3	0.57	1.76	13	2
1:A:19:SER:CB	1:A:120:ALA:HB3	0.56	2.30	18	12
1:A:3:GLU:HG3	1:A:4:LYS:HD2	0.56	1.76	13	3
1:A:85:ASN:H	1:A:85:ASN:ND2	0.56	1.97	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:145:THR:O	1:A:148:LYS:HG2	0.56	2.00	10	1
1:A:57:LEU:HD13	1:A:57:LEU:H	0.56	1.59	12	14
1:A:130:LEU:HD23	1:A:130:LEU:N	0.56	2.15	20	9
1:A:74:ASP:HA	1:A:108:ARG:HE	0.56	1.61	9	13
1:A:5:LEU:HD11	1:A:80:MET:SD	0.56	2.40	3	1
1:A:57:LEU:H	1:A:57:LEU:CD1	0.56	2.13	12	9
1:A:5:LEU:HD11	1:A:80:MET:CG	0.56	2.30	3	6
1:A:2:GLU:HB3	1:A:6:LYS:HE2	0.56	1.77	17	1
1:A:13:VAL:HG13	1:A:116:LEU:HD22	0.55	1.78	14	9
1:A:171:ARG:HB2	1:A:189:HIS:HB2	0.55	1.78	18	3
1:A:173:VAL:HG21	1:A:182:VAL:HG23	0.55	1.76	3	17
1:A:71:THR:O	1:A:75:MET:HB2	0.55	2.01	8	11
1:A:25:CYS:SG	1:A:26:GLU:N	0.55	2.79	7	9
1:A:74:ASP:HA	1:A:108:ARG:NE	0.55	2.16	6	10
1:A:2:GLU:O	1:A:6:LYS:HG2	0.55	2.02	10	13
1:A:4:LYS:HB3	1:A:84:VAL:HG21	0.55	1.78	17	4
1:A:14:VAL:HG22	1:A:21:LYS:CD	0.55	2.30	6	1
1:A:4:LYS:CG	1:A:84:VAL:HG21	0.55	2.31	14	2
1:A:6:LYS:N	1:A:6:LYS:HE2	0.55	2.17	16	2
1:A:119:ASP:HB3	1:A:173:VAL:O	0.55	2.02	11	18
1:A:142:ASN:HB3	1:A:145:THR:HG22	0.55	1.79	4	7
1:A:91:LEU:C	1:A:91:LEU:HD12	0.55	2.22	16	1
1:A:121:GLY:N	1:A:125:MET:HG3	0.54	2.17	7	8
1:A:154:TYR:O	1:A:159:PRO:HD3	0.54	2.02	15	4
1:A:122:PRO:HG3	1:A:150:LEU:HD11	0.54	1.78	19	2
1:A:15:GLY:H	1:A:21:LYS:HE2	0.54	1.62	16	1
1:A:57:LEU:HD22	1:A:58:SER:N	0.54	2.18	5	20
1:A:124:THR:OG1	1:A:176:GLU:HA	0.54	2.03	7	19
1:A:10:ILE:HD12	1:A:109:ILE:HG21	0.54	1.78	10	14
1:A:50:GLY:O	1:A:54:GLY:N	0.54	2.39	4	3
1:A:161:ILE:O	1:A:170:VAL:HG11	0.54	2.03	6	20
1:A:148:LYS:HA	1:A:151:GLU:CG	0.54	2.33	10	1
1:A:130:LEU:O	1:A:134:GLU:N	0.54	2.40	14	15
1:A:130:LEU:HD21	1:A:143:GLU:HB2	0.54	1.80	5	2
1:A:146:ILE:HA	1:A:149:ARG:HG2	0.54	1.79	5	9
1:A:56:LYS:HG3	1:A:57:LEU:H	0.54	1.62	9	11
1:A:142:ASN:O	1:A:144:GLU:N	0.54	2.41	17	20
1:A:91:LEU:HD11	1:A:93:ASP:HB3	0.54	1.80	16	11
1:A:184:SER:HB3	1:A:185:GLN:NE2	0.54	2.18	14	12
1:A:5:LEU:HD21	1:A:80:MET:HG3	0.54	1.79	3	1
1:A:161:ILE:HG22	1:A:170:VAL:HG21	0.54	1.78	19	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:LEU:CD1	1:A:57:LEU:H	0.53	2.16	2	11
1:A:130:LEU:HD13	1:A:141:ASP:OD1	0.53	2.03	2	8
1:A:28:ILE:HG21	1:A:190:LEU:HD12	0.53	1.79	17	2
1:A:126:THR:HA	1:A:146:ILE:HD13	0.53	1.80	19	8
1:A:126:THR:O	1:A:143:GLU:HB2	0.53	2.03	20	1
1:A:120:ALA:HB2	1:A:175:ALA:CB	0.53	2.33	13	15
1:A:173:VAL:HB	1:A:185:GLN:HB2	0.53	1.81	9	19
1:A:14:VAL:HG22	1:A:15:GLY:H	0.53	1.64	12	11
1:A:187:CYS:HA	1:A:190:LEU:HD12	0.53	1.79	12	13
1:A:37:LEU:HD13	1:A:80:MET:SD	0.53	2.44	17	2
1:A:35:THR:HB	1:A:37:LEU:HD23	0.53	1.80	16	1
1:A:84:VAL:HG12	1:A:90:PHE:HE2	0.53	1.64	14	7
1:A:19:SER:HB3	1:A:118:VAL:HG12	0.53	1.81	9	10
1:A:5:LEU:HG	1:A:109:ILE:HG23	0.53	1.81	15	1
1:A:47:VAL:O	1:A:51:SER:N	0.52	2.42	5	8
1:A:157:THR:HG22	1:A:161:ILE:CD1	0.52	2.34	3	1
1:A:15:GLY:N	1:A:21:LYS:HD2	0.52	2.19	10	2
1:A:148:LYS:HA	1:A:151:GLU:HG2	0.52	1.81	10	1
1:A:11:ILE:HB	1:A:90:PHE:O	0.52	2.04	16	12
1:A:14:VAL:O	1:A:117:TYR:HA	0.52	2.04	3	11
1:A:88:LYS:HD3	1:A:89:GLY:H	0.52	1.63	2	20
1:A:25:CYS:HA	1:A:28:ILE:HD12	0.52	1.81	13	10
1:A:73:LEU:HD21	1:A:104:GLU:HG2	0.52	1.81	5	1
1:A:84:VAL:HG23	1:A:85:ASN:N	0.52	2.19	16	19
1:A:181:SER:O	1:A:185:GLN:NE2	0.52	2.42	5	20
1:A:91:LEU:C	1:A:91:LEU:HD23	0.52	2.25	7	1
1:A:73:LEU:H	1:A:73:LEU:CD1	0.52	2.17	12	18
1:A:35:THR:HG21	1:A:83:LYS:CE	0.52	2.34	8	5
1:A:91:LEU:HD21	1:A:93:ASP:HB3	0.52	1.81	7	1
1:A:85:ASN:HD22	1:A:85:ASN:N	0.52	2.03	17	14
1:A:29:VAL:HG21	1:A:36:HIS:HB2	0.52	1.80	12	5
1:A:189:HIS:HD1	1:A:190:LEU:HD22	0.52	1.64	16	1
1:A:11:ILE:HG23	1:A:189:HIS:NE2	0.52	2.20	16	9
1:A:14:VAL:HG22	1:A:21:LYS:HE2	0.52	1.82	16	1
1:A:57:LEU:O	1:A:61:MET:HG3	0.52	2.05	6	19
1:A:115:LEU:HD23	1:A:116:LEU:N	0.52	2.20	5	12
1:A:15:GLY:H	1:A:21:LYS:HD2	0.52	1.65	10	2
1:A:50:GLY:C	1:A:52:ALA:N	0.52	2.63	13	3
1:A:154:TYR:HA	1:A:158:GLU:OE2	0.51	2.05	12	4
1:A:57:LEU:O	1:A:61:MET:HG2	0.51	2.06	11	1
1:A:118:VAL:HA	1:A:173:VAL:HG22	0.51	1.82	3	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:HIS:HA	1:A:91:LEU:HB3	0.51	1.82	7	1
1:A:57:LEU:N	1:A:57:LEU:CD1	0.51	2.74	11	20
1:A:63:LYS:HG2	1:A:65:GLN:HB2	0.51	1.83	19	2
1:A:88:LYS:N	1:A:88:LYS:CD	0.51	2.74	7	18
1:A:14:VAL:HG21	1:A:94:GLY:N	0.51	2.20	6	1
1:A:4:LYS:CB	1:A:84:VAL:HG11	0.51	2.34	11	1
1:A:1:MET:HA	1:A:4:LYS:HD3	0.51	1.82	16	1
1:A:15:GLY:H	1:A:21:LYS:HD3	0.51	1.66	19	8
1:A:68:PRO:O	1:A:72:VAL:HG22	0.51	2.06	17	10
1:A:147:LYS:O	1:A:151:GLU:HG2	0.51	2.05	10	20
1:A:21:LYS:HG2	1:A:118:VAL:HB	0.51	1.81	10	2
1:A:82:ALA:O	1:A:83:LYS:HD3	0.51	2.05	4	7
1:A:106:GLU:HB2	1:A:112:PRO:HD3	0.51	1.83	20	8
1:A:130:LEU:HG	1:A:143:GLU:HG3	0.51	1.83	8	9
1:A:154:TYR:HA	1:A:158:GLU:OE1	0.51	2.05	3	3
1:A:28:ILE:CG2	1:A:190:LEU:HD13	0.51	2.36	5	8
1:A:119:ASP:HB2	1:A:173:VAL:O	0.51	2.06	18	1
1:A:88:LYS:CD	1:A:88:LYS:H	0.51	2.19	7	11
1:A:160:VAL:O	1:A:163:PHE:HB3	0.50	2.06	17	15
1:A:5:LEU:HB3	1:A:6:LYS:HZ3	0.50	1.66	8	1
1:A:51:SER:O	1:A:53:ARG:N	0.50	2.43	12	1
1:A:183:PHE:O	1:A:186:VAL:HG22	0.50	2.07	16	19
1:A:10:ILE:HG22	1:A:113:THR:H	0.50	1.66	16	12
1:A:1:MET:HA	1:A:81:VAL:HB	0.50	1.82	11	10
1:A:21:LYS:HE3	1:A:22:GLY:H	0.50	1.66	5	1
1:A:106:GLU:H	1:A:106:GLU:CD	0.50	2.10	13	1
1:A:2:GLU:HA	1:A:5:LEU:CD2	0.50	2.37	15	1
1:A:179:VAL:HG23	1:A:180:ASP:N	0.50	2.21	3	20
1:A:11:ILE:HG23	1:A:189:HIS:CE1	0.50	2.41	7	2
1:A:85:ASN:N	1:A:85:ASN:HD22	0.50	2.04	16	5
1:A:167:ARG:HG2	1:A:169:ILE:HG23	0.50	1.83	17	1
1:A:29:VAL:O	1:A:33:GLY:HA2	0.50	2.06	6	18
1:A:75:MET:HA	1:A:78:ASP:HB2	0.50	1.83	8	12
1:A:130:LEU:O	1:A:133:GLY:N	0.50	2.45	9	4
1:A:10:ILE:HD11	1:A:12:PHE:CZ	0.50	2.42	19	1
1:A:75:MET:O	1:A:79:ALA:N	0.50	2.45	2	19
1:A:134:GLU:HG3	1:A:135:THR:N	0.50	2.22	6	17
1:A:46:GLU:C	1:A:51:SER:HB2	0.50	2.27	12	1
1:A:175:ALA:C	1:A:177:GLY:H	0.49	2.10	20	20
1:A:130:LEU:CD2	1:A:143:GLU:HB3	0.49	2.35	20	1
1:A:50:GLY:O	1:A:52:ALA:N	0.49	2.45	13	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:THR:HG21	1:A:90:PHE:CE2	0.49	2.43	13	17
1:A:14:VAL:HG22	1:A:15:GLY:N	0.49	2.22	3	11
1:A:42:LEU:HD21	1:A:79:ALA:HB2	0.49	1.83	8	4
1:A:146:ILE:HA	1:A:149:ARG:CG	0.49	2.37	14	7
1:A:190:LEU:N	1:A:190:LEU:CD2	0.49	2.75	17	2
1:A:189:HIS:ND1	1:A:189:HIS:N	0.49	2.61	6	2
1:A:83:LYS:O	1:A:87:SER:N	0.49	2.46	11	5
1:A:43:LEU:HD22	1:A:75:MET:HG2	0.49	1.84	13	1
1:A:121:GLY:O	1:A:124:THR:N	0.49	2.45	19	1
1:A:9:LYS:HG3	1:A:193:LEU:HD11	0.49	1.83	19	4
1:A:13:VAL:HB	1:A:91:LEU:CD2	0.49	2.38	18	2
1:A:24:GLN:NE2	1:A:183:PHE:HB2	0.49	2.23	5	10
1:A:129:LEU:HG	1:A:140:ASP:HB3	0.49	1.84	11	5
1:A:127:GLN:HG3	1:A:128:ARG:N	0.49	2.21	19	1
1:A:42:LEU:HB3	1:A:75:MET:SD	0.49	2.48	3	6
1:A:140:ASP:C	1:A:142:ASN:H	0.49	2.11	17	18
1:A:10:ILE:HD11	1:A:80:MET:CE	0.49	2.38	7	1
1:A:117:TYR:O	1:A:172:LYS:HA	0.49	2.08	20	2
1:A:11:ILE:HG23	1:A:189:HIS:HE1	0.48	1.68	1	2
1:A:12:PHE:HA	1:A:92:ILE:HB	0.48	1.84	16	5
1:A:91:LEU:HD12	1:A:91:LEU:C	0.48	2.29	13	13
1:A:114:LEU:HD13	1:A:169:ILE:O	0.48	2.08	18	9
1:A:76:LEU:O	1:A:80:MET:HG2	0.48	2.07	11	17
1:A:126:THR:C	1:A:143:GLU:HB2	0.48	2.28	20	1
1:A:4:LYS:CB	1:A:84:VAL:HG21	0.48	2.38	17	12
1:A:35:THR:CG2	1:A:37:LEU:HD21	0.48	2.38	12	7
1:A:13:VAL:HG11	1:A:25:CYS:HA	0.48	1.84	7	3
1:A:13:VAL:HG11	1:A:28:ILE:CD1	0.48	2.38	20	1
1:A:179:VAL:O	1:A:183:PHE:HB3	0.48	2.09	4	17
1:A:130:LEU:HG	1:A:141:ASP:HA	0.48	1.84	9	2
1:A:42:LEU:HD13	1:A:75:MET:HB3	0.48	1.83	8	5
1:A:24:GLN:CB	1:A:186:VAL:HG11	0.48	2.38	17	3
1:A:150:LEU:O	1:A:153:TYR:HB3	0.48	2.08	6	12
1:A:77:ARG:HB2	1:A:109:ILE:HD12	0.48	1.86	6	3
1:A:2:GLU:HG2	1:A:109:ILE:O	0.48	2.08	16	11
1:A:151:GLU:O	1:A:154:TYR:HB2	0.48	2.09	11	12
1:A:35:THR:HB	1:A:37:LEU:HD11	0.48	1.85	18	2
1:A:1:MET:O	1:A:4:LYS:HG2	0.48	2.09	16	3
1:A:70:GLU:HG3	1:A:71:THR:N	0.48	2.24	15	12
1:A:5:LEU:HD11	1:A:80:MET:CB	0.48	2.38	17	7
1:A:104:GLU:HB3	1:A:107:ARG:HD3	0.48	1.83	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:MET:HG2	1:A:67:VAL:HG12	0.48	1.85	18	1
1:A:121:GLY:O	1:A:126:THR:HG23	0.48	2.08	20	1
1:A:117:TYR:HB3	1:A:172:LYS:HG2	0.48	1.85	6	18
1:A:174:ASN:H	1:A:185:GLN:HG3	0.48	1.69	13	4
1:A:91:LEU:HD22	1:A:91:LEU:C	0.48	2.27	3	2
1:A:47:VAL:HG13	1:A:54:GLY:HA3	0.48	1.84	12	3
1:A:142:ASN:O	1:A:145:THR:N	0.48	2.47	13	17
1:A:146:ILE:HG23	1:A:149:ARG:HD3	0.47	1.85	6	2
1:A:148:LYS:HD2	1:A:148:LYS:H	0.47	1.67	10	1
1:A:130:LEU:HD11	1:A:143:GLU:HB3	0.47	1.86	20	1
1:A:13:VAL:O	1:A:14:VAL:HB	0.47	2.09	20	1
1:A:131:LYS:N	1:A:131:LYS:HE2	0.47	2.24	4	5
1:A:134:GLU:HB3	1:A:141:ASP:HB2	0.47	1.85	20	4
1:A:52:ALA:C	1:A:54:GLY:N	0.47	2.68	12	1
1:A:106:GLU:C	1:A:108:ARG:N	0.47	2.68	19	4
1:A:36:HIS:HA	1:A:91:LEU:HG	0.47	1.86	9	9
1:A:43:LEU:HA	1:A:46:GLU:HB3	0.47	1.87	20	2
1:A:130:LEU:HD13	1:A:141:ASP:OD2	0.47	2.09	12	1
1:A:130:LEU:CG	1:A:143:GLU:HB3	0.47	2.39	20	1
1:A:130:LEU:O	1:A:134:GLU:HG2	0.47	2.09	1	11
1:A:38:SER:HA	1:A:93:ASP:O	0.47	2.10	5	16
1:A:130:LEU:N	1:A:130:LEU:CD2	0.47	2.78	4	11
1:A:146:ILE:O	1:A:149:ARG:HG2	0.47	2.09	3	1
1:A:63:LYS:HG2	1:A:65:GLN:CB	0.47	2.39	19	2
1:A:14:VAL:CG1	1:A:15:GLY:N	0.47	2.78	6	3
1:A:12:PHE:O	1:A:116:LEU:HB3	0.47	2.09	3	14
1:A:139:VAL:C	1:A:141:ASP:N	0.47	2.68	11	19
1:A:142:ASN:HB2	1:A:149:ARG:HH21	0.47	1.70	17	1
1:A:150:LEU:HD21	1:A:154:TYR:CE1	0.47	2.44	10	7
1:A:131:LYS:N	1:A:131:LYS:HE3	0.47	2.24	14	2
1:A:51:SER:C	1:A:53:ARG:N	0.47	2.68	12	1
1:A:39:THR:HB	1:A:72:VAL:HG12	0.46	1.86	18	5
1:A:124:THR:HG1	1:A:176:GLU:HA	0.46	1.69	8	7
1:A:73:LEU:HD21	1:A:104:GLU:HB3	0.46	1.87	2	1
1:A:60:ILE:O	1:A:64:GLY:N	0.46	2.48	19	5
1:A:4:LYS:HD2	1:A:4:LYS:N	0.46	2.25	15	4
1:A:35:THR:HG21	1:A:83:LYS:HE2	0.46	1.87	2	4
1:A:190:LEU:O	1:A:194:LYS:HD3	0.46	2.10	11	2
1:A:43:LEU:HA	1:A:46:GLU:HB2	0.46	1.87	10	1
1:A:125:MET:O	1:A:129:LEU:HD13	0.46	2.11	1	1
1:A:179:VAL:CG2	1:A:180:ASP:N	0.46	2.78	3	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:MET:HE3	1:A:125:MET:HA	0.46	1.87	13	1
1:A:24:GLN:HG3	1:A:183:PHE:HB2	0.46	1.88	2	1
1:A:157:THR:O	1:A:161:ILE:HG12	0.46	2.10	17	10
1:A:158:GLU:N	1:A:159:PRO:HD2	0.46	2.26	17	11
1:A:53:ARG:HH21	1:A:68:PRO:HB3	0.46	1.71	6	1
1:A:11:ILE:HD11	1:A:193:LEU:HD11	0.46	1.87	11	1
1:A:130:LEU:HD21	1:A:143:GLU:CB	0.46	2.40	20	1
1:A:122:PRO:O	1:A:126:THR:HG21	0.46	2.11	13	5
1:A:69:LEU:HD12	1:A:69:LEU:N	0.46	2.26	14	2
1:A:15:GLY:HA3	1:A:118:VAL:HB	0.46	1.88	8	1
1:A:119:ASP:O	1:A:175:ALA:N	0.46	2.48	18	2
1:A:52:ALA:C	1:A:54:GLY:H	0.46	2.14	12	1
1:A:129:LEU:HB3	1:A:140:ASP:HB3	0.46	1.87	18	2
1:A:17:PRO:HA	1:A:21:LYS:HE3	0.46	1.87	17	2
1:A:12:PHE:CE2	1:A:14:VAL:HG12	0.46	2.46	6	1
1:A:25:CYS:HB2	1:A:91:LEU:HD11	0.46	1.88	7	1
1:A:19:SER:HA	1:A:125:MET:HG2	0.46	1.87	20	1
1:A:126:THR:OG1	1:A:127:GLN:N	0.46	2.48	20	1
1:A:73:LEU:N	1:A:73:LEU:CD1	0.46	2.79	14	10
1:A:60:ILE:HG23	1:A:65:GLN:CB	0.46	2.41	14	6
1:A:53:ARG:O	1:A:55:LYS:N	0.46	2.49	12	12
1:A:38:SER:O	1:A:42:LEU:HD13	0.46	2.11	9	5
1:A:5:LEU:HD12	1:A:109:ILE:HG23	0.46	1.88	20	2
1:A:121:GLY:C	1:A:123:GLU:N	0.46	2.68	19	1
1:A:107:ARG:N	1:A:107:ARG:HD2	0.45	2.25	2	2
1:A:80:MET:HE3	1:A:92:ILE:HD11	0.45	1.88	8	2
1:A:167:ARG:HG3	1:A:169:ILE:HG23	0.45	1.87	17	1
1:A:189:HIS:CE1	1:A:190:LEU:HD22	0.45	2.47	16	1
1:A:126:THR:OG1	1:A:146:ILE:HB	0.45	2.11	19	1
1:A:37:LEU:H	1:A:91:LEU:CD1	0.45	2.24	3	2
1:A:104:GLU:HA	1:A:107:ARG:HB2	0.45	1.86	3	2
1:A:109:ILE:N	1:A:109:ILE:CD1	0.45	2.79	19	7
1:A:9:LYS:HD2	1:A:88:LYS:O	0.45	2.11	14	5
1:A:130:LEU:HD13	1:A:141:ASP:HA	0.45	1.88	13	1
1:A:73:LEU:HD22	1:A:104:GLU:HG3	0.45	1.87	18	1
1:A:9:LYS:HG2	1:A:89:GLY:CA	0.45	2.41	19	11
1:A:42:LEU:HD23	1:A:75:MET:HB3	0.45	1.87	19	7
1:A:5:LEU:HB3	1:A:6:LYS:NZ	0.45	2.26	16	4
1:A:2:GLU:O	1:A:4:LYS:N	0.45	2.50	15	1
1:A:126:THR:HA	1:A:146:ILE:CD1	0.45	2.41	18	4
1:A:2:GLU:HB3	1:A:6:LYS:CE	0.45	2.42	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:HIS:N	1:A:189:HIS:ND1	0.45	2.63	5	1
1:A:39:THR:HA	1:A:42:LEU:HD12	0.45	1.89	8	2
1:A:127:GLN:HG3	1:A:128:ARG:H	0.45	1.71	19	1
1:A:158:GLU:N	1:A:158:GLU:CD	0.45	2.70	3	7
1:A:6:LYS:HZ2	1:A:111:GLN:N	0.45	2.10	19	1
1:A:150:LEU:HD13	1:A:151:GLU:N	0.45	2.27	6	4
1:A:43:LEU:O	1:A:47:VAL:HG23	0.45	2.12	12	1
1:A:146:ILE:HA	1:A:149:ARG:NE	0.45	2.27	20	1
1:A:32:TYR:O	1:A:88:LYS:NZ	0.45	2.50	15	4
1:A:21:LYS:O	1:A:24:GLN:NE2	0.45	2.50	20	1
1:A:114:LEU:HB3	1:A:189:HIS:CE1	0.44	2.47	13	2
1:A:56:LYS:CG	1:A:57:LEU:N	0.44	2.80	7	10
1:A:16:GLY:C	1:A:21:LYS:HD3	0.44	2.32	4	1
1:A:21:LYS:HE3	1:A:21:LYS:N	0.44	2.27	5	1
1:A:114:LEU:HD23	1:A:193:LEU:HB3	0.44	1.88	7	2
1:A:37:LEU:O	1:A:92:ILE:HA	0.44	2.11	7	1
1:A:2:GLU:O	1:A:5:LEU:N	0.44	2.50	13	4
1:A:65:GLN:CG	1:A:66:LEU:N	0.44	2.80	3	1
1:A:111:GLN:O	1:A:111:GLN:HG3	0.44	2.12	4	1
1:A:121:GLY:HA2	1:A:125:MET:SD	0.44	2.52	16	4
1:A:14:VAL:HG21	1:A:94:GLY:H	0.44	1.72	6	1
1:A:5:LEU:HD12	1:A:109:ILE:CG2	0.44	2.42	20	2
1:A:106:GLU:O	1:A:108:ARG:N	0.44	2.50	19	3
1:A:80:MET:SD	1:A:92:ILE:HD11	0.44	2.52	18	1
1:A:6:LYS:HZ1	1:A:109:ILE:HG22	0.44	1.72	19	2
1:A:8:THR:HG23	1:A:88:LYS:O	0.44	2.13	15	4
1:A:145:THR:O	1:A:148:LYS:N	0.44	2.50	13	1
1:A:150:LEU:O	1:A:150:LEU:HD22	0.44	2.13	4	5
1:A:15:GLY:N	1:A:21:LYS:HD3	0.44	2.27	14	5
1:A:35:THR:O	1:A:91:LEU:N	0.44	2.49	7	1
1:A:84:VAL:HG13	1:A:85:ASN:N	0.44	2.28	11	1
1:A:194:LYS:CB	1:A:194:LYS:HZ2	0.44	2.25	15	1
1:A:60:ILE:HG23	1:A:65:GLN:HB3	0.44	1.87	16	4
1:A:164:TYR:C	1:A:170:VAL:HG12	0.44	2.33	20	7
1:A:124:THR:HG21	1:A:175:ALA:O	0.44	2.12	12	2
1:A:9:LYS:HE2	1:A:193:LEU:HD11	0.44	1.89	13	1
1:A:147:LYS:O	1:A:151:GLU:N	0.44	2.51	13	1
1:A:114:LEU:C	1:A:115:LEU:HD12	0.44	2.33	3	1
1:A:54:GLY:HA2	1:A:57:LEU:HD11	0.44	1.90	19	2
1:A:127:GLN:CG	1:A:128:ARG:N	0.44	2.81	19	1
1:A:70:GLU:HG2	1:A:71:THR:N	0.44	2.28	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:LEU:HA	1:A:76:LEU:HB2	0.44	1.90	5	1
1:A:9:LYS:O	1:A:89:GLY:HA2	0.44	2.12	7	1
1:A:47:VAL:CG1	1:A:54:GLY:HA3	0.44	2.42	12	1
1:A:126:THR:HB	1:A:143:GLU:O	0.44	2.12	20	1
1:A:146:ILE:HA	1:A:149:ARG:HE	0.43	1.72	20	1
1:A:104:GLU:HA	1:A:107:ARG:HD3	0.43	1.90	9	1
1:A:5:LEU:HD21	1:A:80:MET:HB2	0.43	1.90	14	4
1:A:10:ILE:CG2	1:A:111:GLN:O	0.43	2.66	19	1
1:A:171:ARG:HB3	1:A:189:HIS:HB2	0.43	1.91	7	1
1:A:119:ASP:OD2	1:A:172:LYS:HB3	0.43	2.13	18	1
1:A:114:LEU:HD11	1:A:189:HIS:HD2	0.43	1.73	20	1
1:A:10:ILE:HG13	1:A:90:PHE:CE1	0.43	2.48	16	8
1:A:2:GLU:HG3	1:A:77:ARG:NE	0.43	2.29	1	3
1:A:148:LYS:N	1:A:148:LYS:CD	0.43	2.82	1	5
1:A:2:GLU:HG3	1:A:77:ARG:HD2	0.43	1.91	2	1
1:A:148:LYS:HA	1:A:151:GLU:HB2	0.43	1.89	13	1
1:A:88:LYS:HD2	1:A:88:LYS:H	0.43	1.74	18	1
1:A:44:ARG:HD2	1:A:61:MET:SD	0.43	2.53	1	1
1:A:106:GLU:HG3	1:A:110:GLY:C	0.43	2.33	16	4
1:A:189:HIS:CD2	1:A:189:HIS:N	0.43	2.84	11	1
1:A:147:LYS:HB2	1:A:147:LYS:NZ	0.43	2.27	2	2
1:A:27:LYS:O	1:A:30:GLN:HB2	0.43	2.14	4	4
1:A:4:LYS:HB3	1:A:84:VAL:CG2	0.43	2.42	17	2
1:A:7:LYS:O	1:A:7:LYS:HD2	0.43	2.14	8	1
1:A:50:GLY:O	1:A:51:SER:C	0.43	2.57	6	2
1:A:30:GLN:HG3	1:A:31:LYS:N	0.43	2.28	17	2
1:A:37:LEU:HD21	1:A:90:PHE:HB2	0.43	1.91	16	1
1:A:3:GLU:HG3	1:A:4:LYS:HD3	0.43	1.90	2	1
1:A:13:VAL:CG2	1:A:91:LEU:HD23	0.43	2.44	18	2
1:A:107:ARG:N	1:A:107:ARG:CD	0.43	2.81	6	1
1:A:12:PHE:HB2	1:A:115:LEU:HD12	0.43	1.90	9	3
1:A:80:MET:HE1	1:A:92:ILE:HG12	0.43	1.90	19	3
1:A:6:LYS:NZ	1:A:109:ILE:HG22	0.43	2.29	16	1
1:A:35:THR:HB	1:A:37:LEU:CD2	0.43	2.43	16	1
1:A:169:ILE:HD12	1:A:170:VAL:N	0.43	2.29	7	6
1:A:131:LYS:HA	1:A:131:LYS:HE2	0.43	1.90	18	2
1:A:110:GLY:O	1:A:111:GLN:HG2	0.43	2.14	19	2
1:A:174:ASN:ND2	1:A:181:SER:O	0.42	2.52	16	2
1:A:6:LYS:HE2	1:A:110:GLY:HA3	0.42	1.90	1	2
1:A:116:LEU:HD12	1:A:189:HIS:HB3	0.42	1.91	1	2
1:A:24:GLN:HE22	1:A:179:VAL:HB	0.42	1.75	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HD13	1:A:28:ILE:N	0.42	2.29	8	1
1:A:14:VAL:HG11	1:A:95:TYR:HB2	0.42	1.90	2	1
1:A:164:TYR:CG	1:A:169:ILE:HD11	0.42	2.50	14	1
1:A:8:THR:HG22	1:A:9:LYS:N	0.42	2.29	11	3
1:A:10:ILE:HG21	1:A:111:GLN:O	0.42	2.13	19	1
1:A:164:TYR:HA	1:A:167:ARG:HB3	0.42	1.91	17	1
1:A:26:GLU:C	1:A:28:ILE:N	0.42	2.71	6	2
1:A:115:LEU:HG	1:A:170:VAL:HG23	0.42	1.90	14	1
1:A:123:GLU:O	1:A:126:THR:HG22	0.42	2.14	19	1
1:A:157:THR:O	1:A:160:VAL:HB	0.42	2.14	3	1
1:A:91:LEU:HD23	1:A:92:ILE:N	0.42	2.30	7	1
1:A:38:SER:O	1:A:42:LEU:HG	0.42	2.15	15	2
1:A:179:VAL:O	1:A:183:PHE:N	0.42	2.53	19	1
1:A:53:ARG:C	1:A:55:LYS:N	0.42	2.73	14	6
1:A:150:LEU:HD21	1:A:154:TYR:HE1	0.42	1.75	7	2
1:A:173:VAL:HG21	1:A:182:VAL:CG2	0.42	2.44	20	2
1:A:17:PRO:O	1:A:125:MET:SD	0.42	2.77	15	2
1:A:85:ASN:CG	1:A:86:THR:HG23	0.42	2.35	15	4
1:A:130:LEU:N	1:A:130:LEU:HD23	0.42	2.29	4	2
1:A:179:VAL:O	1:A:182:VAL:CG1	0.42	2.67	11	5
1:A:2:GLU:C	1:A:4:LYS:N	0.42	2.73	15	1
1:A:186:VAL:O	1:A:190:LEU:CD2	0.42	2.67	16	1
1:A:71:THR:O	1:A:75:MET:N	0.41	2.49	8	2
1:A:142:ASN:C	1:A:144:GLU:N	0.41	2.74	11	3
1:A:126:THR:O	1:A:143:GLU:HG2	0.41	2.15	13	1
1:A:44:ARG:HA	1:A:61:MET:HE1	0.41	1.92	17	1
1:A:66:LEU:HD22	1:A:66:LEU:N	0.41	2.30	18	1
1:A:106:GLU:CD	1:A:106:GLU:H	0.41	2.18	14	1
1:A:104:GLU:HB2	1:A:107:ARG:HB2	0.41	1.91	18	1
1:A:182:VAL:O	1:A:186:VAL:CG1	0.41	2.67	20	1
1:A:106:GLU:HG2	1:A:112:PRO:HD3	0.41	1.92	6	2
1:A:191:ASP:HA	1:A:194:LYS:HD3	0.41	1.92	11	1
1:A:115:LEU:HD13	1:A:169:ILE:HD13	0.41	1.91	20	1
1:A:13:VAL:HG13	1:A:116:LEU:CD2	0.41	2.45	20	1
1:A:115:LEU:HB2	1:A:169:ILE:HD12	0.41	1.92	20	1
1:A:131:LYS:HA	1:A:131:LYS:HD3	0.41	1.71	2	2
1:A:6:LYS:HE2	1:A:6:LYS:H	0.41	1.76	16	1
1:A:33:GLY:C	1:A:88:LYS:NZ	0.41	2.74	16	1
1:A:24:GLN:HB3	1:A:186:VAL:HG21	0.41	1.92	17	1
1:A:19:SER:CB	1:A:120:ALA:HB2	0.41	2.46	19	1
1:A:55:LYS:HD2	1:A:56:LYS:N	0.41	2.29	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:GLU:O	1:A:29:VAL:N	0.41	2.54	20	1
1:A:14:VAL:HG11	1:A:94:GLY:H	0.41	1.75	5	1
1:A:115:LEU:HD23	1:A:116:LEU:H	0.41	1.75	17	1
1:A:5:LEU:HD13	1:A:90:PHE:CZ	0.41	2.51	18	1
1:A:59:GLU:HG3	1:A:60:ILE:HD12	0.41	1.92	19	1
1:A:13:VAL:HA	1:A:116:LEU:HB3	0.41	1.92	6	1
1:A:56:LYS:HG3	1:A:57:LEU:N	0.41	2.30	9	1
1:A:57:LEU:O	1:A:61:MET:CG	0.41	2.69	11	1
1:A:35:THR:HG21	1:A:37:LEU:HD21	0.41	1.93	5	1
1:A:32:TYR:C	1:A:88:LYS:HZ1	0.41	2.19	8	1
1:A:187:CYS:HA	1:A:190:LEU:HD23	0.41	1.92	16	1
1:A:88:LYS:H	1:A:88:LYS:HD2	0.41	1.76	2	1
1:A:24:GLN:NE2	1:A:27:LYS:HD3	0.41	2.31	5	1
1:A:175:ALA:C	1:A:177:GLY:N	0.41	2.74	5	3
1:A:71:THR:HG22	1:A:75:MET:HG3	0.41	1.91	9	1
1:A:9:LYS:NZ	1:A:194:LYS:HG3	0.41	2.30	12	1
1:A:30:GLN:HE21	1:A:30:GLN:HA	0.41	1.76	14	1
1:A:130:LEU:HD22	1:A:141:ASP:CA	0.41	2.41	20	1
1:A:15:GLY:N	1:A:21:LYS:HG2	0.41	2.31	12	1
1:A:131:LYS:O	1:A:131:LYS:HD3	0.41	2.15	18	2
1:A:16:GLY:C	1:A:21:LYS:HE3	0.41	2.36	16	1
1:A:185:GLN:O	1:A:188:THR:HB	0.41	2.15	16	1
1:A:186:VAL:O	1:A:190:LEU:HD23	0.41	2.15	16	1
1:A:131:LYS:HE2	1:A:135:THR:HG23	0.41	1.93	17	1
1:A:5:LEU:O	1:A:8:THR:O	0.40	2.39	17	1
1:A:9:LYS:HD3	1:A:88:LYS:C	0.40	2.36	3	1
1:A:175:ALA:O	1:A:177:GLY:N	0.40	2.54	5	1
1:A:128:ARG:O	1:A:130:LEU:N	0.40	2.54	13	1
1:A:142:ASN:CB	1:A:145:THR:HG22	0.40	2.47	10	1
1:A:22:GLY:HA2	1:A:25:CYS:SG	0.40	2.56	14	1
1:A:173:VAL:HG23	1:A:174:ASN:N	0.40	2.31	18	1
1:A:104:GLU:C	1:A:107:ARG:HG2	0.40	2.37	2	1
1:A:126:THR:O	1:A:130:LEU:HD13	0.40	2.16	5	1
1:A:42:LEU:HB3	1:A:75:MET:HB3	0.40	1.92	7	1
1:A:51:SER:O	1:A:54:GLY:N	0.40	2.51	12	1
1:A:14:VAL:HA	1:A:21:LYS:HB3	0.40	1.93	17	1
1:A:32:TYR:OH	1:A:187:CYS:HB2	0.40	2.16	6	1
1:A:10:ILE:HD11	1:A:80:MET:HE2	0.40	1.93	7	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	184/194 (95%)	148±3 (80±1%)	31±3 (17±2%)	5±1 (3±1%)	6	41
All	All	3680/3880 (95%)	2960 (80%)	620 (17%)	100 (3%)	6	41

All 12 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	143	GLU	20
1	A	176	GLU	20
1	A	51	SER	19
1	A	141	ASP	11
1	A	104	GLU	9
1	A	14	VAL	9
1	A	65	GLN	4
1	A	95	TYR	2
1	A	50	GLY	2
1	A	54	GLY	2
1	A	52	ALA	1
1	A	129	LEU	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	160/167 (96%)	122±3 (76±2%)	38±3 (24±2%)	2	25
All	All	3200/3340 (96%)	2439 (76%)	761 (24%)	2	25

All 77 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	9	LYS	20
1	A	37	LEU	20
1	A	57	LEU	20
1	A	75	MET	20
1	A	83	LYS	20
1	A	85	ASN	20
1	A	88	LYS	20
1	A	90	PHE	20
1	A	108	ARG	20
1	A	114	LEU	20
1	A	145	THR	20
1	A	150	LEU	20
1	A	185	GLN	20
1	A	193	LEU	20
1	A	21	LYS	19
1	A	78	ASP	19
1	A	87	SER	19
1	A	91	LEU	19
1	A	124	THR	19
1	A	126	THR	18
1	A	73	LEU	17
1	A	130	LEU	17
1	A	56	LYS	16
1	A	155	LYS	16
1	A	143	GLU	14
1	A	158	GLU	13
1	A	167	ARG	13
1	A	70	GLU	12
1	A	161	ILE	12
1	A	189	HIS	12
1	A	131	LYS	12
1	A	72	VAL	11
1	A	132	ARG	11
1	A	148	LYS	11
1	A	44	ARG	11
1	A	65	GLN	10
1	A	62	GLU	10
1	A	111	GLN	9
1	A	149	ARG	8
1	A	14	VAL	8
1	A	4	LYS	7
1	A	106	GLU	7
1	A	180	ASP	7

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Mol	Chain	Res	Type	Models (Total)
1	A	61	MET	6
1	A	116	LEU	6
1	A	142	ASN	6
1	A	109	ILE	6
1	A	141	ASP	6
1	A	25	CYS	6
1	A	174	ASN	5
1	A	194	LYS	5
1	A	166	LYS	5
1	A	81	VAL	4
1	A	163	PHE	4
1	A	39	THR	4
1	A	6	LYS	4
1	A	30	GLN	4
1	A	107	ARG	3
1	A	147	LYS	3
1	A	127	GLN	3
1	A	7	LYS	2
1	A	74	ASP	2
1	A	10	ILE	2
1	A	176	GLU	2
1	A	190	LEU	2
1	A	51	SER	2
1	A	5	LEU	2
1	A	63	LYS	1
1	A	80	MET	1
1	A	12	PHE	1
1	A	19	SER	1
1	A	105	PHE	1
1	A	36	HIS	1
1	A	1	MET	1
1	A	76	LEU	1
1	A	55	LYS	1
1	A	125	MET	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

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

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	2008
Number of shifts mapped to atoms	2008
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	188	$-1.16 \pm 0.21$	Should be checked
$^{13}\text{C}_\beta$	161	$0.39 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	167	$-0.11 \pm 0.25$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	182	$0.21 \pm 0.17$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1997 atoms were assigned a chemical shift out of a possible 2554. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	908/938 (97%)	376/385 (98%)	352/372 (95%)	180/181 (99%)
Sidechain	1057/1487 (71%)	684/963 (71%)	365/463 (79%)	8/61 (13%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	32/129 (25%)	18/61 (30%)	14/64 (22%)	0/4 (0%)
Overall	1997/2554 (78%)	1078/1409 (77%)	731/899 (81%)	188/246 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 2007 atoms were assigned a chemical shift out of a possible 2661. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	917/977 (94%)	380/401 (95%)	355/388 (91%)	182/188 (97%)
Sidechain	1058/1543 (69%)	685/998 (69%)	365/482 (76%)	8/63 (13%)
Aromatic	32/141 (23%)	18/67 (27%)	14/69 (20%)	0/5 (0%)
Overall	2007/2661 (75%)	1083/1466 (74%)	734/939 (78%)	190/256 (74%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

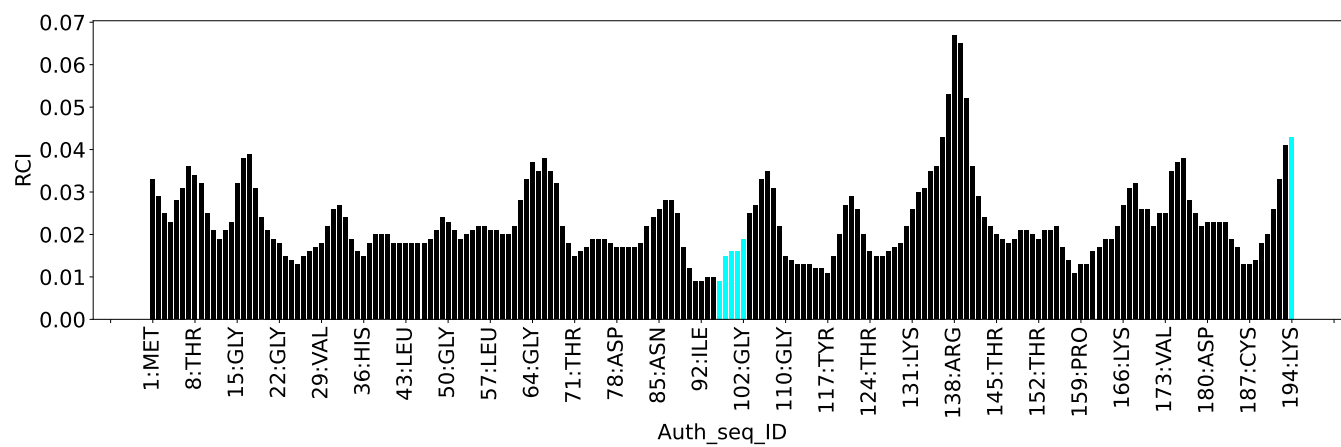
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	111	GLN	CD	173.03	173.59 – 185.85	-5.5
1	A	127	GLN	CD	173.46	173.59 – 185.85	-5.1
1	A	30	GLN	CD	173.48	173.59 – 185.85	-5.1

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

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

Random coil index (RCI) for chain A:





## 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	2467
Intra-residue ( $ i-j =0$ )	876
Sequential ( $ i-j =1$ )	620
Medium range ( $ i-j >1$ and $ i-j <5$ )	548
Long range ( $ i-j \geq 5$ )	423
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	340
Number of unmapped restraints	0
Number of restraints per residue	14.5
Number of long range restraints per residue <sup>1</sup>	2.2

<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)	137.1	0.2
0.2-0.5 (Medium)	86.8	0.5
>0.5 (Large)	138.1	4.04

### 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)	64.2	9.92
10.0-20.0 (Medium)	0.1	11.25
>20.0 (Large)	None	None

## 9 Distance violation analysis ⓘ

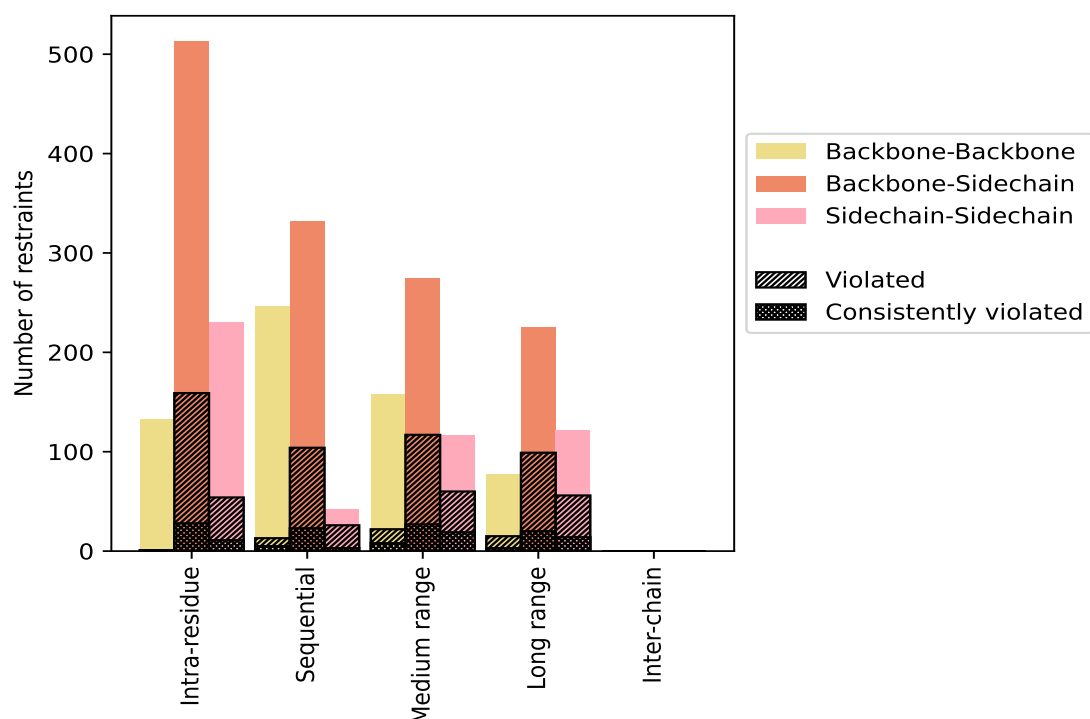
### 9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% <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>
<a href="#">Intra-residue ( i-j =0)</a>	<a href="#">876</a>	<a href="#">35.5</a>	<a href="#">214</a>	<a href="#">24.4</a>	<a href="#">8.7</a>	<a href="#">39</a>	<a href="#">4.5</a>	<a href="#">1.6</a>
Backbone-Backbone	133	5.4	1	0.8	0.0	0	0.0	0.0
Backbone-Sidechain	513	20.8	159	31.0	6.4	28	5.5	1.1
Sidechain-Sidechain	230	9.3	54	23.5	2.2	11	4.8	0.4
<a href="#">Sequential ( i-j =1)</a>	<a href="#">620</a>	<a href="#">25.1</a>	<a href="#">143</a>	<a href="#">23.1</a>	<a href="#">5.8</a>	<a href="#">31</a>	<a href="#">5.0</a>	<a href="#">1.3</a>
Backbone-Backbone	246	10.0	13	5.3	0.5	5	2.0	0.2
Backbone-Sidechain	332	13.5	104	31.3	4.2	23	6.9	0.9
Sidechain-Sidechain	42	1.7	26	61.9	1.1	3	7.1	0.1
<a href="#">Medium range ( i-j &gt;1 &amp;  i-j &lt;5)</a>	<a href="#">548</a>	<a href="#">22.2</a>	<a href="#">199</a>	<a href="#">36.3</a>	<a href="#">8.1</a>	<a href="#">54</a>	<a href="#">9.9</a>	<a href="#">2.2</a>
Backbone-Backbone	158	6.4	22	13.9	0.9	8	5.1	0.3
Backbone-Sidechain	274	11.1	117	42.7	4.7	27	9.9	1.1
Sidechain-Sidechain	116	4.7	60	51.7	2.4	19	16.4	0.8
<a href="#">Long range ( i-j ≥5)</a>	<a href="#">423</a>	<a href="#">17.1</a>	<a href="#">170</a>	<a href="#">40.2</a>	<a href="#">6.9</a>	<a href="#">37</a>	<a href="#">8.7</a>	<a href="#">1.5</a>
Backbone-Backbone	77	3.1	15	19.5	0.6	3	3.9	0.1
Backbone-Sidechain	225	9.1	99	44.0	4.0	20	8.9	0.8
Sidechain-Sidechain	121	4.9	56	46.3	2.3	14	11.6	0.6
<a href="#">Inter-chain</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
<a href="#">Hydrogen bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Disulfide bond</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>	<a href="#">0</a>	<a href="#">0.0</a>	<a href="#">0.0</a>
<a href="#">Total</a>	<a href="#">2467</a>	<a href="#">100.0</a>	<a href="#">726</a>	<a href="#">29.4</a>	<a href="#">29.4</a>	<a href="#">161</a>	<a href="#">6.5</a>	<a href="#">6.5</a>
Backbone-Backbone	614	24.9	51	8.3	2.1	16	2.6	0.6
Backbone-Sidechain	1344	54.5	479	35.6	19.4	98	7.3	4.0
Sidechain-Sidechain	509	20.6	196	38.5	7.9	47	9.2	1.9

<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	97	62	112	84	0	355	0.5	2.35	0.46	0.27
2	94	62	103	95	0	354	0.51	1.77	0.47	0.28
3	90	69	112	93	0	364	0.52	2.34	0.5	0.26
4	97	76	111	85	0	369	0.53	3.13	0.51	0.26
5	95	76	112	90	0	373	0.56	3.13	0.52	0.3
6	89	66	119	88	0	362	0.51	1.87	0.46	0.28
7	98	71	109	94	0	372	0.56	2.61	0.52	0.28
8	101	70	119	87	0	377	0.49	1.82	0.45	0.26
9	96	73	109	89	0	367	0.52	2.57	0.49	0.26
10	99	69	112	91	0	371	0.49	1.85	0.46	0.25

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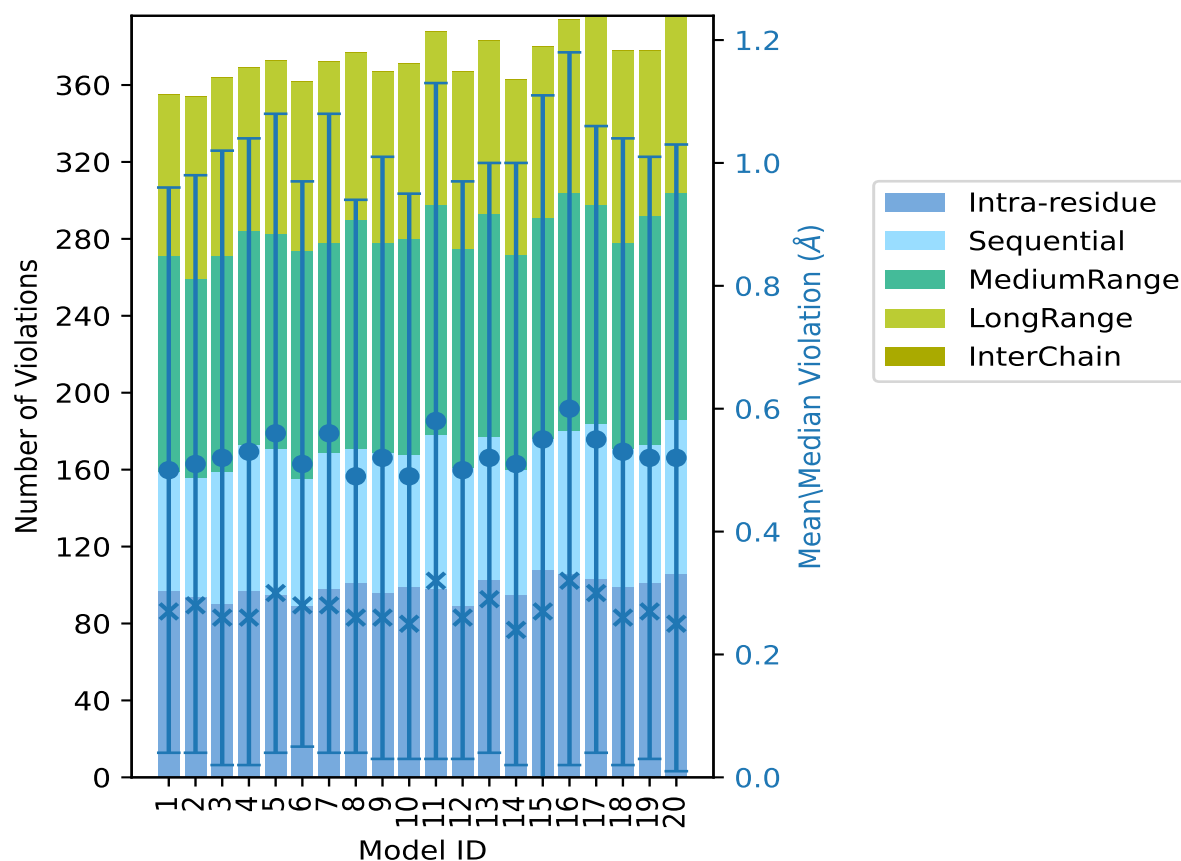
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
11	98	80	120	90	0	388	0.58	3.11	0.55	0.32
12	89	72	114	92	0	367	0.5	2.0	0.47	0.26
13	103	74	116	90	0	383	0.52	1.89	0.48	0.29
14	95	65	112	91	0	363	0.51	1.86	0.49	0.24
15	108	68	115	89	0	380	0.55	4.04	0.56	0.27
16	106	74	124	90	0	394	0.6	2.98	0.58	0.32
17	103	81	114	98	0	396	0.55	3.12	0.51	0.3
18	99	72	107	100	0	378	0.53	2.75	0.51	0.26
19	101	72	119	86	0	378	0.52	3.06	0.49	0.27
20	106	80	118	92	0	396	0.52	3.12	0.51	0.25

<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 ⓘ



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

### 9.3 Distance violation statistics for the ensemble

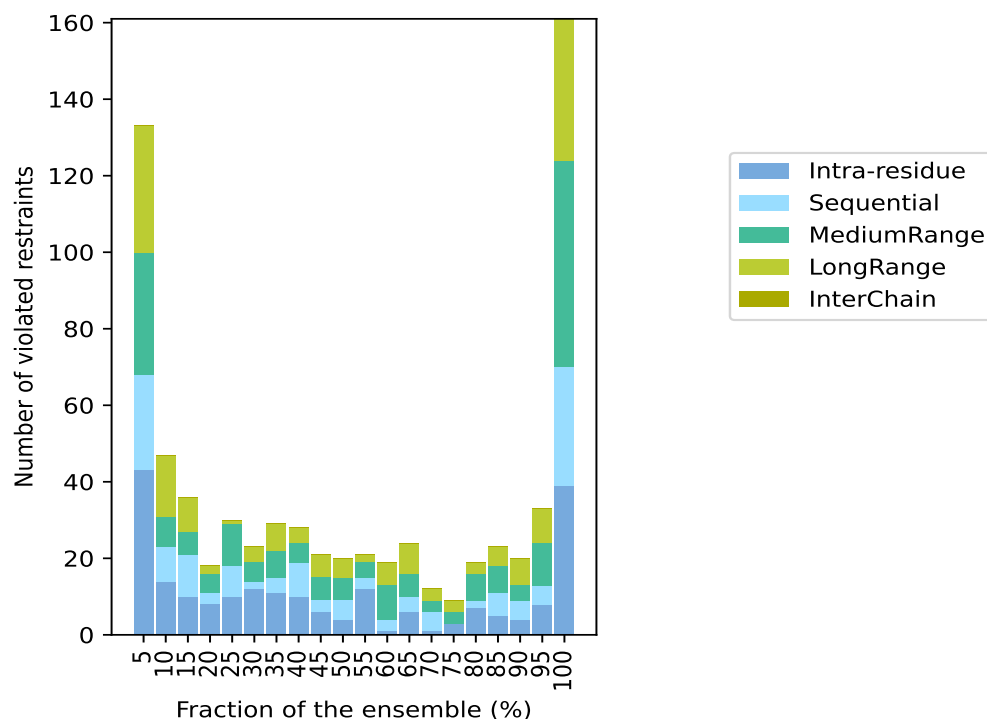
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1741(IR:662, SQ:477, MR:349, LR:253, IC:0) restraints are 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>	%
43	25	32	33	0	133	1	5.0
14	9	8	16	0	47	2	10.0
10	11	6	9	0	36	3	15.0
8	3	5	2	0	18	4	20.0
10	8	11	1	0	30	5	25.0
12	2	5	4	0	23	6	30.0
11	4	7	7	0	29	7	35.0
10	9	5	4	0	28	8	40.0
6	3	6	6	0	21	9	45.0
4	5	6	5	0	20	10	50.0
12	3	4	2	0	21	11	55.0
1	3	9	6	0	19	12	60.0
6	4	6	8	0	24	13	65.0
1	5	3	3	0	12	14	70.0
3	0	3	3	0	9	15	75.0
7	2	7	3	0	19	16	80.0
5	6	7	5	0	23	17	85.0
4	5	4	7	0	20	18	90.0
8	5	11	9	0	33	19	95.0
39	31	54	37	0	161	20	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](#)

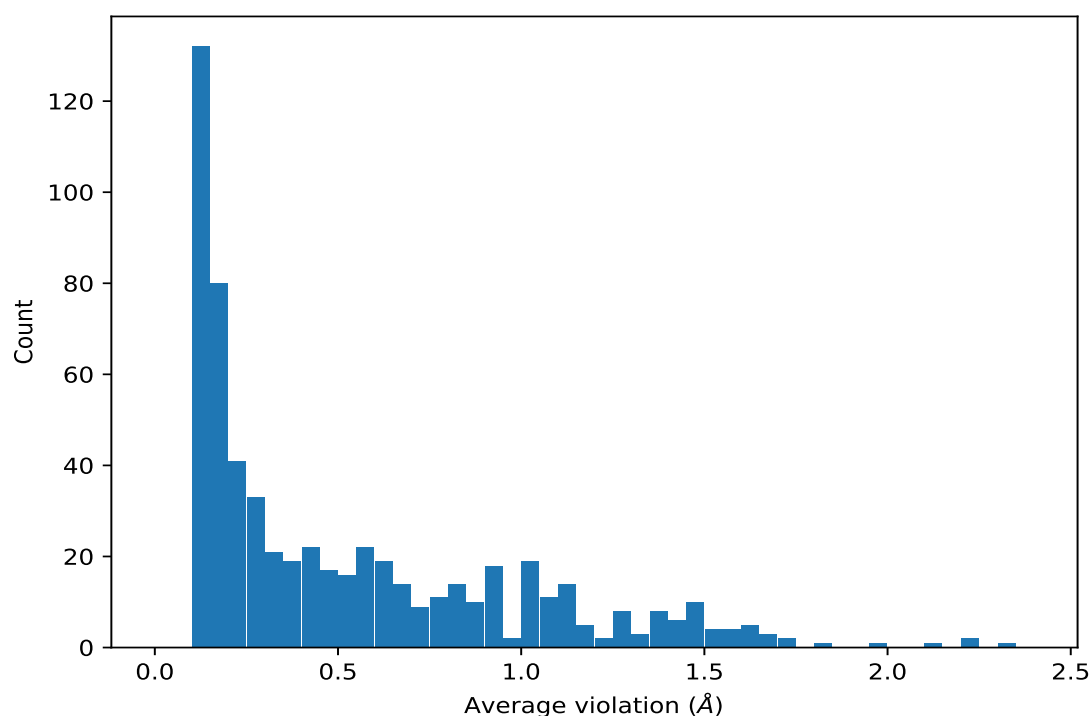


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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)
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	20	1.97	0.67	1.6
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	20	1.7	0.03	1.7
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	20	1.68	0.13	1.71
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	20	1.64	0.05	1.63
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	20	1.64	0.11	1.68
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	20	1.62	0.01	1.62
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	20	1.57	0.07	1.6
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	20	1.51	0.06	1.52
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	20	1.51	0.06	1.52
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	20	1.5	0.53	1.5
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	20	1.49	0.05	1.5
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	20	1.46	0.08	1.46
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	20	1.43	0.27	1.52
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	20	1.36	0.4	1.53
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	20	1.36	0.4	1.53
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG23	20	1.36	0.4	1.53

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	20	1.36	0.07	1.38
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	20	1.36	0.09	1.37
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	20	1.29	0.14	1.34
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	20	1.29	0.03	1.27
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	20	1.27	0.13	1.31
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	20	1.26	0.15	1.28
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	20	1.22	0.16	1.27
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	20	1.21	0.05	1.2
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	20	1.18	0.07	1.17
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	20	1.13	0.4	1.04
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	20	1.12	0.17	1.14
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	20	1.07	0.05	1.06
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	20	1.05	0.07	1.04
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	20	1.05	0.04	1.04
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	20	1.05	0.19	1.06
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	20	1.03	0.45	1.21
(1,13)	1:34:A:TYR:HE2	1:193:A:LEU:HG	20	1.03	0.45	1.21
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	20	1.02	0.24	1.04
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	20	1.01	0.06	1.02
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	20	1.01	0.02	1.01
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	20	0.99	0.24	0.92
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	20	0.98	0.25	0.98
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	20	0.94	0.09	0.92
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	20	0.93	0.1	0.92
(1,17)	1:114:A:LEU:HD11	1:114:A:LEU:H	20	0.93	0.1	0.92
(1,17)	1:114:A:LEU:HD13	1:193:A:LEU:H	20	0.93	0.1	0.92
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	20	0.91	0.05	0.91
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	20	0.9	0.15	0.91
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	20	0.88	0.01	0.88
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	20	0.84	0.01	0.84
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	20	0.84	0.78	0.22
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	20	0.79	0.82	0.18
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	20	0.79	0.32	0.8
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	20	0.77	0.38	0.96
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	20	0.76	0.07	0.76
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	20	0.7	0.01	0.7
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	20	0.69	0.08	0.67
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	20	0.69	0.16	0.72
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	20	0.68	0.1	0.63
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	20	0.68	0.48	1.03
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	20	0.64	0.16	0.72
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	20	0.64	0.67	0.26

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	20	0.63	0.03	0.64
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	20	0.63	0.22	0.55
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	20	0.63	0.17	0.6
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	20	0.62	0.57	0.39
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD11	20	0.62	0.57	0.39
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	20	0.6	0.56	0.22
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	20	0.59	0.13	0.63
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	20	0.59	0.04	0.58
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	20	0.59	0.02	0.59
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	20	0.58	0.2	0.62
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	20	0.57	0.61	0.18
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	20	0.57	0.1	0.59
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	20	0.55	0.08	0.56
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	20	0.55	0.13	0.57
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	20	0.55	0.13	0.57
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	20	0.54	0.12	0.57
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	20	0.54	0.08	0.53
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	20	0.51	0.12	0.52
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	20	0.5	0.09	0.52
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	20	0.48	0.19	0.59
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	20	0.48	0.51	0.24
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	20	0.48	0.04	0.48
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	20	0.47	0.13	0.49
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	20	0.45	0.14	0.4
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	20	0.44	0.06	0.44
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	20	0.43	0.27	0.3
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	20	0.43	0.04	0.44
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	20	0.43	0.04	0.44
(2,488)	1:73:A:LEU:HD13	1:72:A:VAL:HA	20	0.43	0.04	0.44
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	20	0.42	0.12	0.4
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	20	0.41	0.01	0.42
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	20	0.4	0.1	0.4
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	20	0.39	0.08	0.4
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	20	0.39	0.12	0.36
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	20	0.38	0.0	0.38
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	20	0.38	0.05	0.36
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	20	0.37	0.08	0.4
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	20	0.37	0.02	0.36
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	20	0.37	0.01	0.37
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	20	0.34	0.07	0.37
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	20	0.34	0.06	0.38
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	20	0.34	0.02	0.33

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	20	0.33	0.13	0.3
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	20	0.32	0.12	0.32
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	20	0.31	0.04	0.32
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	20	0.3	0.01	0.3
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	20	0.3	0.36	0.21
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	20	0.29	0.04	0.3
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	20	0.29	0.16	0.2
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	20	0.29	0.07	0.3
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	20	0.29	0.09	0.34
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	20	0.29	0.01	0.29
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	20	0.26	0.03	0.27
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	20	0.26	0.02	0.26
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	20	0.26	0.01	0.26
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	20	0.26	0.03	0.27
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	20	0.25	0.04	0.24
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	20	0.25	0.01	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	20	0.25	0.01	0.26
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	20	0.24	0.01	0.24
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	20	0.24	0.02	0.24
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	20	0.24	0.01	0.24
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	20	0.24	0.02	0.24
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	20	0.24	0.03	0.24
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	20	0.24	0.03	0.24
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	20	0.23	0.03	0.24
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	20	0.23	0.28	0.13
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	20	0.23	0.01	0.23
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	20	0.22	0.03	0.22
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	20	0.22	0.03	0.22
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	20	0.22	0.03	0.23
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	20	0.22	0.03	0.22
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	20	0.22	0.05	0.21
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	20	0.21	0.02	0.22
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	20	0.21	0.04	0.22
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	20	0.2	0.03	0.2
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	20	0.2	0.04	0.2
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	20	0.2	0.03	0.19
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	20	0.2	0.02	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	20	0.19	0.01	0.2
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	20	0.19	0.03	0.18
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	20	0.19	0.02	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	20	0.19	0.0	0.19
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	20	0.19	0.15	0.16

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	20	0.18	0.03	0.18
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	20	0.18	0.03	0.18
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	20	0.18	0.03	0.18
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	20	0.17	0.03	0.17
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	20	0.17	0.02	0.18
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	20	0.17	0.07	0.16
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	20	0.17	0.02	0.17
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	20	0.17	0.03	0.16
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	20	0.17	0.01	0.17
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	20	0.17	0.02	0.17
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	20	0.17	0.02	0.18
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	20	0.17	0.03	0.16
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	20	0.17	0.02	0.17
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	20	0.16	0.04	0.17
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	20	0.16	0.03	0.17
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	20	0.16	0.01	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	20	0.16	0.01	0.16
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	20	0.16	0.03	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	20	0.16	0.01	0.15
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	20	0.15	0.01	0.15
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	20	0.15	0.02	0.15
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	20	0.14	0.02	0.13
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	20	0.14	0.0	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	20	0.14	0.01	0.14
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	20	0.14	0.01	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	20	0.12	0.01	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	20	0.12	0.01	0.12
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	19	1.63	0.12	1.63
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	19	1.45	0.17	1.44
(1,15)	1:125:A:MET:HB3	1:126:A:THR:HG22	19	1.45	0.17	1.44
(1,15)	1:68:A:PRO:HB3	1:71:A:THR:HG21	19	1.45	0.17	1.44
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	19	1.43	0.04	1.43
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	19	1.0	0.64	1.48
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	19	0.92	0.13	0.98
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	19	0.91	0.83	0.23
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	19	0.81	0.03	0.82
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	19	0.73	0.08	0.72
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	19	0.72	0.27	0.83
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	19	0.56	0.42	0.31
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	19	0.41	0.1	0.44
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	19	0.4	0.28	0.16
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	19	0.37	0.58	0.13

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	19	0.32	0.06	0.32
(1,11)	1:184:A:SER:HB2	1:185:A:GLN:HG2	19	0.32	0.06	0.32
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	19	0.22	0.03	0.22
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	19	0.21	0.02	0.21
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	19	0.18	0.04	0.17
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	19	0.18	0.03	0.19
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	19	0.16	0.02	0.16
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	19	0.16	0.02	0.16
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	19	0.15	0.02	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	19	0.15	0.01	0.15
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	19	0.15	0.02	0.16
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	19	0.15	0.02	0.15
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	19	0.15	0.01	0.15
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	19	0.14	0.02	0.14
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	19	0.14	0.02	0.13
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	19	0.13	0.02	0.12
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	19	0.13	0.01	0.13
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	19	0.13	0.01	0.13
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	19	0.13	0.02	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	19	0.11	0.01	0.12
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	19	0.11	0.01	0.11
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	18	1.37	0.19	1.36
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	18	1.25	0.8	1.78
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	18	1.04	0.04	1.05
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	18	0.94	0.51	1.2
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	18	0.78	0.81	0.15
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	18	0.77	0.72	0.16
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	18	0.69	0.01	0.69
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	18	0.69	0.51	1.08
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	18	0.39	0.22	0.27
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	18	0.38	0.36	0.12
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	18	0.3	0.01	0.3
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	18	0.25	0.09	0.24
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	18	0.23	0.04	0.24
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	18	0.2	0.02	0.2
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	18	0.15	0.02	0.15
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	18	0.15	0.02	0.14
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	18	0.14	0.03	0.13
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	18	0.13	0.03	0.13
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	18	0.13	0.02	0.12
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	18	0.11	0.01	0.11
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	17	1.33	0.05	1.33

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	17	1.26	0.54	1.56
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	17	1.14	0.19	1.21
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	17	0.94	0.28	0.97
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	17	0.9	0.26	0.82
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	17	0.53	0.1	0.56
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	17	0.53	0.6	0.14
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	17	0.5	0.56	0.14
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	17	0.32	0.06	0.33
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	17	0.29	0.04	0.28
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	17	0.19	0.01	0.2
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	17	0.17	0.11	0.12
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	17	0.16	0.04	0.15
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	17	0.15	0.02	0.15
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	17	0.14	0.04	0.13
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	17	0.14	0.02	0.14
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	17	0.14	0.02	0.13
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	17	0.14	0.02	0.13
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	17	0.13	0.02	0.13
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	17	0.13	0.02	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	17	0.12	0.01	0.13
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	17	0.12	0.02	0.11
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	16	1.19	0.1	1.22
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	16	1.16	0.11	1.16
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	16	1.05	0.45	1.06
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	16	1.03	0.36	0.94
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	16	1.03	0.34	1.16
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	16	0.58	0.35	0.69
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	16	0.43	0.32	0.26
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	16	0.41	0.52	0.28
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	16	0.41	0.03	0.42
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	16	0.34	0.54	0.14
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	16	0.25	0.12	0.24
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	16	0.22	0.32	0.13
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	16	0.2	0.06	0.22
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	16	0.16	0.02	0.16
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	16	0.15	0.02	0.15
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	16	0.15	0.03	0.16
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	16	0.12	0.01	0.12
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	16	0.12	0.01	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	16	0.11	0.01	0.11
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	15	0.69	0.07	0.67
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	15	0.63	0.22	0.67

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	15	0.4	0.72	0.13
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	15	0.37	0.09	0.42
(1,25)	1:72:A:VAL:HB	1:69:A:LEU:HA	15	0.37	0.09	0.42
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	15	0.18	0.02	0.18
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	15	0.15	0.06	0.14
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	15	0.15	0.03	0.14
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	15	0.14	0.04	0.14
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	15	0.13	0.02	0.14
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	14	1.66	0.41	1.77
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	14	0.68	0.43	0.78
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	14	0.62	0.36	0.69
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	14	0.4	0.59	0.14
(1,32)	1:50:A:GLY:H	1:51:A:SER:HB2	14	0.4	0.59	0.14
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	14	0.27	0.25	0.14
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	14	0.26	0.09	0.24
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	14	0.25	0.18	0.14
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	14	0.25	0.07	0.25
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	14	0.23	0.38	0.12
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	14	0.12	0.01	0.12
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	14	0.11	0.01	0.11
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	14	0.11	0.01	0.11
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	13	1.59	0.08	1.59
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	13	0.93	0.13	0.91
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	13	0.87	0.1	0.89
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	13	0.86	0.4	1.07
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	13	0.85	0.15	0.82
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	13	0.67	0.13	0.71
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	13	0.59	0.41	0.45
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	13	0.55	0.02	0.55
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	13	0.53	0.18	0.51
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	13	0.53	0.13	0.55
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	13	0.51	0.71	0.14
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	13	0.43	0.0	0.43
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	13	0.28	0.0	0.28
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	13	0.17	0.02	0.17
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	13	0.17	0.03	0.16
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	13	0.15	0.03	0.16
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	13	0.15	0.02	0.15
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	13	0.15	0.04	0.14
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	13	0.13	0.03	0.12
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	13	0.12	0.02	0.12
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	13	0.12	0.02	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	13	0.12	0.01	0.11
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	13	0.11	0.01	0.11
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	13	0.1	0.0	0.1
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	12	1.48	0.07	1.46
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	12	1.45	0.06	1.44
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	12	1.42	0.05	1.44
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	12	1.33	0.02	1.33
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	12	1.25	0.66	1.6
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	12	1.12	0.15	1.11
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	12	1.11	0.29	0.93
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	12	1.05	0.55	1.1
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	12	0.65	0.08	0.64
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	12	0.61	0.18	0.58
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	12	0.57	0.54	0.12
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	12	0.55	0.1	0.54
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	12	0.36	0.37	0.24
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD11	12	0.36	0.37	0.24
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	12	0.29	0.48	0.15
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	12	0.26	0.08	0.23
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	12	0.22	0.01	0.22
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	12	0.21	0.1	0.16
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	12	0.16	0.07	0.13
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	12	0.12	0.01	0.12
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	11	1.63	0.02	1.64
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	11	1.0	0.02	1.01
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	11	0.84	0.31	0.99
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	11	0.76	0.01	0.75
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	11	0.74	0.54	1.1
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	11	0.59	0.0	0.59
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	11	0.46	0.14	0.51
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	11	0.37	0.02	0.37
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	11	0.32	0.27	0.25
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	11	0.25	0.06	0.27
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	11	0.16	0.01	0.16
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	11	0.15	0.07	0.12
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	11	0.12	0.01	0.12
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	11	0.12	0.01	0.12
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	11	0.12	0.02	0.12
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	11	0.12	0.01	0.12
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	11	0.11	0.01	0.11
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	11	0.11	0.01	0.11
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	10	1.56	0.01	1.56

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	10	1.47	0.18	1.58
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	10	1.12	0.51	1.37
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	10	1.07	0.49	1.27
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	10	0.87	0.25	0.98
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	10	0.81	0.04	0.82
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	10	0.81	0.44	1.1
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	10	0.81	0.16	0.76
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	10	0.79	0.32	0.76
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	10	0.72	0.02	0.71
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	10	0.68	0.16	0.76
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	10	0.61	0.0	0.61
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	10	0.54	0.01	0.54
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	10	0.38	0.15	0.38
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	10	0.17	0.04	0.18
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	10	0.16	0.11	0.12
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	10	0.16	0.03	0.16
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	10	0.14	0.03	0.16
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	10	0.14	0.03	0.12
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	10	0.12	0.02	0.11
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	9	1.38	0.45	1.58
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	9	1.13	0.02	1.14
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	9	1.03	0.35	1.08
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	9	1.02	0.05	0.99
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	9	0.89	0.02	0.88
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	9	0.6	0.01	0.6
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	9	0.46	0.14	0.53
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	9	0.46	0.29	0.6
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	9	0.39	0.46	0.15
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	9	0.3	0.03	0.31
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	9	0.29	0.43	0.14
(1,3)	1:9:A:LYS:HE2	1:88:A:LYS:HG2	9	0.25	0.05	0.26
(1,3)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	9	0.25	0.05	0.26
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	9	0.24	0.02	0.24
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	9	0.21	0.1	0.15
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	9	0.16	0.0	0.16
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	9	0.14	0.02	0.14
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	9	0.13	0.02	0.13
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	9	0.13	0.01	0.12
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	9	0.13	0.02	0.12
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	9	0.12	0.02	0.12
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	9	0.12	0.02	0.11
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	8	1.74	0.03	1.75

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	8	1.57	0.01	1.58
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	8	1.48	0.09	1.52
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	8	1.1	0.14	1.04
(2,319)	1:66:A:LEU:HD23	1:66:A:LEU:HA	8	1.04	0.54	1.27
(2,319)	1:66:A:LEU:HD21	1:66:A:LEU:HA	8	1.04	0.54	1.27
(2,319)	1:66:A:LEU:HD22	1:66:A:LEU:HA	8	1.04	0.54	1.27
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	8	1.02	0.35	1.15
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	8	1.0	0.57	0.78
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	8	0.92	0.13	0.9
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	8	0.83	0.06	0.8
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	8	0.83	0.06	0.8
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	8	0.81	0.01	0.81
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	8	0.59	0.38	0.86
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	8	0.55	0.06	0.56
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	8	0.4	0.76	0.11
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	8	0.4	0.12	0.42
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	8	0.34	0.49	0.15
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	8	0.3	0.07	0.3
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	8	0.29	0.46	0.11
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	8	0.18	0.01	0.18
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	8	0.16	0.03	0.16
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	8	0.14	0.03	0.14
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	8	0.14	0.01	0.14
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	8	0.13	0.01	0.13
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	8	0.12	0.02	0.12
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	8	0.12	0.02	0.12
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	8	0.12	0.01	0.12
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	8	0.11	0.01	0.11
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	8	0.11	0.01	0.11
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	8	0.1	0.0	0.1
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	7	1.13	0.02	1.11
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	7	1.07	0.24	1.14
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	7	1.05	0.62	1.52
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	7	1.01	0.03	1.02
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	7	0.89	0.5	1.2
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	7	0.81	0.62	1.17
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	7	0.71	0.33	0.84
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	7	0.66	0.03	0.67
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	7	0.62	1.2	0.14
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	7	0.55	1.03	0.12
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	7	0.48	0.16	0.53
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	7	0.47	0.18	0.48

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,22)	1:38:A:SER:HA	1:91:A:LEU:HD13	7	0.45	0.51	0.24
(1,22)	1:38:A:SER:HA	1:14:A:VAL:HG21	7	0.45	0.51	0.24
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	7	0.4	0.03	0.42
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	7	0.39	0.01	0.39
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	7	0.33	0.22	0.21
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	7	0.3	0.05	0.32
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	7	0.24	0.1	0.21
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	7	0.23	0.06	0.23
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	7	0.17	0.03	0.19
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	7	0.16	0.04	0.15
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	7	0.15	0.05	0.14
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	7	0.13	0.04	0.11
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	7	0.12	0.01	0.13
(1,8)	1:81:A:VAL:HA	1:81:A:VAL:HG22	7	0.12	0.0	0.12
(1,8)	1:47:A:VAL:HG21	1:47:A:VAL:HA	7	0.12	0.0	0.12
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	7	0.12	0.02	0.13
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	7	0.12	0.02	0.11
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	7	0.11	0.01	0.12
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	7	0.11	0.01	0.11
(2,2366)	1:2:A:GLU:H	1:3:A:GLU:HG2	6	1.5	0.03	1.5
(2,314)	1:166:A:LYS:HB2	1:166:A:LYS:HD2	6	1.18	0.1	1.19
(2,883)	1:162:A:ALA:HB1	1:166:A:LYS:HE3	6	1.14	0.55	1.17
(2,1276)	1:7:A:LYS:H	1:7:A:LYS:HE2	6	1.11	0.04	1.12
(2,2306)	1:163:A:PHE:H	1:166:A:LYS:HD2	6	1.07	0.08	1.06
(2,1699)	1:53:A:ARG:H	1:53:A:ARG:HD2	6	0.93	0.04	0.92
(2,2024)	1:95:A:TYR:H	1:14:A:VAL:HG22	6	0.83	0.35	0.94
(2,217)	1:138:A:ARG:HD2	1:133:A:GLY:HA3	6	0.75	0.2	0.65
(2,37)	1:166:A:LYS:HD2	1:163:A:PHE:HA	6	0.73	0.19	0.72
(2,40)	1:166:A:LYS:HD2	1:166:A:LYS:HE3	6	0.62	0.0	0.62
(2,644)	1:123:A:GLU:HG3	1:124:A:THR:HB	6	0.59	0.02	0.6
(2,311)	1:143:A:GLU:HG3	1:130:A:LEU:HD12	6	0.54	0.44	0.49
(2,1708)	1:143:A:GLU:H	1:130:A:LEU:HD12	6	0.45	0.48	0.12
(2,1447)	1:152:A:THR:H	1:149:A:ARG:HD3	6	0.41	0.06	0.4
(2,1336)	1:149:A:ARG:H	1:149:A:ARG:HD3	6	0.26	0.07	0.26
(2,1204)	1:51:A:SER:H	1:51:A:SER:HB2	6	0.16	0.01	0.16
(2,212)	1:169:A:ILE:HG22	1:169:A:ILE:HG13	6	0.16	0.03	0.16
(2,231)	1:161:A:ILE:HD12	1:161:A:ILE:HB	6	0.15	0.03	0.16
(2,848)	1:5:A:LEU:HG	1:2:A:GLU:HG2	6	0.14	0.02	0.15
(2,295)	1:68:A:PRO:HA	1:68:A:PRO:HB2	6	0.14	0.03	0.12
(2,607)	1:34:A:TYR:HE2	1:34:A:TYR:HA	6	0.12	0.04	0.11
(2,302)	1:2:A:GLU:HA	1:2:A:GLU:HG2	6	0.12	0.01	0.11
(2,23)	1:7:A:LYS:HA	1:7:A:LYS:HB2	6	0.1	0.0	0.1

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1293)	1:161:A:ILE:H	1:161:A:ILE:HG13	5	1.05	0.02	1.05
(2,529)	1:162:A:ALA:HB2	1:161:A:ILE:HG13	5	1.04	0.06	1.07
(2,477)	1:161:A:ILE:HG13	1:160:A:VAL:HB	5	0.93	0.03	0.92
(2,1705)	1:3:A:GLU:H	1:4:A:LYS:HD2	5	0.77	0.46	0.78
(2,852)	1:161:A:ILE:HG22	1:161:A:ILE:HG12	5	0.68	0.01	0.67
(2,1399)	1:55:A:LYS:H	1:55:A:LYS:HB3	5	0.6	0.0	0.6
(2,1320)	1:41:A:ASP:H	1:41:A:ASP:HB2	5	0.51	0.01	0.51
(2,223)	1:132:A:ARG:HA	1:132:A:ARG:HD2	5	0.5	0.35	0.25
(2,1457)	1:38:A:SER:H	1:41:A:ASP:HB2	5	0.47	0.11	0.42
(2,2371)	1:7:A:LYS:H	1:6:A:LYS:HG2	5	0.36	0.03	0.37
(2,1424)	1:44:A:ARG:H	1:44:A:ARG:HD3	5	0.29	0.37	0.11
(2,462)	1:134:A:GLU:HG3	1:131:A:LYS:HE2	5	0.25	0.2	0.17
(2,937)	1:6:A:LYS:HG3	1:6:A:LYS:HB3	5	0.18	0.0	0.18
(2,841)	1:60:A:ILE:HG12	1:56:A:LYS:HA	5	0.17	0.02	0.17
(2,930)	1:174:A:ASN:HB3	1:176:A:GLU:HB2	5	0.15	0.04	0.14
(2,44)	1:30:A:GLN:HB2	1:30:A:GLN:HG2	5	0.15	0.03	0.15
(2,1878)	1:87:A:SER:H	1:90:A:PHE:HD2	5	0.13	0.02	0.13
(2,1801)	1:44:A:ARG:H	1:43:A:LEU:HD22	5	0.13	0.01	0.13
(2,517)	1:179:A:VAL:HG22	1:180:A:ASP:HB2	5	0.13	0.01	0.13
(2,1417)	1:58:A:SER:H	1:58:A:SER:HB3	5	0.13	0.02	0.13
(2,1473)	1:175:A:ALA:H	1:174:A:ASN:HB2	5	0.12	0.01	0.12
(2,1392)	1:79:A:ALA:H	1:81:A:VAL:H	5	0.12	0.02	0.12
(2,1845)	1:107:A:ARG:H	1:106:A:GLU:HG3	5	0.12	0.02	0.12
(2,2142)	1:71:A:THR:H	1:69:A:LEU:H	5	0.12	0.01	0.12
(2,2381)	1:177:A:GLY:H	1:177:A:GLY:HA3	5	0.12	0.01	0.11
(2,528)	1:192:A:ALA:HB2	1:188:A:THR:HG21	5	0.12	0.02	0.11
(2,530)	1:60:A:ILE:HG22	1:66:A:LEU:HA	5	0.11	0.01	0.11
(2,666)	1:87:A:SER:HB2	1:83:A:LYS:HG2	5	0.11	0.0	0.11
(2,2139)	1:45:A:SER:H	1:48:A:SER:H	5	0.11	0.01	0.1
(2,2029)	1:142:A:ASN:H	1:145:A:THR:HG21	5	0.1	0.0	0.1
(2,2106)	1:160:A:VAL:H	1:163:A:PHE:HB3	4	1.43	0.12	1.38
(1,18)	1:130:A:LEU:HD22	1:129:A:LEU:HB3	4	1.42	1.25	1.37
(1,18)	1:130:A:LEU:HD22	1:129:A:LEU:HB2	4	1.42	1.25	1.37
(2,2102)	1:27:A:LYS:H	1:26:A:GLU:HG2	4	1.1	0.01	1.1
(2,409)	1:107:A:ARG:HD2	1:106:A:GLU:HG2	4	0.9	0.67	0.86
(2,2154)	1:135:A:THR:H	1:131:A:LYS:HD3	4	0.89	0.75	0.88
(1,26)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	4	0.8	0.02	0.82
(2,74)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	4	0.78	0.03	0.8
(2,1365)	1:111:A:GLN:H	1:111:A:GLN:HG2	4	0.73	0.38	0.84
(2,2294)	1:28:A:ILE:H	1:26:A:GLU:HG2	4	0.61	0.03	0.6
(2,868)	1:160:A:VAL:HG12	1:163:A:PHE:HB3	4	0.4	0.15	0.36
(2,1072)	1:143:A:GLU:H	1:143:A:GLU:HG3	4	0.27	0.25	0.14

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1287)	1:163:A:PHE:H	1:163:A:PHE:HB3	4	0.23	0.04	0.22
(2,1150)	1:106:A:GLU:H	1:106:A:GLU:HB2	4	0.18	0.02	0.18
(2,297)	1:44:A:ARG:HG2	1:44:A:ARG:HA	4	0.16	0.02	0.16
(2,515)	1:182:A:VAL:HG22	1:118:A:VAL:HA	4	0.13	0.02	0.12
(2,1678)	1:141:A:ASP:H	1:138:A:ARG:HB2	4	0.12	0.01	0.12
(2,1337)	1:62:A:GLU:H	1:62:A:GLU:HG3	4	0.11	0.0	0.11
(2,556)	1:34:A:TYR:HD1	1:29:A:VAL:HG12	4	0.11	0.0	0.11
(2,1588)	1:13:A:VAL:H	1:91:A:LEU:HD12	3	2.23	0.15	2.34
(2,795)	1:34:A:TYR:HB2	1:91:A:LEU:HD22	3	2.1	0.47	2.21
(2,1596)	1:46:A:GLU:H	1:47:A:VAL:HG12	3	1.82	0.04	1.81
(2,2418)	1:31:A:LYS:H	1:30:A:GLN:HB2	3	1.35	0.0	1.35
(2,1159)	1:47:A:VAL:H	1:47:A:VAL:HG12	3	1.13	0.02	1.12
(2,785)	1:140:A:ASP:HB3	1:149:A:ARG:HD3	3	0.9	0.13	0.94
(2,225)	1:166:A:LYS:HB2	1:166:A:LYS:HE2	3	0.8	0.01	0.8
(2,393)	1:91:A:LEU:HA	1:91:A:LEU:HD12	3	0.73	0.05	0.71
(2,899)	1:76:A:LEU:HD12	1:75:A:MET:HB2	3	0.68	0.82	0.1
(2,2214)	1:189:A:HIS:H	1:190:A:LEU:HG	3	0.63	0.58	0.24
(2,265)	1:53:A:ARG:HG2	1:53:A:ARG:HD2	3	0.6	0.0	0.6
(2,227)	1:106:A:GLU:HA	1:106:A:GLU:HG3	3	0.49	0.0	0.49
(2,2020)	1:110:A:GLY:H	1:111:A:GLN:HG2	3	0.46	0.43	0.18
(2,1774)	1:100:A:GLN:H	1:163:A:PHE:HB3	3	0.24	0.07	0.29
(2,2101)	1:27:A:LYS:H	1:25:A:CYS:HB2	3	0.24	0.08	0.25
(2,2268)	1:37:A:LEU:H	1:91:A:LEU:HG	3	0.24	0.09	0.19
(2,1388)	1:30:A:GLN:H	1:30:A:GLN:HG2	3	0.21	0.0	0.21
(2,836)	1:155:A:LYS:HD2	1:154:A:TYR:HB3	3	0.19	0.01	0.2
(2,422)	1:41:A:ASP:HB2	1:44:A:ARG:HB2	3	0.17	0.06	0.15
(2,2278)	1:115:A:LEU:H	1:114:A:LEU:HD12	3	0.16	0.01	0.15
(2,492)	1:170:A:VAL:HG11	1:172:A:LYS:H	3	0.15	0.02	0.15
(2,1779)	1:155:A:LYS:H	1:155:A:LYS:HB3	3	0.13	0.0	0.13
(2,1869)	1:31:A:LYS:H	1:28:A:ILE:HG22	3	0.13	0.02	0.13
(2,1835)	1:111:A:GLN:H	1:6:A:LYS:HA	3	0.13	0.02	0.11
(2,1511)	1:93:A:ASP:H	1:37:A:LEU:HB2	3	0.12	0.03	0.1
(2,292)	1:72:A:VAL:HB	1:72:A:VAL:HG22	3	0.11	0.01	0.11
(2,1746)	1:156:A:ALA:H	1:155:A:LYS:HB2	3	0.11	0.01	0.12
(2,505)	1:118:A:VAL:H	1:118:A:VAL:HG12	3	0.11	0.0	0.11
(2,869)	1:160:A:VAL:HG12	1:157:A:THR:HA	3	0.11	0.01	0.11
(2,989)	1:11:A:ILE:HB	1:11:A:ILE:HG22	3	0.11	0.01	0.1
(2,1242)	1:121:A:GLY:H	1:120:A:ALA:H	3	0.11	0.01	0.11
(2,2264)	1:175:A:ALA:H	1:176:A:GLU:HB2	3	0.11	0.01	0.11
(2,1672)	1:39:A:THR:H	1:93:A:ASP:HA	3	0.11	0.01	0.11
(2,1974)	1:18:A:GLY:H	1:17:A:PRO:HB2	3	0.11	0.0	0.11
(2,2130)	1:25:A:CYS:H	1:21:A:LYS:HA	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(2,1539)	1:119:A:ASP:H	1:173:A:VAL:HG12	3	0.1	0.0	0.1
(2,213)	1:11:A:ILE:HG22	1:190:A:LEU:HD22	2	2.32	0.44	2.32
(2,895)	1:130:A:LEU:HD22	1:130:A:LEU:HA	2	2.22	0.01	2.22
(2,1736)	1:81:A:VAL:H	1:5:A:LEU:HD22	2	1.67	1.55	1.67
(2,1472)	1:36:A:HIS:H	1:37:A:LEU:HD12	2	1.49	1.39	1.49
(2,1627)	1:130:A:LEU:H	1:130:A:LEU:HD22	2	1.3	0.04	1.3
(2,769)	1:132:A:ARG:HD3	1:129:A:LEU:HA	2	1.28	0.0	1.28
(2,1720)	1:132:A:ARG:H	1:131:A:LYS:HD3	2	1.17	0.01	1.17
(2,931)	1:7:A:LYS:HA	1:7:A:LYS:HD3	2	1.11	0.1	1.11
(2,1718)	1:60:A:ILE:H	1:61:A:MET:HG2	2	0.92	0.01	0.92
(2,779)	1:9:A:LYS:HE2	1:11:A:ILE:HD12	2	0.88	0.58	0.88
(2,963)	1:61:A:MET:HG2	1:57:A:LEU:HB2	2	0.88	0.1	0.88
(2,1609)	1:84:A:VAL:H	1:85:A:ASN:HB3	2	0.58	0.48	0.58
(2,277)	1:134:A:GLU:HB2	1:134:A:GLU:HA	2	0.56	0.0	0.56
(2,29)	1:194:A:LYS:HB3	1:194:A:LYS:HE2	2	0.54	0.01	0.54
(2,1942)	1:15:A:GLY:H	1:21:A:LYS:HE2	2	0.5	0.06	0.5
(2,823)	1:65:A:GLN:HG2	1:60:A:ILE:HA	2	0.47	0.0	0.47
(2,1017)	1:171:A:ARG:HD3	1:171:A:ARG:HA	2	0.34	0.08	0.34
(2,904)	1:194:A:LYS:HB3	1:192:A:ALA:H	2	0.32	0.14	0.32
(2,466)	1:190:A:LEU:HG	1:190:A:LEU:HD12	2	0.26	0.01	0.26
(2,573)	1:153:A:TYR:HD1	1:15:A:GLY:HA3	2	0.26	0.15	0.26
(2,457)	1:189:A:HIS:HB3	1:114:A:LEU:HD12	2	0.24	0.03	0.24
(2,828)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	2	0.22	0.12	0.22
(2,2157)	1:16:A:GLY:H	1:119:A:ASP:HB2	2	0.2	0.09	0.2
(2,1967)	1:20:A:GLY:H	1:21:A:LYS:HB2	2	0.19	0.07	0.19
(2,714)	1:36:A:HIS:HA	1:91:A:LEU:HB2	2	0.15	0.01	0.15
(2,1973)	1:18:A:GLY:H	1:125:A:MET:HG2	2	0.15	0.05	0.15
(2,1770)	1:144:A:GLU:H	1:145:A:THR:HA	2	0.14	0.03	0.14
(2,1152)	1:47:A:VAL:H	1:47:A:VAL:HB	2	0.14	0.02	0.14
(2,2151)	1:15:A:GLY:H	1:16:A:GLY:H	2	0.14	0.03	0.14
(2,946)	1:138:A:ARG:HG3	1:138:A:ARG:HA	2	0.14	0.01	0.14
(2,2032)	1:93:A:ASP:H	1:12:A:PHE:HA	2	0.13	0.02	0.13
(2,2160)	1:102:A:GLY:H	1:105:A:PHE:H	2	0.13	0.03	0.13
(2,81)	1:57:A:LEU:HD22	1:43:A:LEU:HB3	2	0.12	0.02	0.12
(2,1798)	1:61:A:MET:H	1:57:A:LEU:HA	2	0.12	0.02	0.12
(2,2047)	1:118:A:VAL:H	1:175:A:ALA:HB2	2	0.12	0.02	0.12
(2,376)	1:176:A:GLU:HA	1:124:A:THR:HG21	2	0.12	0.01	0.12
(2,916)	1:34:A:TYR:HE2	1:32:A:TYR:HB2	2	0.12	0.0	0.12
(2,2153)	1:15:A:GLY:H	1:94:A:GLY:H	2	0.12	0.01	0.12
(2,165)	1:112:A:PRO:HA	1:10:A:ILE:HG22	2	0.12	0.02	0.12
(2,921)	1:72:A:VAL:HA	1:73:A:LEU:HG	2	0.12	0.02	0.12
(2,1096)	1:174:A:ASN:H	1:174:A:ASN:HB3	2	0.12	0.02	0.12

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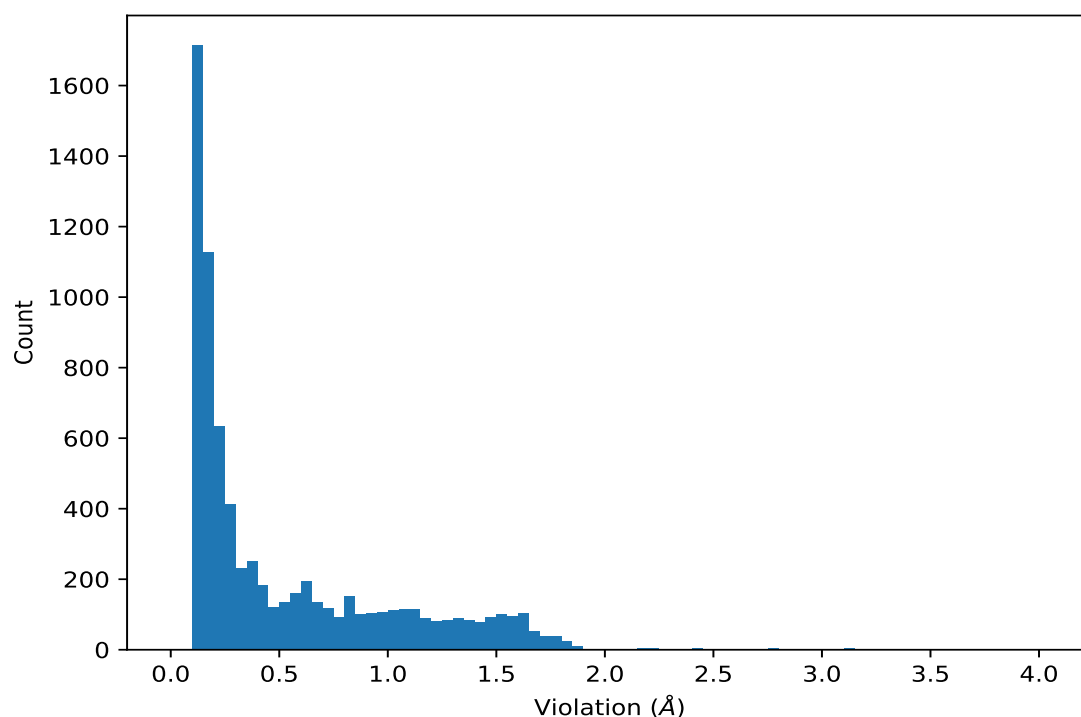
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,5)	1:151:A:GLU:HG3	1:148:A:LYS:HA	2	0.12	0.0	0.12
(2,912)	1:73:A:LEU:HG	1:105:A:PHE:H	2	0.12	0.0	0.12
(2,1933)	1:58:A:SER:H	1:57:A:LEU:HD22	2	0.12	0.0	0.12
(2,298)	1:41:A:ASP:HB2	1:41:A:ASP:HA	2	0.11	0.0	0.11
(2,1432)	1:37:A:LEU:H	1:37:A:LEU:HB3	2	0.11	0.0	0.11
(2,123)	1:47:A:VAL:HB	1:47:A:VAL:HG12	2	0.1	0.0	0.1

<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)
(2,1043)	1:81:A:VAL:HA	1:5:A:LEU:HD22	15	4.04
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	15	3.55
(2,1736)	1:81:A:VAL:H	1:5:A:LEU:HD22	15	3.22
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	4	3.13
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	5	3.13
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	17	3.12
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	20	3.12
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	11	3.11
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	19	3.06
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	16	2.98
(2,1472)	1:36:A:HIS:H	1:37:A:LEU:HD12	16	2.88
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	4	2.87
(2,213)	1:11:A:ILE:HG22	1:190:A:LEU:HD22	16	2.76
(1,18)	1:130:A:LEU:HD22	1:129:A:LEU:HB2	5	2.76
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	18	2.75
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	16	2.74
(2,795)	1:34:A:TYR:HB2	1:91:A:LEU:HD22	7	2.61
(1,18)	1:130:A:LEU:HD22	1:129:A:LEU:HB3	9	2.57
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	7	2.53
(2,1935)	1:83:A:LYS:H	1:84:A:VAL:HG22	11	2.49
(2,965)	1:37:A:LEU:HD12	1:90:A:PHE:HA	16	2.41
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	11	2.41
(2,2128)	1:35:A:THR:H	1:37:A:LEU:HD12	16	2.4
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	16	2.39
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	1	2.35
(2,1588)	1:13:A:VAL:H	1:91:A:LEU:HD12	3	2.34
(2,1588)	1:13:A:VAL:H	1:91:A:LEU:HD12	18	2.34
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	3	2.29
(2,709)	1:83:A:LYS:HA	1:84:A:VAL:HG22	11	2.28
(2,938)	1:84:A:VAL:HG12	1:5:A:LEU:HA	11	2.24
(2,895)	1:130:A:LEU:HD22	1:130:A:LEU:HA	5	2.23
(2,2247)	1:86:A:THR:H	1:84:A:VAL:HG22	11	2.22
(2,895)	1:130:A:LEU:HD22	1:130:A:LEU:HA	9	2.21
(2,795)	1:34:A:TYR:HB2	1:91:A:LEU:HD22	18	2.21
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	17	2.19
(2,484)	1:37:A:LEU:HD12	1:35:A:THR:HB	16	2.19
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	11	2.16
(2,1853)	1:111:A:GLN:H	1:5:A:LEU:HD12	15	2.14
(2,1588)	1:13:A:VAL:H	1:91:A:LEU:HD12	7	2.02
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	12	2.0
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	4	1.94
(2,481)	1:91:A:LEU:H	1:37:A:LEU:HD12	16	1.91
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	13	1.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	16	1.89
(1,15)	1:68:A:PRO:HB3	1:71:A:THR:HG21	13	1.89
(2,213)	1:11:A:ILE:HG22	1:190:A:LEU:HD22	17	1.88
(2,1596)	1:46:A:GLU:H	1:47:A:VAL:HG12	6	1.87
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	20	1.86
(1,32)	1:50:A:GLY:H	1:51:A:SER:HB2	14	1.86
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	10	1.85
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	7	1.85
(2,899)	1:76:A:LEU:HD12	1:75:A:MET:HB2	17	1.85
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	16	1.85
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	14	1.84
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	15	1.84
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	14	1.84
(1,32)	1:50:A:GLY:H	1:51:A:SER:HB2	5	1.84
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	1	1.83
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	5	1.82
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	8	1.82
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	18	1.82
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	18	1.82
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	10	1.81
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	7	1.81
(2,1596)	1:46:A:GLU:H	1:47:A:VAL:HG12	13	1.81
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	11	1.81
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	12	1.81
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	17	1.81
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	16	1.8
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	7	1.8
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	12	1.8
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	11	1.8
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	20	1.8
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	10	1.8
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	13	1.8
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	18	1.8
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	19	1.8
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	19	1.79
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	11	1.79
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	16	1.79
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	20	1.79
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	13	1.79
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	16	1.79
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	20	1.79
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	4	1.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	9	1.78
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	11	1.78
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	3	1.78
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	4	1.78
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	17	1.78
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	7	1.78
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	3	1.78
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	7	1.78
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	16	1.78
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	17	1.78
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	4	1.78
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	2	1.77
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	2	1.77
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	6	1.77
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	8	1.77
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	17	1.77
(2,1596)	1:46:A:GLU:H	1:47:A:VAL:HG12	12	1.77
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	4	1.77
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	18	1.77
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	20	1.76
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	14	1.76
(2,883)	1:162:A:ALA:HB1	1:166:A:LYS:HE3	5	1.76
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	14	1.76
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	2	1.76
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	6	1.76
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	20	1.76
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	3	1.75
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	7	1.75
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	18	1.75
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	18	1.75
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	7	1.75
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	13	1.74
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	10	1.74
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	15	1.74
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	20	1.74
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	11	1.74
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	15	1.74
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	1	1.73
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	11	1.73
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	17	1.73
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	17	1.73
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	4	1.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	16	1.73
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	3	1.73
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	8	1.73
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	10	1.73
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	14	1.73
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	1	1.73
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	19	1.73
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	16	1.72
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	17	1.72
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	10	1.72
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	20	1.72
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	16	1.72
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	2	1.72
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	7	1.72
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	18	1.72
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	14	1.72
(2,1402)	1:84:A:VAL:H	1:84:A:VAL:HG22	11	1.71
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	1	1.71
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	2	1.71
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	4	1.71
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	6	1.71
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	9	1.71
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	8	1.7
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	11	1.7
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	20	1.7
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	13	1.7
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	11	1.7
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	13	1.7
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	9	1.69
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	6	1.69
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	9	1.69
(2,884)	1:109:A:ILE:HG22	1:6:A:LYS:HE3	15	1.69
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	15	1.69
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	2	1.69
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	3	1.69
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	6	1.69
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	8	1.69
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	19	1.69
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	8	1.69
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	5	1.69
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	16	1.69
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	19	1.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	14	1.69
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	5	1.69
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	2	1.68
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	8	1.68
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	12	1.68
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	14	1.68
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	9	1.68
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	3	1.68
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	5	1.67
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	17	1.67
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	11	1.67
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	4	1.67
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	20	1.67
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	11	1.66
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	17	1.66
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	17	1.66
(2,883)	1:162:A:ALA:HB1	1:166:A:LYS:HE3	18	1.66
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	1	1.66
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	12	1.66
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	17	1.66
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	15	1.66
(2,409)	1:107:A:ARG:HD2	1:106:A:GLU:HG2	6	1.66
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	9	1.66
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	10	1.66
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	16	1.66
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	20	1.66
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	7	1.65
(2,2232)	1:169:A:ILE:H	1:167:A:ARG:HB2	17	1.65
(2,2154)	1:135:A:THR:H	1:131:A:LYS:HD3	17	1.65
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	10	1.65
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	2	1.65
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	5	1.65
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	13	1.65
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	10	1.65
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	2	1.65
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	5	1.65
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	12	1.65
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	14	1.65
(2,126)	1:84:A:VAL:HG22	1:81:A:VAL:HA	11	1.65
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	5	1.64
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	6	1.64
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	14	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	16	1.64
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	13	1.64
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	3	1.64
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	6	1.64
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	8	1.64
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	4	1.64
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	20	1.64
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	9	1.64
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	19	1.64
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	14	1.64
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	8	1.64
(2,463)	1:60:A:ILE:HG12	1:63:A:LYS:HB3	11	1.64
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	4	1.64
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	8	1.64
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	7	1.64
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	19	1.64
(1,22)	1:38:A:SER:HA	1:14:A:VAL:HG21	7	1.64
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	11	1.64
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	12	1.63
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	4	1.63
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	11	1.63
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	15	1.63
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	18	1.63
(2,2192)	1:85:A:ASN:HD21	1:84:A:VAL:HG22	11	1.63
(2,2106)	1:160:A:VAL:H	1:163:A:PHE:HB3	20	1.63
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	5	1.63
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	19	1.63
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	13	1.63
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	12	1.63
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	16	1.63
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	10	1.63
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	14	1.63
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	11	1.63
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	12	1.63
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	15	1.63
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	1	1.63
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	4	1.63
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	8	1.62
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	15	1.62
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	17	1.62
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	2	1.62
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	9	1.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	10	1.62
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	13	1.62
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	14	1.62
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	20	1.62
(2,2154)	1:135:A:THR:H	1:131:A:LYS:HD3	11	1.62
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	15	1.62
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	15	1.62
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	7	1.62
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	10	1.62
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	16	1.62
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	4	1.62
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	14	1.62
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	3	1.62
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	7	1.62
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	12	1.62
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	9	1.62
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD11	3	1.62
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	2	1.62
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	6	1.62
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	7	1.62
(2,319)	1:66:A:LEU:HD22	1:66:A:LEU:HA	13	1.62
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	16	1.62
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	1	1.61
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	7	1.61
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	16	1.61
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	17	1.61
(2,1705)	1:3:A:GLU:H	1:4:A:LYS:HD2	2	1.61
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	3	1.61
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	3	1.61
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	9	1.61
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	12	1.61
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	18	1.61
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	7	1.61
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	19	1.61
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	19	1.61
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	20	1.61
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	17	1.61
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	18	1.61
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	15	1.61
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	15	1.61
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	5	1.6
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	12	1.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	8	1.6
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	14	1.6
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	15	1.6
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	13	1.6
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	18	1.6
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	10	1.6
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	7	1.6
(2,883)	1:162:A:ALA:HB1	1:166:A:LYS:HE3	16	1.6
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	1	1.6
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	5	1.6
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	9	1.6
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	2	1.6
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	7	1.6
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	20	1.6
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	11	1.6
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	2	1.6
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	17	1.6
(2,2409)	1:90:A:PHE:H	1:88:A:LYS:HE3	3	1.59
(2,2277)	1:69:A:LEU:H	1:70:A:GLU:HB2	19	1.59
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	13	1.59
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	2	1.59
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	16	1.59
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	13	1.59
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	18	1.59
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	5	1.59
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	19	1.59
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	20	1.59
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	11	1.59
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	3	1.59
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	1	1.58
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	13	1.58
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	17	1.58
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	20	1.58
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	17	1.58
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	2	1.58
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	9	1.58
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	17	1.58
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	7	1.58
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	11	1.58
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	19	1.58
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	4	1.58
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	9	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	7	1.58
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	8	1.58
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	16	1.58
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	3	1.58
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	7	1.58
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	3	1.58
(2,326)	1:124:A:THR:HG21	1:177:A:GLY:HA3	15	1.58
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	5	1.58
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	17	1.58
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	8	1.58
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	5	1.57
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	5	1.57
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	11	1.57
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	11	1.57
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	20	1.57
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	1	1.57
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	2	1.57
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	6	1.57
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	19	1.57
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	3	1.57
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	13	1.57
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	10	1.57
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	1	1.57
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	8	1.57
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	15	1.57
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	4	1.57
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	3	1.57
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	10	1.57
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	15	1.57
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	20	1.57
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	6	1.56
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	4	1.56
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	12	1.56
(2,2038)	1:57:A:LEU:H	1:56:A:LYS:HD3	19	1.56
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	16	1.56
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	15	1.56
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	15	1.56
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	8	1.56
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	6	1.56
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	18	1.56
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	9	1.56
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	7	1.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	6	1.56
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	14	1.56
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	2	1.56
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	14	1.56
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	4	1.56
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	12	1.56
(2,2366)	1:2:A:GLU:H	1:3:A:GLU:HG2	20	1.55
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	16	1.55
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	20	1.55
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	16	1.55
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	13	1.55
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	9	1.55
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	5	1.55
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	11	1.55
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	4	1.55
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	16	1.55
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	1	1.55
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	6	1.55
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	1	1.55
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	13	1.55
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	18	1.55
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	14	1.55
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	2	1.55
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	15	1.55
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	19	1.55
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	5	1.55
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	7	1.55
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	10	1.55
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	20	1.54
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	11	1.54
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	7	1.54
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	10	1.54
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	4	1.54
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	16	1.54
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	1	1.54
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	9	1.54
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	5	1.54
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	5	1.54
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	9	1.54
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	12	1.54
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	17	1.54
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	19	1.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	13	1.54
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	2	1.54
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	9	1.54
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	1	1.54
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	3	1.54
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	4	1.54
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	16	1.54
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	20	1.54
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	6	1.54
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	19	1.54
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	6	1.54
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	13	1.54
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	16	1.54
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	11	1.54
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	4	1.53
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	1	1.53
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	16	1.53
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	8	1.53
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	13	1.53
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	19	1.53
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	20	1.53
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	20	1.53
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	16	1.53
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	8	1.53
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	13	1.53
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	19	1.53
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	1	1.53
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	6	1.53
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	10	1.53
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	19	1.53
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	8	1.53
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	11	1.53
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD11	18	1.53
(2,36)	1:62:A:GLU:HB2	1:59:A:GLU:HA	18	1.53
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	1	1.53
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	20	1.53
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	1	1.53
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	3	1.52
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	18	1.52
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	6	1.52
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	9	1.52
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	12	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	15	1.52
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	19	1.52
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	16	1.52
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	12	1.52
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	2	1.52
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	7	1.52
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	16	1.52
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	6	1.52
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	9	1.52
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	10	1.52
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	17	1.52
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	19	1.52
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	18	1.52
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	12	1.51
(2,2366)	1:2:A:GLU:H	1:3:A:GLU:HG2	4	1.51
(2,2366)	1:2:A:GLU:H	1:3:A:GLU:HG2	11	1.51
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	12	1.51
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	3	1.51
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	12	1.51
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	19	1.51
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	18	1.51
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	20	1.51
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	1	1.51
(2,935)	1:6:A:LYS:HG2	1:2:A:GLU:HB2	15	1.51
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	18	1.51
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	9	1.51
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	6	1.51
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	7	1.51
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	9	1.51
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	1	1.51
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	3	1.51
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	16	1.5
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	13	1.5
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	8	1.5
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	9	1.5
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	1	1.5
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	4	1.5
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	5	1.5
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	14	1.5
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	13	1.5
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	6	1.5
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	20	1.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	15	1.5
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	12	1.5
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	7	1.5
(1,13)	1:34:A:TYR:HE2	1:193:A:LEU:HG	5	1.5
(2,2366)	1:2:A:GLU:H	1:3:A:GLU:HG2	19	1.49
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	13	1.49
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	20	1.49
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	14	1.49
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	15	1.49
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	16	1.49
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	18	1.49
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	3	1.49
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	19	1.49
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	12	1.49
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	15	1.49
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	6	1.49
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	16	1.49
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	5	1.49
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	13	1.49
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	16	1.49
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	18	1.49
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	13	1.49
(2,409)	1:107:A:ARG:HD2	1:106:A:GLU:HG2	9	1.49
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	6	1.49
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	11	1.49
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	3	1.49
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	16	1.49
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	13	1.48
(2,2366)	1:2:A:GLU:H	1:3:A:GLU:HG2	6	1.48
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	15	1.48
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	8	1.48
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	10	1.48
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	11	1.48
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	3	1.48
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	6	1.48
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	17	1.48
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	13	1.48
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	18	1.48
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	14	1.48
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	16	1.48
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	14	1.48
(2,795)	1:34:A:TYR:HB2	1:91:A:LEU:HD22	3	1.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	7	1.48
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	12	1.48
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	3	1.48
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	4	1.48
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	4	1.47
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	9	1.47
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	14	1.47
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	18	1.47
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	2	1.47
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	8	1.47
(2,784)	1:172:A:LYS:HE3	1:158:A:GLU:HG3	17	1.47
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	20	1.47
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	5	1.47
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	14	1.47
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	8	1.47
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	7	1.47
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	20	1.47
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	18	1.46
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	19	1.46
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	5	1.46
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	7	1.46
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	10	1.46
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	18	1.46
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	7	1.46
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	17	1.46
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	7	1.46
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	14	1.46
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	17	1.46
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	10	1.46
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	12	1.46
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	20	1.46
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	10	1.46
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	18	1.46
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	2	1.46
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	19	1.46
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	16	1.46
(2,779)	1:9:A:LYS:HE2	1:11:A:ILE:HD12	7	1.46
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	13	1.46
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	14	1.46
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	14	1.46
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	15	1.45
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	16	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	7	1.45
(2,2214)	1:189:A:HIS:H	1:190:A:LEU:HG	16	1.45
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	2	1.45
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	5	1.45
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	9	1.45
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	9	1.45
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	11	1.45
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	14	1.45
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	16	1.45
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	20	1.45
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	15	1.45
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	1	1.45
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	6	1.44
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	18	1.44
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	7	1.44
(2,2366)	1:2:A:GLU:H	1:3:A:GLU:HG2	14	1.44
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	2	1.44
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	11	1.44
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	1	1.44
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	2	1.44
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	4	1.44
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	11	1.44
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	18	1.44
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	16	1.44
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	13	1.44
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	19	1.44
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	9	1.44
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	16	1.44
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	17	1.44
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	8	1.44
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	15	1.43
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	3	1.43
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	9	1.43
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	1	1.43
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	20	1.43
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	20	1.43
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	7	1.43
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	11	1.43
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	19	1.43
(2,2106)	1:160:A:VAL:H	1:163:A:PHE:HB3	4	1.43
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	11	1.43
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	20	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	11	1.43
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	6	1.43
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	2	1.43
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	7	1.43
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	20	1.43
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	1	1.43
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	8	1.43
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	19	1.43
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	5	1.43
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	3	1.42
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	7	1.42
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	19	1.42
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	16	1.42
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	19	1.42
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	15	1.42
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	7	1.42
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	4	1.42
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	10	1.42
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	3	1.42
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	15	1.42
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	5	1.42
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	19	1.42
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	17	1.42
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	2	1.42
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	18	1.42
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	16	1.42
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	9	1.41
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	16	1.41
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	20	1.41
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	12	1.41
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	14	1.41
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	3	1.41
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	10	1.41
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	13	1.41
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	19	1.41
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	1	1.41
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	3	1.41
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	20	1.41
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	14	1.41
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	9	1.4
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	20	1.4
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	5	1.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	8	1.4
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	7	1.4
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	3	1.4
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	17	1.4
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	3	1.4
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	2	1.4
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	9	1.4
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	12	1.39
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	13	1.39
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	1	1.39
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	9	1.39
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	7	1.39
(2,1005)	1:57:A:LEU:HB2	1:54:A:GLY:HA3	12	1.39
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	20	1.39
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	11	1.39
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	16	1.39
(2,2398)	1:27:A:LYS:H	1:28:A:ILE:HG12	11	1.38
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	8	1.38
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	15	1.38
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	18	1.38
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	5	1.38
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	1	1.38
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	3	1.38
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	17	1.38
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	18	1.38
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	4	1.38
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	17	1.38
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	5	1.38
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	14	1.38
(2,319)	1:66:A:LEU:HD22	1:66:A:LEU:HA	19	1.38
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	4	1.38
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	15	1.38
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	12	1.38
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	11	1.37
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	6	1.37
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	14	1.37
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	14	1.37
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	16	1.37
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	2	1.37
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	7	1.37
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	11	1.37
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	12	1.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	11	1.37
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	4	1.37
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	11	1.37
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	15	1.37
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	5	1.37
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	15	1.37
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	20	1.37
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	19	1.37
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	10	1.37
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	16	1.37
(2,319)	1:66:A:LEU:HD22	1:66:A:LEU:HA	7	1.37
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	2	1.37
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	4	1.37
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	19	1.37
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	19	1.36
(2,2352)	1:169:A:ILE:H	1:167:A:ARG:HG2	3	1.36
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	9	1.36
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	13	1.36
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	5	1.36
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	17	1.36
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	7	1.36
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	3	1.36
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	4	1.36
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	13	1.36
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	2	1.36
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	20	1.36
(2,2418)	1:31:A:LYS:H	1:30:A:GLN:HB2	8	1.35
(2,2418)	1:31:A:LYS:H	1:30:A:GLN:HB2	17	1.35
(2,2418)	1:31:A:LYS:H	1:30:A:GLN:HB2	20	1.35
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	11	1.35
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	19	1.35
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	13	1.35
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	3	1.35
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	16	1.35
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	20	1.35
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	10	1.35
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	19	1.35
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	12	1.35
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	11	1.35
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	18	1.35
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	2	1.35
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	5	1.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	8	1.35
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	2	1.35
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	8	1.35
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	15	1.35
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	14	1.35
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	15	1.35
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG22	10	1.35
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	17	1.34
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	5	1.34
(2,2206)	1:26:A:GLU:H	1:28:A:ILE:HG12	6	1.34
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	5	1.34
(2,2106)	1:160:A:VAL:H	1:163:A:PHE:HB3	16	1.34
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	6	1.34
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	8	1.34
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	17	1.34
(2,1627)	1:130:A:LEU:H	1:130:A:LEU:HD22	9	1.34
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	4	1.34
(2,898)	1:34:A:TYR:HB3	1:32:A:TYR:H	17	1.34
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	11	1.34
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	10	1.34
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	7	1.34
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	10	1.34
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	19	1.34
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	1	1.34
(2,458)	1:21:A:LYS:HB2	1:118:A:VAL:HG22	5	1.34
(2,319)	1:66:A:LEU:HD23	1:66:A:LEU:HA	17	1.34
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	20	1.34
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	15	1.34
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	5	1.33
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	11	1.33
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	5	1.33
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	2	1.33
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	17	1.33
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	12	1.33
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	14	1.33
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	7	1.33
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	19	1.33
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	6	1.33
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	15	1.33
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	8	1.33
(2,1251)	1:172:A:LYS:H	1:117:A:TYR:HB2	18	1.33
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	14	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	18	1.33
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	10	1.33
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	19	1.33
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	3	1.33
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	18	1.33
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	15	1.33
(1,21)	1:90:A:PHE:HA	1:28:A:ILE:HG23	8	1.33
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	14	1.32
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	4	1.32
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	16	1.32
(2,2106)	1:160:A:VAL:H	1:163:A:PHE:HB3	14	1.32
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	12	1.32
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	18	1.32
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	12	1.32
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	19	1.32
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	3	1.32
(2,1458)	1:145:A:THR:H	1:146:A:ILE:HG12	6	1.32
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	19	1.32
(2,862)	1:76:A:LEU:HD22	1:37:A:LEU:HB2	17	1.32
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	3	1.32
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	1	1.32
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	16	1.32
(2,267)	1:147:A:LYS:HA	1:147:A:LYS:HD2	5	1.32
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	17	1.32
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	6	1.32
(1,15)	1:125:A:MET:HB3	1:126:A:THR:HG22	16	1.32
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	5	1.31
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	9	1.31
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	10	1.31
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	9	1.31
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	15	1.31
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	2	1.31
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	10	1.31
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	13	1.31
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	17	1.31
(2,941)	1:169:A:ILE:HG13	1:167:A:ARG:HB2	17	1.31
(2,837)	1:155:A:LYS:HD2	1:154:A:TYR:HD1	8	1.31
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	8	1.31
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	10	1.31
(2,431)	1:164:A:TYR:HB3	1:160:A:VAL:HG12	5	1.31
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	4	1.31
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	4	1.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	8	1.3
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	4	1.3
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	14	1.3
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	2	1.3
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	18	1.3
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	14	1.3
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	12	1.3
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	10	1.3
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	3	1.3
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	9	1.3
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	13	1.3
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	10	1.3
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	18	1.3
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	10	1.29
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	8	1.29
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	12	1.29
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	1	1.29
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	9	1.29
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	15	1.29
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	15	1.29
(2,824)	1:125:A:MET:HB2	1:18:A:GLY:HA3	13	1.29
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	19	1.29
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	9	1.29
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	13	1.29
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	18	1.29
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	18	1.29
(1,13)	1:34:A:TYR:HE2	1:193:A:LEU:HG	20	1.29
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	1	1.28
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	2	1.28
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	3	1.28
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	1	1.28
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	3	1.28
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	20	1.28
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	9	1.28
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	15	1.28
(2,769)	1:132:A:ARG:HD3	1:129:A:LEU:HA	5	1.28
(2,769)	1:132:A:ARG:HD3	1:129:A:LEU:HA	16	1.28
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	14	1.28
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	7	1.28
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	12	1.28
(2,314)	1:166:A:LYS:HB2	1:166:A:LYS:HD2	5	1.28
(2,314)	1:166:A:LYS:HB2	1:166:A:LYS:HD2	16	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,314)	1:166:A:LYS:HB2	1:166:A:LYS:HD2	18	1.28
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	10	1.27
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	8	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	4	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	5	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	6	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	7	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	11	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	13	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	17	1.27
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	18	1.27
(2,1897)	1:25:A:CYS:H	1:28:A:ILE:HG12	13	1.27
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	18	1.27
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	7	1.27
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	14	1.27
(2,778)	1:167:A:ARG:HD2	1:169:A:ILE:HG22	18	1.27
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	10	1.27
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	15	1.27
(1,15)	1:125:A:MET:HB3	1:120:A:ALA:HB1	2	1.27
(1,13)	1:34:A:TYR:HE2	1:193:A:LEU:HG	12	1.27
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	12	1.26
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	10	1.26
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	6	1.26
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	2	1.26
(2,2196)	1:124:A:THR:H	1:123:A:GLU:HB2	15	1.26
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	13	1.26
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	20	1.26
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	18	1.26
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	20	1.26
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	17	1.26
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	5	1.26
(2,1627)	1:130:A:LEU:H	1:130:A:LEU:HD22	5	1.26
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	2	1.26
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	3	1.26
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	4	1.26
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	4	1.26
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	8	1.25
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	17	1.25
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	7	1.25
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	12	1.25
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	15	1.25
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	8	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	13	1.25
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	1	1.25
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	5	1.25
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	1	1.25
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	9	1.25
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	1	1.25
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	9	1.25
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	3	1.25
(2,752)	1:40:A:GLY:HA3	1:43:A:LEU:HD22	5	1.25
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	14	1.25
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	13	1.25
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	6	1.25
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	9	1.25
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	13	1.25
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	5	1.24
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	10	1.24
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	15	1.24
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	12	1.24
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	6	1.24
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	7	1.24
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	16	1.24
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	14	1.24
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	13	1.24
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	4	1.24
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	7	1.24
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	1	1.24
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	17	1.24
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	7	1.24
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	5	1.23
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	7	1.23
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	18	1.23
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	12	1.23
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	14	1.23
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	18	1.23
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	15	1.23
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	9	1.23
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	13	1.23
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	7	1.23
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	17	1.23
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	5	1.23
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	7	1.23
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	2	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	17	1.22
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	3	1.22
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	20	1.22
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	18	1.22
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	13	1.22
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	9	1.22
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	3	1.22
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	20	1.22
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	14	1.22
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	2	1.22
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	7	1.22
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	19	1.22
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	20	1.22
(2,2413)	1:29:A:VAL:H	1:34:A:TYR:HB3	17	1.21
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	4	1.21
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	4	1.21
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	5	1.21
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	6	1.21
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	14	1.21
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	12	1.21
(2,931)	1:7:A:LYS:HA	1:7:A:LYS:HD3	8	1.21
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	6	1.21
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	5	1.21
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	1	1.21
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	10	1.21
(2,319)	1:66:A:LEU:HD21	1:66:A:LEU:HA	12	1.21
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	19	1.21
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	3	1.21
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	5	1.21
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	9	1.21
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	10	1.21
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	14	1.21
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	11	1.2
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	8	1.2
(2,2307)	1:144:A:GLU:H	1:146:A:ILE:HG12	6	1.2
(2,2306)	1:163:A:PHE:H	1:166:A:LYS:HD2	15	1.2
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	18	1.2
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	4	1.2
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	11	1.2
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	17	1.2
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	20	1.2
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	11	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	5	1.2
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	17	1.2
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	5	1.2
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	8	1.2
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	11	1.2
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	17	1.2
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	11	1.2
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	1	1.2
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	13	1.2
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	18	1.2
(2,2024)	1:95:A:TYR:H	1:14:A:VAL:HG22	5	1.19
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	14	1.19
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	10	1.19
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	20	1.19
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	8	1.19
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	12	1.19
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	19	1.19
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	14	1.19
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	2	1.19
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	11	1.19
(2,320)	1:5:A:LEU:HD22	1:5:A:LEU:HA	15	1.19
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	5	1.19
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	12	1.19
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	15	1.19
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	18	1.19
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	18	1.19
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	6	1.19
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	17	1.19
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	1	1.18
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	6	1.18
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	19	1.18
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	8	1.18
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	3	1.18
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	6	1.18
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	8	1.18
(2,1720)	1:132:A:ARG:H	1:131:A:LYS:HD3	11	1.18
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	15	1.18
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	9	1.18
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	3	1.18
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	4	1.18
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	4	1.18
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	5	1.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	6	1.18
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	18	1.18
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	2	1.18
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	16	1.17
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	16	1.17
(2,1720)	1:132:A:ARG:H	1:131:A:LYS:HD3	17	1.17
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	17	1.17
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	5	1.17
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	8	1.17
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	4	1.17
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	8	1.17
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	12	1.17
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	11	1.17
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	4	1.17
(2,319)	1:66:A:LEU:HD21	1:66:A:LEU:HA	4	1.17
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	3	1.17
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	9	1.17
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	12	1.17
(1,15)	1:125:A:MET:HB3	1:126:A:THR:HG22	5	1.17
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	14	1.16
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	15	1.16
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	16	1.16
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	1	1.16
(2,1708)	1:143:A:GLU:H	1:130:A:LEU:HD12	9	1.16
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	13	1.16
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	3	1.16
(2,1276)	1:7:A:LYS:H	1:7:A:LYS:HE2	7	1.16
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	15	1.16
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	16	1.16
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	10	1.16
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	15	1.16
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	6	1.16
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	20	1.16
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	18	1.16
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	8	1.16
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	9	1.16
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	13	1.16
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	10	1.16
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	5	1.16
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	10	1.16
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	13	1.16
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	16	1.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	19	1.16
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	4	1.16
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	15	1.16
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	9	1.15
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	11	1.15
(2,1159)	1:47:A:VAL:H	1:47:A:VAL:HG12	12	1.15
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	10	1.15
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	16	1.15
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	9	1.15
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	4	1.15
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	12	1.15
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	18	1.15
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	12	1.15
(2,217)	1:138:A:ARG:HD2	1:133:A:GLY:HA3	9	1.15
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	15	1.15
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	4	1.14
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	17	1.14
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	9	1.14
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	16	1.14
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	6	1.14
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	16	1.14
(2,2024)	1:95:A:TYR:H	1:14:A:VAL:HG22	17	1.14
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	4	1.14
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	2	1.14
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	17	1.14
(2,1365)	1:111:A:GLN:H	1:111:A:GLN:HG2	4	1.14
(2,1276)	1:7:A:LYS:H	1:7:A:LYS:HE2	4	1.14
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	9	1.14
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	14	1.14
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	12	1.14
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	16	1.14
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	14	1.14
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	12	1.14
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	7	1.14
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	1	1.14
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	20	1.14
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	1	1.14
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	2	1.14
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	14	1.14
(1,17)	1:114:A:LEU:HD11	1:114:A:LEU:H	5	1.14
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	2	1.13
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	17	1.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	19	1.13
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	7	1.13
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	16	1.13
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	5	1.13
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	7	1.13
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	5	1.13
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	13	1.13
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	19	1.13
(2,1276)	1:7:A:LYS:H	1:7:A:LYS:HE2	18	1.13
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	6	1.13
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	17	1.13
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	6	1.13
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	6	1.13
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	18	1.13
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	1	1.13
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	11	1.13
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	1	1.13
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	14	1.13
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	11	1.13
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	5	1.12
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	20	1.12
(2,2306)	1:163:A:PHE:H	1:166:A:LYS:HD2	19	1.12
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	9	1.12
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	11	1.12
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	14	1.12
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	6	1.12
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	15	1.12
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	12	1.12
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	15	1.12
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	16	1.12
(2,1276)	1:7:A:LYS:H	1:7:A:LYS:HE2	6	1.12
(2,1159)	1:47:A:VAL:H	1:47:A:VAL:HG12	13	1.12
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	8	1.12
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	5	1.12
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	5	1.12
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	20	1.12
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	4	1.12
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	3	1.12
(2,311)	1:143:A:GLU:HG3	1:130:A:LEU:HD12	20	1.12
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	13	1.12
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	13	1.11
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	5	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2102)	1:27:A:LYS:H	1:26:A:GLU:HG2	10	1.11
(2,2102)	1:27:A:LYS:H	1:26:A:GLU:HG2	20	1.11
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	15	1.11
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	6	1.11
(2,1159)	1:47:A:VAL:H	1:47:A:VAL:HG12	6	1.11
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	18	1.11
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	1	1.11
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	8	1.11
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	7	1.11
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	4	1.11
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	13	1.11
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	17	1.11
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	15	1.11
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	15	1.11
(2,721)	1:156:A:ALA:HA	1:155:A:LYS:HE2	12	1.11
(2,529)	1:162:A:ALA:HB2	1:161:A:ILE:HG13	4	1.11
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	17	1.11
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	13	1.11
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	8	1.11
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	9	1.1
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	19	1.1
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	19	1.1
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	7	1.1
(2,2102)	1:27:A:LYS:H	1:26:A:GLU:HG2	13	1.1
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	16	1.1
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	5	1.1
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	19	1.1
(2,1708)	1:143:A:GLU:H	1:130:A:LEU:HD12	5	1.1
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	11	1.1
(2,1366)	1:111:A:GLN:H	1:111:A:GLN:HB2	4	1.1
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	1	1.1
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	10	1.1
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	15	1.1
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	17	1.1
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	18	1.1
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	19	1.1
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	5	1.1
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	14	1.1
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	16	1.1
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	12	1.1
(2,796)	1:78:A:ASP:HB2	1:75:A:MET:HG2	20	1.1
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	11	1.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	5	1.1
(2,314)	1:166:A:LYS:HB2	1:166:A:LYS:HD2	15	1.1
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	2	1.1
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	6	1.09
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	13	1.09
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	14	1.09
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	15	1.09
(2,2102)	1:27:A:LYS:H	1:26:A:GLU:HG2	6	1.09
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	9	1.09
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	8	1.09
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	11	1.09
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	16	1.09
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	17	1.09
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	10	1.09
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	18	1.09
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	5	1.09
(2,55)	1:116:A:LEU:HD12	1:116:A:LEU:HB3	16	1.09
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	7	1.09
(1,17)	1:114:A:LEU:HD11	1:114:A:LEU:H	11	1.09
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	1	1.08
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	2	1.08
(2,2306)	1:163:A:PHE:H	1:166:A:LYS:HD2	6	1.08
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	17	1.08
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	9	1.08
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	18	1.08
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	14	1.08
(2,1293)	1:161:A:ILE:H	1:161:A:ILE:HG13	2	1.08
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	6	1.08
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	16	1.08
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	14	1.08
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	7	1.08
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	13	1.08
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	16	1.08
(2,529)	1:162:A:ALA:HB2	1:161:A:ILE:HG13	3	1.08
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	18	1.08
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	17	1.08
(2,395)	1:122:A:PRO:HD3	1:121:A:GLY:HA3	19	1.08
(2,314)	1:166:A:LYS:HB2	1:166:A:LYS:HD2	6	1.08
(1,17)	1:114:A:LEU:HD11	1:114:A:LEU:H	15	1.08
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	4	1.07
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	8	1.07
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	10	1.07

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	19	1.07
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	10	1.07
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	6	1.07
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	8	1.07
(2,2024)	1:95:A:TYR:H	1:14:A:VAL:HG22	20	1.07
(2,2020)	1:110:A:GLY:H	1:111:A:GLN:HG2	4	1.07
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	1	1.07
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	8	1.07
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	9	1.07
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	12	1.07
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	20	1.07
(2,1276)	1:7:A:LYS:H	1:7:A:LYS:HE2	2	1.07
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	7	1.07
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	15	1.07
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	20	1.07
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	14	1.07
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	19	1.07
(2,529)	1:162:A:ALA:HB2	1:161:A:ILE:HG13	11	1.07
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	18	1.07
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	20	1.07
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	5	1.07
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	13	1.07
(2,383)	1:85:A:ASN:HA	1:84:A:VAL:HG22	11	1.07
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	13	1.07
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	20	1.07
(1,17)	1:114:A:LEU:HD13	1:193:A:LEU:H	16	1.07
(2,2335)	1:90:A:PHE:H	1:34:A:TYR:HB2	9	1.06
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	10	1.06
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	3	1.06
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	12	1.06
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	15	1.06
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	14	1.06
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	5	1.06
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	20	1.06
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	8	1.06
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	16	1.06
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	19	1.06
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	14	1.06
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	3	1.06
(2,1293)	1:161:A:ILE:H	1:161:A:ILE:HG13	4	1.06
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	3	1.06
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	11	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	16	1.06
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	19	1.06
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	8	1.06
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	17	1.06
(2,314)	1:166:A:LYS:HB2	1:166:A:LYS:HD2	19	1.06
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	4	1.06
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	9	1.06
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	14	1.06
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	12	1.05
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	18	1.05
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	20	1.05
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	4	1.05
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	18	1.05
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	20	1.05
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	3	1.05
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	6	1.05
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	10	1.05
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	12	1.05
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	12	1.05
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	11	1.05
(2,1609)	1:84:A:VAL:H	1:85:A:ASN:HB3	7	1.05
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	7	1.05
(2,1293)	1:161:A:ILE:H	1:161:A:ILE:HG13	3	1.05
(2,1293)	1:161:A:ILE:H	1:161:A:ILE:HG13	15	1.05
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	3	1.05
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	2	1.05
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	7	1.05
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	16	1.05
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	3	1.05
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	11	1.05
(2,215)	1:44:A:ARG:HD3	1:41:A:ASP:HA	11	1.05
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	20	1.05
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	6	1.05
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	11	1.04
(2,2306)	1:163:A:PHE:H	1:166:A:LYS:HD2	16	1.04
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	4	1.04
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	6	1.04
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	2	1.04
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	5	1.04
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	6	1.04
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	16	1.04
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	2	1.04

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	11	1.04
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	17	1.04
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	9	1.04
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	12	1.04
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	13	1.04
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	8	1.04
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	10	1.04
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	12	1.04
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	20	1.04
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	13	1.04
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	6	1.04
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	20	1.04
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	5	1.04
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	7	1.03
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	16	1.03
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	20	1.03
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	15	1.03
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	7	1.03
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	2	1.03
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	3	1.03
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	8	1.03
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	10	1.03
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	3	1.03
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	8	1.03
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	19	1.03
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	3	1.03
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	14	1.03
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	7	1.03
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	2	1.03
(2,1424)	1:44:A:ARG:H	1:44:A:ARG:HD3	11	1.03
(2,1276)	1:7:A:LYS:H	1:7:A:LYS:HE2	19	1.03
(2,785)	1:140:A:ASP:HB3	1:149:A:ARG:HD3	20	1.03
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	17	1.03
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	20	1.03
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	4	1.03
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	14	1.03
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	5	1.03
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	10	1.03
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	15	1.03
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	11	1.03
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	16	1.03
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	16	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	8	1.03
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	10	1.02
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	13	1.02
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	14	1.02
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	3	1.02
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	3	1.02
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	1	1.02
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	13	1.02
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	1	1.02
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	15	1.02
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	18	1.02
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	10	1.02
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	15	1.02
(2,1293)	1:161:A:ILE:H	1:161:A:ILE:HG13	11	1.02
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	2	1.02
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	13	1.02
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	12	1.02
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	2	1.02
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	17	1.02
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	15	1.01
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	17	1.01
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	6	1.01
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	7	1.01
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	8	1.01
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	17	1.01
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	13	1.01
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	7	1.01
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	7	1.01
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	9	1.01
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	20	1.01
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	1	1.01
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	14	1.01
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	7	1.01
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	11	1.01
(2,1699)	1:53:A:ARG:H	1:53:A:ARG:HD2	4	1.01
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	1	1.01
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	17	1.01
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	18	1.01
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	1	1.01
(2,931)	1:7:A:LYS:HA	1:7:A:LYS:HD3	1	1.01
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	14	1.01
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	10	1.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	9	1.01
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	9	1.01
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	1	1.01
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	4	1.0
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	12	1.0
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	13	1.0
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	18	1.0
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	1	1.0
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	9	1.0
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	15	1.0
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	18	1.0
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	5	1.0
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	6	1.0
(2,754)	1:54:A:GLY:HA3	1:57:A:LEU:HD22	12	1.0
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	3	1.0
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	3	1.0
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	14	1.0
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	15	1.0
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	14	1.0
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	2	1.0
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	12	0.99
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	14	0.99
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	11	0.99
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	8	0.99
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	17	0.99
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	1	0.99
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	17	0.99
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	11	0.99
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	17	0.99
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	11	0.99
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	3	0.99
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	9	0.99
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	15	0.99
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	6	0.99
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	19	0.99
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	11	0.99
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	2	0.99
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	18	0.99
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	7	0.99
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	17	0.99
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	8	0.99
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	10	0.99

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	12	0.99
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	13	0.99
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	15	0.99
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	18	0.99
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	13	0.99
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	4	0.99
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	7	0.98
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	6	0.98
(2,2306)	1:163:A:PHE:H	1:166:A:LYS:HD2	5	0.98
(2,2306)	1:163:A:PHE:H	1:166:A:LYS:HD2	18	0.98
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	14	0.98
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	19	0.98
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	10	0.98
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	2	0.98
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	9	0.98
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	14	0.98
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	7	0.98
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	19	0.98
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	8	0.98
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	9	0.98
(2,963)	1:61:A:MET:HG2	1:57:A:LEU:HB2	18	0.98
(2,882)	1:146:A:ILE:HG22	1:149:A:ARG:HD2	3	0.98
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	13	0.98
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	4	0.98
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	13	0.98
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	11	0.98
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	4	0.98
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	1	0.98
(2,529)	1:162:A:ALA:HB2	1:161:A:ILE:HG13	15	0.98
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	10	0.98
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	4	0.98
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	17	0.98
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	4	0.98
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	17	0.98
(2,2391)	1:154:A:TYR:H	1:153:A:TYR:HB2	3	0.97
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	5	0.97
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	16	0.97
(2,2283)	1:119:A:ASP:H	1:172:A:LYS:HB2	11	0.97
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	1	0.97
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	3	0.97
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	15	0.97
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	16	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	10	0.97
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	16	0.97
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	16	0.97
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	16	0.97
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	8	0.97
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	2	0.97
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	10	0.97
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	9	0.97
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	4	0.97
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	7	0.97
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	2	0.97
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	2	0.97
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	12	0.97
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	8	0.97
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	17	0.96
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	12	0.96
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	18	0.96
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	6	0.96
(2,1131)	1:65:A:GLN:H	1:65:A:GLN:HB3	20	0.96
(2,923)	1:71:A:THR:HB	1:74:A:ASP:HB3	11	0.96
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	1	0.96
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	9	0.96
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	19	0.96
(2,776)	1:108:A:ARG:HD2	1:77:A:ARG:HA	7	0.96
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	5	0.96
(2,477)	1:161:A:ILE:HG13	1:160:A:VAL:HB	2	0.96
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	12	0.96
(2,37)	1:166:A:LYS:HD2	1:163:A:PHE:HA	15	0.96
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	10	0.96
(2,2336)	1:34:A:TYR:H	1:88:A:LYS:HE3	11	0.95
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	2	0.95
(2,2120)	1:142:A:ASN:H	1:142:A:ASN:HD22	8	0.95
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	5	0.95
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	1	0.95
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	3	0.95
(2,608)	1:34:A:TYR:HE2	1:194:A:LYS:HD2	15	0.95
(2,477)	1:161:A:ILE:HG13	1:160:A:VAL:HB	4	0.95
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	11	0.95
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	11	0.95
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	16	0.95
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	7	0.95
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	20	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	2	0.95
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	2	0.94
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	12	0.94
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	11	0.94
(2,2201)	1:170:A:VAL:H	1:168:A:GLY:HA3	17	0.94
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	13	0.94
(2,1991)	1:133:A:GLY:H	1:134:A:GLU:HB2	18	0.94
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	7	0.94
(2,1841)	1:111:A:GLN:H	1:6:A:LYS:HE3	3	0.94
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	2	0.94
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	14	0.94
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	2	0.94
(2,785)	1:140:A:ASP:HB3	1:149:A:ARG:HD3	13	0.94
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	17	0.94
(2,529)	1:162:A:ALA:HB2	1:161:A:ILE:HG13	2	0.94
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	12	0.94
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	10	0.94
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	15	0.94
(2,223)	1:132:A:ARG:HA	1:132:A:ARG:HD2	16	0.94
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	1	0.94
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	4	0.94
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	2	0.94
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	17	0.94
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	19	0.94
(2,37)	1:166:A:LYS:HD2	1:163:A:PHE:HA	19	0.94
(2,2233)	1:148:A:LYS:H	1:147:A:LYS:HB2	10	0.93
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	1	0.93
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	10	0.93
(2,1718)	1:60:A:ILE:H	1:61:A:MET:HG2	17	0.93
(2,1699)	1:53:A:ARG:H	1:53:A:ARG:HD2	2	0.93
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	9	0.93
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	17	0.93
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	7	0.93
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	16	0.93
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	2	0.93
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	1	0.93
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	1	0.93
(2,223)	1:132:A:ARG:HA	1:132:A:ARG:HD2	5	0.93
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	16	0.93
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	12	0.93
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	18	0.93
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	6	0.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1718)	1:60:A:ILE:H	1:61:A:MET:HG2	18	0.92
(2,1699)	1:53:A:ARG:H	1:53:A:ARG:HD2	7	0.92
(2,1699)	1:53:A:ARG:H	1:53:A:ARG:HD2	19	0.92
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	11	0.92
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	18	0.92
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	6	0.92
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	17	0.92
(2,477)	1:161:A:ILE:HG13	1:160:A:VAL:HB	3	0.92
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	19	0.92
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	5	0.92
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	6	0.92
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	1	0.92
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	14	0.92
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	19	0.92
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	3	0.92
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	19	0.92
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	8	0.91
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	13	0.91
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	5	0.91
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	14	0.91
(2,1699)	1:53:A:ARG:H	1:53:A:ARG:HD2	16	0.91
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	4	0.91
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	10	0.91
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	12	0.91
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	13	0.91
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	3	0.91
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	10	0.91
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	19	0.91
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	16	0.91
(2,477)	1:161:A:ILE:HG13	1:160:A:VAL:HB	15	0.91
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	2	0.91
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	20	0.91
(2,311)	1:143:A:GLU:HG3	1:130:A:LEU:HD12	9	0.91
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	20	0.91
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	2	0.91
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	12	0.91
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	19	0.91
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	5	0.91
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	10	0.91
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	13	0.91
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	10	0.91
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	11	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	12	0.91
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	9	0.9
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	13	0.9
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	16	0.9
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	19	0.9
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	6	0.9
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	16	0.9
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	19	0.9
(2,441)	1:59:A:GLU:HG3	1:60:A:ILE:HG12	19	0.9
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	18	0.9
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	2	0.9
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	3	0.9
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	16	0.9
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	5	0.9
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	3	0.9
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	9	0.9
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	18	0.9
(2,28)	1:127:A:GLN:HG2	1:127:A:GLN:HA	19	0.9
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	15	0.9
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	7	0.9
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	5	0.89
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	13	0.89
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	20	0.89
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	3	0.89
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	7	0.89
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	8	0.89
(2,477)	1:161:A:ILE:HG13	1:160:A:VAL:HB	11	0.89
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	18	0.89
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	9	0.89
(1,17)	1:114:A:LEU:HD11	1:114:A:LEU:H	20	0.89
(1,13)	1:34:A:TYR:HE2	1:193:A:LEU:HG	11	0.89
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	5	0.89
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	3	0.88
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	18	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	1	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	6	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	7	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	8	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	9	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	10	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	14	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	16	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	19	0.88
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	17	0.88
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	1	0.88
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	7	0.88
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	18	0.88
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	5	0.88
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	17	0.88
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	5	0.88
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	12	0.88
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	5	0.88
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	3	0.88
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	5	0.88
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	10	0.88
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	8	0.88
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	2	0.87
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	3	0.87
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	4	0.87
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	11	0.87
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	12	0.87
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	15	0.87
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	17	0.87
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	18	0.87
(2,2202)	1:23:A:THR:H	1:25:A:CYS:HB2	19	0.87
(2,1699)	1:53:A:ARG:H	1:53:A:ARG:HD2	17	0.87
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	6	0.87
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	7	0.87
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	2	0.87
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	14	0.87
(2,789)	1:74:A:ASP:HB3	1:71:A:THR:HG21	11	0.87
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	15	0.87
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	11	0.87
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	20	0.87
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	15	0.87
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	3	0.87
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	10	0.87
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	6	0.87
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	4	0.87
(2,311)	1:143:A:GLU:HG3	1:130:A:LEU:HD12	5	0.87
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	7	0.87
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	11	0.87
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	12	0.87
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	18	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	1	0.87
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	4	0.87
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	8	0.87
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	13	0.87
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	20	0.87
(2,2088)	1:141:A:ASP:H	1:142:A:ASN:HD22	8	0.86
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	13	0.86
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	18	0.86
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	2	0.86
(2,1075)	1:3:A:GLU:H	1:3:A:GLU:HB2	8	0.86
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	12	0.86
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	1	0.86
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	1	0.86
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	13	0.86
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	20	0.86
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	14	0.86
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	18	0.86
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	3	0.85
(2,2240)	1:144:A:GLU:H	1:144:A:GLU:HB2	20	0.85
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	20	0.85
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	15	0.85
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	9	0.85
(2,1365)	1:111:A:GLN:H	1:111:A:GLN:HG2	1	0.85
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	5	0.85
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	6	0.85
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	15	0.85
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	15	0.85
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	11	0.85
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	17	0.85
(2,773)	1:44:A:ARG:HD2	1:61:A:MET:HG2	11	0.85
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	17	0.85
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	2	0.85
(2,217)	1:138:A:ARG:HD2	1:133:A:GLY:HA3	16	0.85
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	13	0.85
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	9	0.85
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	20	0.85
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	9	0.85
(2,2357)	1:121:A:GLY:H	1:122:A:PRO:HD2	19	0.84
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	9	0.84
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	17	0.84
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	14	0.84
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	13	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	11	0.84
(2,1481)	1:11:A:ILE:H	1:90:A:PHE:HB3	20	0.84
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	8	0.84
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	16	0.84
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	17	0.84
(2,1365)	1:111:A:GLN:H	1:111:A:GLN:HG2	5	0.84
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	19	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	1	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	3	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	6	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	7	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	8	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	12	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	13	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	17	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	18	0.84
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	19	0.84
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	13	0.84
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	4	0.84
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	15	0.84
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	6	0.84
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	16	0.84
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	13	0.84
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	7	0.84
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	16	0.84
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	20	0.84
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	8	0.84
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	9	0.84
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	13	0.84
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	6	0.84
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	1	0.84
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	16	0.83
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	17	0.83
(2,1946)	1:22:A:GLY:H	1:25:A:CYS:HB2	19	0.83
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	7	0.83
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	12	0.83
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	13	0.83
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	15	0.83
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	10	0.83
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	11	0.83
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	14	0.83
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	18	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	20	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	2	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	4	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	5	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	9	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	10	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	11	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	14	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	16	0.83
(2,950)	1:122:A:PRO:HG2	1:122:A:PRO:HA	20	0.83
(2,806)	1:117:A:TYR:HB3	1:157:A:THR:HG21	20	0.83
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	1	0.83
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	16	0.83
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	4	0.83
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	7	0.83
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	11	0.83
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	12	0.83
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	17	0.83
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	10	0.83
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	17	0.83
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	13	0.83
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	16	0.83
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	9	0.83
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	17	0.83
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	4	0.82
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	20	0.82
(2,2024)	1:95:A:TYR:H	1:14:A:VAL:HG22	4	0.82
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	11	0.82
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	1	0.82
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	13	0.82
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	2	0.82
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	11	0.82
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	12	0.82
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	13	0.82
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	9	0.82
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	11	0.82
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	16	0.82
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	17	0.82
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	14	0.82
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	20	0.82
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	2	0.82
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	6	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	3	0.82
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	4	0.82
(2,37)	1:166:A:LYS:HD2	1:163:A:PHE:HA	6	0.82
(1,26)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	12	0.82
(1,26)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	17	0.82
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	11	0.82
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	16	0.81
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	2	0.81
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	13	0.81
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	3	0.81
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	11	0.81
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	16	0.81
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	9	0.81
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	10	0.81
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	16	0.81
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	1	0.81
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	9	0.81
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	12	0.81
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	15	0.81
(2,858)	1:76:A:LEU:HD12	1:75:A:MET:HB3	17	0.81
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	5	0.81
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	5	0.81
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	12	0.81
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	1	0.81
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	8	0.81
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	7	0.81
(2,225)	1:166:A:LYS:HB2	1:166:A:LYS:HE2	15	0.81
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	11	0.81
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	20	0.81
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	1	0.81
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	8	0.81
(2,74)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	12	0.81
(1,26)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	4	0.81
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	2	0.81
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	10	0.81
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	11	0.8
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	6	0.8
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	13	0.8
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	11	0.8
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	4	0.8
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	2	0.8
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	8	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	20	0.8
(2,1705)	1:3:A:GLU:H	1:4:A:LYS:HD2	5	0.8
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	1	0.8
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	4	0.8
(2,1446)	1:7:A:LYS:H	1:7:A:LYS:HB3	19	0.8
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	11	0.8
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	3	0.8
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	8	0.8
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	19	0.8
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	5	0.8
(2,393)	1:91:A:LEU:HA	1:91:A:LEU:HD12	7	0.8
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	6	0.8
(2,225)	1:166:A:LYS:HB2	1:166:A:LYS:HE2	6	0.8
(2,132)	1:44:A:ARG:HA	1:44:A:ARG:HG3	11	0.8
(2,74)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	17	0.8
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	4	0.8
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	3	0.8
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	7	0.8
(1,19)	1:182:A:VAL:HG21	1:20:A:GLY:H	3	0.8
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD21	18	0.8
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	12	0.79
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	13	0.79
(2,810)	1:119:A:ASP:HB3	1:174:A:ASN:HB3	18	0.79
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	9	0.79
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	10	0.79
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	14	0.79
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	9	0.79
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	2	0.79
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	17	0.79
(2,74)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	4	0.79
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	16	0.79
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	18	0.79
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	2	0.79
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	6	0.79
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	14	0.79
(2,2327)	1:5:A:LEU:H	1:5:A:LEU:HB2	15	0.78
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	15	0.78
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	6	0.78
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	15	0.78
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	15	0.78
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	19	0.78
(2,1705)	1:3:A:GLU:H	1:4:A:LYS:HD2	17	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	3	0.78
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	1	0.78
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	7	0.78
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	6	0.78
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	15	0.78
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	9	0.78
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	4	0.78
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	3	0.78
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	4	0.78
(2,225)	1:166:A:LYS:HB2	1:166:A:LYS:HE2	19	0.78
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	13	0.78
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	4	0.78
(1,4)	1:43:A:LEU:HB3	1:43:A:LEU:HD23	1	0.78
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	8	0.77
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	7	0.77
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	10	0.77
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	18	0.77
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	9	0.77
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	3	0.77
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	16	0.77
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	16	0.77
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	7	0.77
(2,963)	1:61:A:MET:HG2	1:57:A:LEU:HB2	17	0.77
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	8	0.77
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	13	0.77
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	19	0.77
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	17	0.77
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	16	0.77
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	19	0.77
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	1	0.77
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	12	0.77
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	1	0.76
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	4	0.76
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	14	0.76
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	1	0.76
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	3	0.76
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	5	0.76
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	15	0.76
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	16	0.76
(2,418)	1:141:A:ASP:HB3	1:133:A:GLY:HA3	4	0.76
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	14	0.76
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	12	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	18	0.76
(1,26)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	1	0.76
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	8	0.76
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	11	0.76
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	19	0.76
(1,17)	1:37:A:LEU:HD13	1:90:A:PHE:HD2	14	0.76
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	16	0.75
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	7	0.75
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	7	0.75
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	13	0.75
(2,1629)	1:41:A:ASP:H	1:44:A:ARG:HB3	11	0.75
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	13	0.75
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	4	0.75
(2,1445)	1:63:A:LYS:H	1:62:A:GLU:HG3	13	0.75
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	3	0.75
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	6	0.75
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	8	0.75
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	12	0.75
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	20	0.75
(2,860)	1:76:A:LEU:HD12	1:73:A:LEU:HA	17	0.75
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	16	0.75
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	18	0.75
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	19	0.75
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	18	0.75
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	10	0.75
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	10	0.75
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	5	0.75
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	15	0.75
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	18	0.74
(2,2254)	1:129:A:LEU:H	1:128:A:ARG:HB2	5	0.74
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	12	0.74
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	7	0.74
(2,1850)	1:35:A:THR:H	1:83:A:LYS:HG3	11	0.74
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	15	0.74
(2,1415)	1:61:A:MET:H	1:61:A:MET:HB2	11	0.74
(2,1100)	1:178:A:SER:H	1:178:A:SER:HB3	10	0.74
(2,883)	1:162:A:ALA:HB1	1:166:A:LYS:HE3	6	0.74
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	17	0.74
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	13	0.74
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	10	0.74
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	14	0.74
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	5	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	9	0.74
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	18	0.74
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	2	0.74
(2,74)	1:63:A:LYS:HE2	1:63:A:LYS:HB2	1	0.74
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	15	0.74
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	6	0.74
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	10	0.74
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	8	0.73
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	14	0.73
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	20	0.73
(2,990)	1:169:A:ILE:HG22	1:167:A:ARG:HG2	4	0.73
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	3	0.73
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	10	0.73
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	10	0.73
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	18	0.73
(2,785)	1:140:A:ASP:HB3	1:149:A:ARG:HD3	17	0.73
(2,771)	1:119:A:ASP:HB2	1:117:A:TYR:HB2	19	0.73
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	8	0.73
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	20	0.73
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	20	0.73
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	1	0.73
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	2	0.73
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	17	0.73
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	19	0.73
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	10	0.73
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	4	0.73
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	5	0.72
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	16	0.72
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	17	0.72
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	2	0.72
(2,1989)	1:177:A:GLY:H	1:125:A:MET:HB3	18	0.72
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	12	0.72
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	14	0.72
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	20	0.72
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	6	0.72
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	5	0.72
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	5	0.72
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	12	0.72
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	15	0.72
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	1	0.72
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	10	0.72
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	13	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	20	0.72
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	7	0.72
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	1	0.72
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	7	0.72
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	4	0.72
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	20	0.71
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	5	0.71
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	17	0.71
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	10	0.71
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	2	0.71
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	3	0.71
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	12	0.71
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	15	0.71
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	19	0.71
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	9	0.71
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	15	0.71
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	15	0.71
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	2	0.71
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	14	0.71
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	19	0.71
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	20	0.71
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	2	0.71
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	15	0.71
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	6	0.71
(2,393)	1:91:A:LEU:HA	1:91:A:LEU:HD12	3	0.71
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	8	0.71
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	15	0.71
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	6	0.71
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	20	0.7
(2,2262)	1:36:A:HIS:H	1:83:A:LYS:HG3	18	0.7
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	20	0.7
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	6	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	1	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	4	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	5	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	8	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	9	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	10	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	11	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	13	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	14	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	16	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	17	0.7
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	20	0.7
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	5	0.7
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	8	0.7
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	10	0.7
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	11	0.7
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	16	0.7
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	20	0.7
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	4	0.7
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	1	0.7
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	1	0.7
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	20	0.7
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	9	0.7
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	9	0.7
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	7	0.7
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	20	0.7
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	1	0.7
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	6	0.7
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	19	0.7
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	1	0.7
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	8	0.7
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	8	0.69
(2,2021)	1:110:A:GLY:H	1:106:A:GLU:HB3	7	0.69
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	5	0.69
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	17	0.69
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	12	0.69
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	7	0.69
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	1	0.69
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	3	0.69
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	6	0.69
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	17	0.69
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	19	0.69
(2,1076)	1:2:A:GLU:H	1:1:A:MET:HB3	16	0.69
(2,1072)	1:143:A:GLU:H	1:143:A:GLU:HG3	20	0.69
(2,852)	1:161:A:ILE:HG22	1:161:A:ILE:HG12	11	0.69
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	3	0.69
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	19	0.69
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	3	0.69
(2,820)	1:106:A:GLU:HG2	1:111:A:GLN:HA	13	0.69
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	4	0.69
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	14	0.69
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	2	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	12	0.69
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	13	0.69
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	5	0.69
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	7	0.69
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	19	0.69
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	8	0.69
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	14	0.69
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	19	0.69
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	3	0.69
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	17	0.69
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	5	0.68
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	9	0.68
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	13	0.68
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	14	0.68
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	15	0.68
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	17	0.68
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	19	0.68
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	15	0.68
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	17	0.68
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	19	0.68
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	7	0.68
(2,1290)	1:127:A:GLN:H	1:127:A:GLN:HB2	19	0.68
(2,1252)	1:172:A:LYS:H	1:172:A:LYS:HB3	18	0.68
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	2	0.68
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	7	0.68
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	12	0.68
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	13	0.68
(2,1176)	1:134:A:GLU:H	1:134:A:GLU:HB2	18	0.68
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	19	0.68
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	11	0.68
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	9	0.68
(2,852)	1:161:A:ILE:HG22	1:161:A:ILE:HG12	4	0.68
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	7	0.68
(2,753)	1:40:A:GLY:HA3	1:44:A:ARG:HB3	11	0.68
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	3	0.68
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	8	0.68
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	16	0.68
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	7	0.68
(2,393)	1:91:A:LEU:HA	1:91:A:LEU:HD12	18	0.68
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	17	0.68
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	2	0.68
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	8	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	6	0.68
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	8	0.68
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	8	0.68
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	18	0.68
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	1	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	2	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	3	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	4	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	6	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	10	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	12	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	16	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	18	0.67
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	3	0.67
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	9	0.67
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	11	0.67
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	6	0.67
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	18	0.67
(2,852)	1:161:A:ILE:HG22	1:161:A:ILE:HG12	2	0.67
(2,852)	1:161:A:ILE:HG22	1:161:A:ILE:HG12	3	0.67
(2,852)	1:161:A:ILE:HG22	1:161:A:ILE:HG12	15	0.67
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	2	0.67
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	13	0.67
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	14	0.67
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	11	0.67
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	12	0.67
(2,378)	1:190:A:LEU:HA	1:190:A:LEU:HD22	16	0.67
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	4	0.67
(2,217)	1:138:A:ARG:HD2	1:133:A:GLY:HA3	3	0.67
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	4	0.67
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	8	0.67
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	7	0.67
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	11	0.67
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	11	0.66
(2,2410)	1:85:A:ASN:HD22	1:85:A:ASN:HB3	20	0.66
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	6	0.66
(2,2234)	1:148:A:LYS:H	1:148:A:LYS:HB2	10	0.66
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	7	0.66
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	16	0.66
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	17	0.66
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	4	0.66
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	6	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	6	0.66
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	17	0.66
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	13	0.66
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	19	0.66
(2,2294)	1:28:A:ILE:H	1:26:A:GLU:HG2	13	0.65
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	6	0.65
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	8	0.65
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	9	0.65
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	14	0.65
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	10	0.65
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	10	0.65
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	9	0.65
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	20	0.65
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	14	0.65
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	1	0.65
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	12	0.65
(2,780)	1:63:A:LYS:HE2	1:60:A:ILE:HG12	2	0.65
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	9	0.65
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	10	0.65
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	5	0.65
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	8	0.65
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	8	0.65
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	9	0.65
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	10	0.65
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	12	0.65
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	13	0.65
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	3	0.65
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	14	0.65
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	13	0.65
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	12	0.65
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	15	0.65
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	14	0.64
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	11	0.64
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	9	0.64
(2,2390)	1:88:A:LYS:H	1:9:A:LYS:HD2	3	0.64
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	18	0.64
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	5	0.64
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	15	0.64
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	20	0.64
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	5	0.64
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	9	0.64
(2,868)	1:160:A:VAL:HG12	1:163:A:PHE:HB3	20	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	6	0.64
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	10	0.64
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	9	0.64
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	2	0.64
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	17	0.64
(2,462)	1:134:A:GLU:HG3	1:131:A:LYS:HE2	5	0.64
(2,415)	1:171:A:ARG:HD3	1:171:A:ARG:HB2	9	0.64
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	4	0.64
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	19	0.64
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	20	0.64
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	9	0.64
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	18	0.64
(2,52)	1:194:A:LYS:HG3	1:194:A:LYS:HE3	12	0.64
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	11	0.63
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	19	0.63
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	4	0.63
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	12	0.63
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	15	0.63
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	18	0.63
(2,1457)	1:38:A:SER:H	1:41:A:ASP:HB2	13	0.63
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	1	0.63
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	2	0.63
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	9	0.63
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	14	0.63
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	16	0.63
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	19	0.63
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	18	0.63
(2,883)	1:162:A:ALA:HB1	1:166:A:LYS:HE3	19	0.63
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	12	0.63
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	16	0.63
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	2	0.63
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	14	0.63
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	2	0.63
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	10	0.63
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	17	0.63
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	12	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	1	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	2	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	3	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	5	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	6	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	14	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	15	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	16	0.63
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	18	0.63
(2,217)	1:138:A:ARG:HD2	1:133:A:GLY:HA3	20	0.63
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	9	0.63
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	10	0.63
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	14	0.63
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	1	0.63
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	6	0.63
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	12	0.63
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	20	0.63
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	17	0.62
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	1	0.62
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	10	0.62
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	2	0.62
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	18	0.62
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	19	0.62
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	11	0.62
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	14	0.62
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	16	0.62
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	20	0.62
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	11	0.62
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	13	0.62
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	7	0.62
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	11	0.62
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	13	0.62
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	15	0.62
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	17	0.62
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	7	0.62
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	19	0.62
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	20	0.62
(2,669)	1:109:A:ILE:HA	1:5:A:LEU:HB3	15	0.62
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	5	0.62
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	13	0.62
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	17	0.62
(2,217)	1:138:A:ARG:HD2	1:133:A:GLY:HA3	2	0.62
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	7	0.62
(2,40)	1:166:A:LYS:HD2	1:166:A:LYS:HE3	5	0.62
(2,40)	1:166:A:LYS:HD2	1:166:A:LYS:HE3	6	0.62
(2,40)	1:166:A:LYS:HD2	1:166:A:LYS:HE3	15	0.62
(2,40)	1:166:A:LYS:HD2	1:166:A:LYS:HE3	16	0.62
(2,40)	1:166:A:LYS:HD2	1:166:A:LYS:HE3	18	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	2	0.62
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	14	0.62
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	17	0.62
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	10	0.62
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	2	0.61
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	6	0.61
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	18	0.61
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	6	0.61
(2,2294)	1:28:A:ILE:H	1:26:A:GLU:HG2	10	0.61
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	1	0.61
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	4	0.61
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	12	0.61
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	17	0.61
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	18	0.61
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	5	0.61
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	2	0.61
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	6	0.61
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	4	0.61
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	1	0.61
(2,1399)	1:55:A:LYS:H	1:55:A:LYS:HB3	11	0.61
(2,1399)	1:55:A:LYS:H	1:55:A:LYS:HB3	20	0.61
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	20	0.61
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	17	0.61
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	10	0.61
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	1	0.61
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	3	0.61
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	14	0.61
(2,644)	1:123:A:GLU:HG3	1:124:A:THR:HB	5	0.61
(2,644)	1:123:A:GLU:HG3	1:124:A:THR:HB	12	0.61
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	4	0.61
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	10	0.61
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	7	0.61
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	4	0.61
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	17	0.61
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	11	0.61
(2,263)	1:74:A:ASP:HA	1:108:A:ARG:HG2	9	0.61
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	7	0.61
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	7	0.61
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	8	0.61
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	11	0.61
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	13	0.61
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	17	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	20	0.61
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	6	0.61
(2,40)	1:166:A:LYS:HD2	1:166:A:LYS:HE3	19	0.61
(2,37)	1:166:A:LYS:HD2	1:163:A:PHE:HA	16	0.61
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	1	0.6
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	16	0.6
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	12	0.6
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	13	0.6
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	11	0.6
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	14	0.6
(2,2294)	1:28:A:ILE:H	1:26:A:GLU:HG2	20	0.6
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	10	0.6
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	19	0.6
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	3	0.6
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	12	0.6
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	2	0.6
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	1	0.6
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	10	0.6
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	14	0.6
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	4	0.6
(2,1399)	1:55:A:LYS:H	1:55:A:LYS:HB3	7	0.6
(2,1399)	1:55:A:LYS:H	1:55:A:LYS:HB3	16	0.6
(2,1399)	1:55:A:LYS:H	1:55:A:LYS:HB3	18	0.6
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	1	0.6
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	8	0.6
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	1	0.6
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	9	0.6
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	18	0.6
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	19	0.6
(2,644)	1:123:A:GLU:HG3	1:124:A:THR:HB	9	0.6
(2,644)	1:123:A:GLU:HG3	1:124:A:THR:HB	19	0.6
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	19	0.6
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	3	0.6
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	20	0.6
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	5	0.6
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	5	0.6
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	6	0.6
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	9	0.6
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	12	0.6
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	16	0.6
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	6	0.6
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	9	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	2	0.6
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	3	0.6
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	4	0.6
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	5	0.6
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	7	0.6
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	14	0.6
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	17	0.6
(2,265)	1:53:A:ARG:HG2	1:53:A:ARG:HD2	13	0.6
(2,265)	1:53:A:ARG:HG2	1:53:A:ARG:HD2	15	0.6
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	1	0.6
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	4	0.6
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	10	0.6
(2,133)	1:181:A:SER:HB2	1:181:A:SER:HA	14	0.6
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	9	0.6
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	16	0.6
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	20	0.59
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	8	0.59
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	12	0.59
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	5	0.59
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	11	0.59
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	17	0.59
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	7	0.59
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	2	0.59
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	17	0.59
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	18	0.59
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	18	0.59
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	8	0.59
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	1	0.59
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	7	0.59
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	7	0.59
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	11	0.59
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	8	0.59
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	11	0.59
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	19	0.59
(2,379)	1:108:A:ARG:HA	1:108:A:ARG:HD2	2	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	1	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	3	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	5	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	8	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	10	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	12	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	15	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	16	0.59
(2,346)	1:178:A:SER:HA	1:178:A:SER:HB2	20	0.59
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	1	0.59
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	6	0.59
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	8	0.59
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	9	0.59
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	10	0.59
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	12	0.59
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	19	0.59
(2,265)	1:53:A:ARG:HG2	1:53:A:ARG:HD2	6	0.59
(2,217)	1:138:A:ARG:HD2	1:133:A:GLY:HA3	5	0.59
(2,102)	1:132:A:ARG:HB2	1:132:A:ARG:HD3	19	0.59
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	5	0.59
(2,17)	1:176:A:GLU:HA	1:176:A:GLU:HG3	19	0.59
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	2	0.58
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	7	0.58
(2,2294)	1:28:A:ILE:H	1:26:A:GLU:HG2	6	0.58
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	11	0.58
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	16	0.58
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	3	0.58
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	16	0.58
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	9	0.58
(2,1546)	1:192:A:ALA:H	1:191:A:ASP:HB2	13	0.58
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	19	0.58
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	2	0.58
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	6	0.58
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	9	0.58
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	13	0.58
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	8	0.58
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	3	0.58
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	6	0.58
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	1	0.58
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	6	0.58
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	8	0.58
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	2	0.58
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	7	0.58
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	18	0.58
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	3	0.58
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	15	0.58
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	1	0.58
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	2	0.58
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	17	0.57
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	5	0.57
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	15	0.57
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	19	0.57
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	18	0.57
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	17	0.57
(2,2077)	1:62:A:GLU:H	1:60:A:ILE:HG12	13	0.57
(2,2076)	1:130:A:LEU:H	1:143:A:GLU:HG2	20	0.57
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	11	0.57
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	2	0.57
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	10	0.57
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	12	0.57
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	11	0.57
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	2	0.57
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	7	0.57
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	9	0.57
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	2	0.57
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	3	0.57
(2,1007)	1:76:A:LEU:HB3	1:76:A:LEU:HD22	17	0.57
(2,918)	1:91:A:LEU:HD13	1:92:A:ILE:H	7	0.57
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	13	0.57
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	10	0.57
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	12	0.57
(2,644)	1:123:A:GLU:HG3	1:124:A:THR:HB	14	0.57
(2,644)	1:123:A:GLU:HG3	1:124:A:THR:HB	16	0.57
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	8	0.57
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	19	0.57
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	14	0.57
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	15	0.57
(2,277)	1:134:A:GLU:HB2	1:134:A:GLU:HA	14	0.57
(2,49)	1:194:A:LYS:HG2	1:194:A:LYS:HA	6	0.57
(2,37)	1:166:A:LYS:HD2	1:163:A:PHE:HA	18	0.57
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	14	0.57
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	1	0.56
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	3	0.56
(2,1942)	1:15:A:GLY:H	1:21:A:LYS:HE2	5	0.56
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	1	0.56
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	8	0.56
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	11	0.56
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	10	0.56
(2,1457)	1:38:A:SER:H	1:41:A:ASP:HB2	17	0.56
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	19	0.56
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	4	0.56
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	5	0.56
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	12	0.56
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	7	0.56
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	12	0.56
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	6	0.56
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	15	0.56
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	8	0.56
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	6	0.56
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	7	0.56
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	8	0.56
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	19	0.56
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	14	0.56
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	10	0.56
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	20	0.56
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	1	0.56
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	3	0.56
(2,277)	1:134:A:GLU:HB2	1:134:A:GLU:HA	4	0.56
(2,177)	1:132:A:ARG:HD2	1:132:A:ARG:HB2	19	0.56
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	8	0.56
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	18	0.56
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	8	0.55
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	10	0.55
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	3	0.55
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	6	0.55
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	13	0.55
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	6	0.55
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	10	0.55
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	12	0.55
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	15	0.55
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	18	0.55
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	2	0.55
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	3	0.55
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	4	0.55
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	20	0.55
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	19	0.55
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	14	0.55
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	17	0.55
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	1	0.55
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	9	0.55
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	12	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	3	0.55
(2,439)	1:151:A:GLU:HG3	1:147:A:LYS:HG2	20	0.55
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	6	0.55
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	8	0.55
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	14	0.55
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	2	0.55
(2,29)	1:194:A:LYS:HB3	1:194:A:LYS:HE2	4	0.55
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	2	0.54
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	9	0.54
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	13	0.54
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	3	0.54
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	20	0.54
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	13	0.54
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	8	0.54
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	17	0.54
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	16	0.54
(2,1447)	1:152:A:THR:H	1:149:A:ARG:HD3	3	0.54
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	8	0.54
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	8	0.54
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	5	0.54
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	10	0.54
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	1	0.54
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	2	0.54
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	8	0.54
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	5	0.54
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	4	0.54
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	8	0.54
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	13	0.54
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	16	0.54
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	17	0.54
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	12	0.54
(1,22)	1:38:A:SER:HA	1:91:A:LEU:HD13	20	0.54
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	9	0.53
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	16	0.53
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	7	0.53
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	1	0.53
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	10	0.53
(2,1944)	1:15:A:GLY:H	1:14:A:VAL:HG22	6	0.53
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	7	0.53
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	20	0.53
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	9	0.53
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	4	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	13	0.53
(2,775)	1:93:A:ASP:HB2	1:22:A:GLY:HA3	11	0.53
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	5	0.53
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	6	0.53
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	17	0.53
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	13	0.53
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	17	0.53
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	2	0.53
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	19	0.53
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	8	0.53
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	16	0.53
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	7	0.53
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	12	0.53
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	11	0.53
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	18	0.53
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	11	0.53
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	16	0.53
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	6	0.53
(2,440)	1:62:A:GLU:HG2	1:59:A:GLU:HA	11	0.53
(2,29)	1:194:A:LYS:HB3	1:194:A:LYS:HE2	15	0.53
(1,20)	1:173:A:VAL:HG11	1:186:A:VAL:HB	20	0.53
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	17	0.52
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	3	0.52
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	16	0.52
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	16	0.52
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	4	0.52
(2,1663)	1:139:A:VAL:H	1:138:A:ARG:HG3	4	0.52
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	19	0.52
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	15	0.52
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	18	0.52
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	20	0.52
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	15	0.52
(2,967)	1:116:A:LEU:HD12	1:189:A:HIS:HB2	15	0.52
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	9	0.52
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	19	0.52
(2,761)	1:91:A:LEU:HB2	1:90:A:PHE:HB3	18	0.52
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	13	0.52
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	14	0.52
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	18	0.52
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	5	0.52
(2,372)	1:194:A:LYS:HA	1:9:A:LYS:HE3	7	0.52
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	5	0.52
(1,13)	1:34:A:TYR:HE2	1:193:A:LEU:HG	7	0.52
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	14	0.51
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	9	0.51
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	4	0.51
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	12	0.51
(2,1544)	1:67:A:VAL:H	1:66:A:LEU:HB3	13	0.51
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	14	0.51
(2,1320)	1:41:A:ASP:H	1:41:A:ASP:HB2	6	0.51
(2,1320)	1:41:A:ASP:H	1:41:A:ASP:HB2	8	0.51
(2,1320)	1:41:A:ASP:H	1:41:A:ASP:HB2	14	0.51
(2,1320)	1:41:A:ASP:H	1:41:A:ASP:HB2	17	0.51
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	11	0.51
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	2	0.51
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	6	0.51
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	8	0.51
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	16	0.51
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	12	0.51
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	10	0.51
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	12	0.51
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	15	0.51
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	16	0.51
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	4	0.51
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	8	0.51
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	9	0.51
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	14	0.51
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	18	0.51
(2,404)	1:18:A:GLY:HA3	1:132:A:ARG:HG2	10	0.51
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	13	0.51
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	9	0.51
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	17	0.51
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	5	0.51
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	11	0.51
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	9	0.51
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	1	0.5
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	18	0.5
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	1	0.5
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	4	0.5
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	18	0.5
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	3	0.5
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	9	0.5
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	4	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	13	0.5
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	15	0.5
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	8	0.5
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	5	0.5
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	12	0.5
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	17	0.5
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	17	0.5
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	13	0.5
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	3	0.5
(2,735)	1:142:A:ASN:HA	1:141:A:ASP:HB2	11	0.5
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	17	0.5
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	9	0.5
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	15	0.5
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	17	0.5
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	14	0.5
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	1	0.49
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	13	0.49
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	2	0.49
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	10	0.49
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	14	0.49
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	16	0.49
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	16	0.49
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	11	0.49
(2,1320)	1:41:A:ASP:H	1:41:A:ASP:HB2	13	0.49
(2,949)	1:109:A:ILE:HG22	1:5:A:LEU:HD13	15	0.49
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	13	0.49
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	14	0.49
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	4	0.49
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	12	0.49
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	1	0.49
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	17	0.49
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	4	0.49
(2,227)	1:106:A:GLU:HA	1:106:A:GLU:HG3	13	0.49
(2,227)	1:106:A:GLU:HA	1:106:A:GLU:HG3	14	0.49
(2,227)	1:106:A:GLU:HA	1:106:A:GLU:HG3	19	0.49
(2,73)	1:83:A:LYS:HE2	1:83:A:LYS:HB2	16	0.49
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	5	0.49
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	5	0.48
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	13	0.48
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	20	0.48
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	18	0.48
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	13	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	15	0.48
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	20	0.48
(2,1765)	1:128:A:ARG:H	1:127:A:GLN:HB2	19	0.48
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	8	0.48
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	18	0.48
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	5	0.48
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	13	0.48
(2,1405)	1:83:A:LYS:H	1:83:A:LYS:HE2	16	0.48
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	18	0.48
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	10	0.48
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	15	0.48
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	1	0.48
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	5	0.48
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	11	0.48
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	16	0.48
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	5	0.48
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	7	0.48
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	16	0.48
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	4	0.48
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	12	0.47
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	19	0.47
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	20	0.47
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	5	0.47
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	12	0.47
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	17	0.47
(2,1849)	1:70:A:GLU:H	1:69:A:LEU:HB2	20	0.47
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	9	0.47
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	1	0.47
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	10	0.47
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	12	0.47
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	6	0.47
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	19	0.47
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	3	0.47
(2,904)	1:194:A:LYS:HB3	1:192:A:ALA:H	11	0.47
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	6	0.47
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	18	0.47
(2,823)	1:65:A:GLN:HG2	1:60:A:ILE:HA	9	0.47
(2,823)	1:65:A:GLN:HG2	1:60:A:ILE:HA	20	0.47
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	2	0.47
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	10	0.47
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	1	0.47
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	16	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	18	0.47
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	9	0.47
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	13	0.47
(2,37)	1:166:A:LYS:HD2	1:163:A:PHE:HA	5	0.47
(1,14)	1:149:A:ARG:HD3	1:146:A:ILE:HD13	3	0.47
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	16	0.47
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	4	0.46
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	3	0.46
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	1	0.46
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	7	0.46
(2,1848)	1:107:A:ARG:H	1:106:A:GLU:HB2	12	0.46
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	6	0.46
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	15	0.46
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	8	0.46
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	16	0.46
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	11	0.46
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	17	0.46
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	9	0.46
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	20	0.46
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	3	0.46
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	11	0.46
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	13	0.46
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	19	0.46
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	10	0.46
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	3	0.46
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	11	0.46
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	10	0.46
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	13	0.46
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	4	0.45
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	15	0.45
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	13	0.45
(2,1968)	1:20:A:GLY:H	1:21:A:LYS:HG2	8	0.45
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	13	0.45
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	13	0.45
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	14	0.45
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	12	0.45
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	19	0.45
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	8	0.45
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	3	0.45
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD11	11	0.45
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	18	0.45
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	17	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	18	0.45
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	10	0.45
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	11	0.45
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	12	0.45
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	4	0.45
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	14	0.45
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	20	0.45
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	8	0.45
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	11	0.45
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	20	0.45
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	7	0.44
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	7	0.44
(2,2024)	1:95:A:TYR:H	1:14:A:VAL:HG22	16	0.44
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	3	0.44
(2,1942)	1:15:A:GLY:H	1:21:A:LYS:HE2	16	0.44
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	9	0.44
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	20	0.44
(2,1292)	1:124:A:THR:H	1:124:A:THR:HG21	19	0.44
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	10	0.44
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	16	0.44
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	5	0.44
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	15	0.44
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	7	0.44
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	1	0.44
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	13	0.44
(2,488)	1:73:A:LEU:HD13	1:72:A:VAL:HA	14	0.44
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	1	0.44
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	16	0.44
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	19	0.44
(2,195)	1:127:A:GLN:HG3	1:127:A:GLN:HB2	19	0.44
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	3	0.44
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	7	0.44
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	7	0.43
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	17	0.43
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	18	0.43
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	10	0.43
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	3	0.43
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	6	0.43
(2,883)	1:162:A:ALA:HB1	1:166:A:LYS:HE3	15	0.43
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	2	0.43
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	4	0.43
(2,670)	1:109:A:ILE:HA	1:108:A:ARG:HG2	8	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	13	0.43
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	7	0.43
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	15	0.43
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	7	0.43
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	19	0.43
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	2	0.43
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	9	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	1	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	3	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	6	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	9	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	10	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	14	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	15	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	16	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	18	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	19	0.43
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	20	0.43
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	6	0.43
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	13	0.43
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	17	0.43
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	15	0.42
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	19	0.42
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	12	0.42
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	12	0.42
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	6	0.42
(2,1914)	1:71:A:THR:H	1:70:A:GLU:HB2	19	0.42
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	10	0.42
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	16	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	1	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	7	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	8	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	9	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	10	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	12	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	15	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	16	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	17	0.42
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	20	0.42
(2,1656)	1:123:A:GLU:H	1:122:A:PRO:HD2	19	0.42
(2,1457)	1:38:A:SER:H	1:41:A:ASP:HB2	14	0.42
(2,1447)	1:152:A:THR:H	1:149:A:ARG:HD3	19	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	1	0.42
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	7	0.42
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	8	0.42
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	12	0.42
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	15	0.42
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	1	0.42
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	4	0.42
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	6	0.42
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	13	0.42
(2,1017)	1:171:A:ARG:HD3	1:171:A:ARG:HA	9	0.42
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	4	0.42
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	8	0.42
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	1	0.42
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	2	0.42
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	6	0.42
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	18	0.42
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	6	0.42
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	19	0.42
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	12	0.42
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	13	0.42
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	12	0.42
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	4	0.42
(2,308)	1:108:A:ARG:HD2	1:108:A:ARG:HG2	8	0.42
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	1	0.42
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	7	0.42
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	15	0.42
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	17	0.42
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	18	0.42
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	19	0.42
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	15	0.42
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	5	0.41
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	20	0.41
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	10	0.41
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	3	0.41
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	6	0.41
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	13	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	2	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	3	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	4	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	5	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	6	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	14	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	18	0.41
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	19	0.41
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	17	0.41
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	17	0.41
(2,1447)	1:152:A:THR:H	1:149:A:ARG:HD3	1	0.41
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	10	0.41
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	4	0.41
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	6	0.41
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	16	0.41
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	7	0.41
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	13	0.41
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	7	0.41
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	15	0.41
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	19	0.41
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	9	0.41
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	4	0.41
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	17	0.41
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	7	0.41
(2,573)	1:153:A:TYR:HD1	1:15:A:GLY:HA3	8	0.41
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	6	0.41
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	9	0.41
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	18	0.41
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	15	0.41
(2,342)	1:124:A:THR:HA	1:127:A:GLN:HG3	19	0.41
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	15	0.41
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	6	0.41
(1,25)	1:4:A:LYS:HB2	1:4:A:LYS:HA	5	0.41
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	13	0.4
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	2	0.4
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	6	0.4
(2,2371)	1:7:A:LYS:H	1:6:A:LYS:HG2	11	0.4
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	15	0.4
(2,1670)	1:138:A:ARG:H	1:137:A:GLY:HA3	13	0.4
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	6	0.4
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	17	0.4
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	19	0.4
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	3	0.4
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	7	0.4
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	15	0.4
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	2	0.4
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	4	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	10	0.4
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	2	0.4
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	5	0.4
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	10	0.4
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	11	0.4
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	10	0.4
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	1	0.4
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	5	0.4
(2,868)	1:160:A:VAL:HG12	1:163:A:PHE:HB3	4	0.4
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	12	0.4
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	3	0.4
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	7	0.4
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	11	0.4
(2,649)	1:186:A:VAL:HA	1:189:A:HIS:HB2	15	0.4
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	3	0.4
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	6	0.4
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	2	0.4
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	15	0.4
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	20	0.4
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	9	0.4
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	18	0.4
(1,25)	1:72:A:VAL:HB	1:69:A:LEU:HA	8	0.4
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	9	0.4
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	9	0.4
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	8	0.39
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	10	0.39
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	12	0.39
(2,2371)	1:7:A:LYS:H	1:6:A:LYS:HG2	17	0.39
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	16	0.39
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	8	0.39
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	10	0.39
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	13	0.39
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	15	0.39
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	20	0.39
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	4	0.39
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	16	0.39
(2,1447)	1:152:A:THR:H	1:149:A:ARG:HD3	13	0.39
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	1	0.39
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	5	0.39
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	7	0.39
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	10	0.39
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	13	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	14	0.39
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	15	0.39
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	16	0.39
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	12	0.39
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	18	0.39
(2,1336)	1:149:A:ARG:H	1:149:A:ARG:HD3	13	0.39
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	6	0.39
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	3	0.39
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	9	0.39
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	12	0.39
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	16	0.39
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	18	0.39
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	4	0.39
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	16	0.39
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	17	0.39
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	18	0.39
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	9	0.39
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	1	0.39
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	11	0.39
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	16	0.39
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	3	0.39
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	1	0.39
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	15	0.39
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	3	0.39
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	4	0.39
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	12	0.39
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	5	0.39
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	6	0.39
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	11	0.39
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	16	0.39
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	12	0.39
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	13	0.39
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	19	0.39
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	11	0.39
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	19	0.39
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	4	0.38
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	19	0.38
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	2	0.38
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	7	0.38
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	6	0.38
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	8	0.38
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	11	0.38
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	16	0.38
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	20	0.38
(2,1747)	1:4:A:LYS:H	1:4:A:LYS:HD2	2	0.38
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	10	0.38
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	16	0.38
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	17	0.38
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	18	0.38
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	11	0.38
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	17	0.38
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	10	0.38
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	19	0.38
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	12	0.38
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	19	0.38
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	13	0.38
(2,986)	1:75:A:MET:HA	1:75:A:MET:HG2	20	0.38
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	15	0.38
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	20	0.38
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	11	0.38
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	17	0.38
(2,488)	1:73:A:LEU:HD12	1:72:A:VAL:HA	8	0.38
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	20	0.38
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	5	0.38
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	6	0.38
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	11	0.38
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	13	0.38
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	1	0.38
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	4	0.38
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	1	0.38
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	10	0.38
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	15	0.38
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	13	0.38
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	18	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	1	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	2	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	3	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	4	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	5	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	6	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	7	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	8	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	9	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	10	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	11	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	14	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	15	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	16	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	17	0.38
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	20	0.38
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	9	0.37
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	19	0.37
(2,2393)	1:107:A:ARG:H	1:107:A:ARG:HB3	2	0.37
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	7	0.37
(2,2371)	1:7:A:LYS:H	1:6:A:LYS:HG2	5	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	1	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	3	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	8	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	10	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	11	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	12	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	13	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	17	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	19	0.37
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	11	0.37
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	10	0.37
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	2	0.37
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	7	0.37
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	17	0.37
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	18	0.37
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	13	0.37
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	8	0.37
(2,1457)	1:38:A:SER:H	1:41:A:ASP:HB2	8	0.37
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	1	0.37
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	14	0.37
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	16	0.37
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	20	0.37
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	11	0.37
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	7	0.37
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	15	0.37
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	17	0.37
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	18	0.37
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	19	0.37
(2,964)	1:81:A:VAL:HB	1:1:A:MET:HG2	2	0.37
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	16	0.37
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	11	0.37
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	8	0.37
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	10	0.37
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	14	0.37
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	20	0.37
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	11	0.37
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	8	0.37
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	14	0.37
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	8	0.37
(2,448)	1:127:A:GLN:HG2	1:126:A:THR:HG21	19	0.37
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	20	0.37
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	2	0.37
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	8	0.37
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	17	0.37
(2,271)	1:60:A:ILE:HD12	1:60:A:ILE:HG12	18	0.37
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	12	0.37
(1,13)	1:34:A:TYR:HE2	1:9:A:LYS:HD2	19	0.37
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	4	0.36
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	5	0.36
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	6	0.36
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	9	0.36
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	14	0.36
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	18	0.36
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	20	0.36
(2,2268)	1:37:A:LEU:H	1:91:A:LEU:HG	7	0.36
(2,1971)	1:20:A:GLY:H	1:21:A:LYS:HE2	8	0.36
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	7	0.36
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	11	0.36
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	1	0.36
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	12	0.36
(2,1786)	1:78:A:ASP:H	1:75:A:MET:HG2	13	0.36
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	15	0.36
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	19	0.36
(2,1705)	1:3:A:GLU:H	1:4:A:LYS:HD2	9	0.36
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	11	0.36
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	13	0.36
(2,1457)	1:38:A:SER:H	1:41:A:ASP:HB2	6	0.36
(2,1447)	1:152:A:THR:H	1:149:A:ARG:HD3	2	0.36
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	13	0.36
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	1	0.36
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	6	0.36
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	9	0.36
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	14	0.36
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	20	0.36
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	8	0.36
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	12	0.36
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	10	0.36
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	12	0.36
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	1	0.36
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	2	0.36
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	3	0.36
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	5	0.36
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	8	0.36
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	9	0.36
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	16	0.36
(2,981)	1:87:A:SER:HB2	1:86:A:THR:HG21	11	0.36
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	6	0.36
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	8	0.36
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	20	0.36
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	8	0.36
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	5	0.36
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	10	0.36
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	15	0.36
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	20	0.36
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	6	0.36
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	8	0.36
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	12	0.36
(2,488)	1:73:A:LEU:HD11	1:72:A:VAL:HA	2	0.36
(2,488)	1:73:A:LEU:HD13	1:72:A:VAL:HA	11	0.36
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	3	0.36
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	6	0.36
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	17	0.36
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	11	0.36
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	17	0.36
(1,22)	1:38:A:SER:HA	1:91:A:LEU:HD13	16	0.36
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	10	0.36
(2,2424)	1:89:A:GLY:H	1:87:A:SER:HB3	11	0.35
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	5	0.35
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	10	0.35
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	17	0.35
(2,1447)	1:152:A:THR:H	1:149:A:ARG:HD3	15	0.35
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	4	0.35
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	16	0.35
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	18	0.35
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	2	0.35
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	9	0.35
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	13	0.35
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	14	0.35
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	16	0.35
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	11	0.35
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	14	0.35
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	1	0.35
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	7	0.35
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	19	0.35
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	5	0.35
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	9	0.35
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	12	0.35
(2,756)	1:15:A:GLY:HA3	1:21:A:LYS:HB2	5	0.35
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	11	0.35
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	9	0.35
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	2	0.35
(1,32)	1:50:A:GLY:H	1:51:A:SER:HB2	18	0.35
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	15	0.35
(1,11)	1:184:A:SER:HB2	1:185:A:GLN:HG2	17	0.35
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	12	0.34
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	14	0.34
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	18	0.34
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	5	0.34
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	5	0.34
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	13	0.34
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	15	0.34
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	9	0.34
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	7	0.34
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	14	0.34
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	3	0.34
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	12	0.34
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	14	0.34
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	16	0.34
(2,1353)	1:136:A:SER:H	1:136:A:SER:HB2	13	0.34
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	5	0.34
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	8	0.34
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	4	0.34
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	12	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,896)	1:34:A:TYR:HB2	1:91:A:LEU:HB3	7	0.34
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	4	0.34
(2,828)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	17	0.34
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	3	0.34
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	6	0.34
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	8	0.34
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	14	0.34
(2,766)	1:121:A:GLY:HA3	1:122:A:PRO:HG2	16	0.34
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	13	0.34
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	4	0.34
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	7	0.34
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	8	0.34
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	14	0.34
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	1	0.34
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	14	0.34
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	4	0.34
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	6	0.34
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	4	0.34
(2,175)	1:132:A:ARG:HD3	1:128:A:ARG:HB2	18	0.34
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	12	0.34
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	5	0.34
(1,11)	1:184:A:SER:HB2	1:185:A:GLN:HG2	18	0.34
(1,3)	1:9:A:LYS:HE2	1:88:A:LYS:HG2	2	0.34
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	3	0.33
(2,2371)	1:7:A:LYS:H	1:6:A:LYS:HG2	4	0.33
(2,2304)	1:132:A:ARG:H	1:130:A:LEU:HB3	9	0.33
(2,2101)	1:27:A:LYS:H	1:25:A:CYS:HB2	13	0.33
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	7	0.33
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	4	0.33
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	18	0.33
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	13	0.33
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	11	0.33
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	12	0.33
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	2	0.33
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	3	0.33
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	9	0.33
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	10	0.33
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	18	0.33
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	6	0.33
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	11	0.33
(2,926)	1:179:A:VAL:HA	1:178:A:SER:HB2	10	0.33
(2,868)	1:160:A:VAL:HG12	1:163:A:PHE:HB3	16	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	19	0.33
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	2	0.33
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	4	0.33
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	12	0.33
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	10	0.33
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	6	0.33
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	17	0.33
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	7	0.33
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	8	0.33
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	5	0.33
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	11	0.33
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	1	0.33
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	4	0.33
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	7	0.33
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	12	0.33
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	15	0.33
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	16	0.33
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	8	0.33
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	4	0.32
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	8	0.32
(2,2348)	1:2:A:GLU:H	1:2:A:GLU:HB3	15	0.32
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	16	0.32
(2,2248)	1:86:A:THR:H	1:86:A:THR:HG21	9	0.32
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	18	0.32
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	11	0.32
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	17	0.32
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	19	0.32
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	5	0.32
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	8	0.32
(2,1705)	1:3:A:GLU:H	1:4:A:LYS:HD2	4	0.32
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	17	0.32
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	11	0.32
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	1	0.32
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	7	0.32
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	5	0.32
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	1	0.32
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	2	0.32
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	3	0.32
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	4	0.32
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	7	0.32
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	17	0.32
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	20	0.32
(2,1078)	1:147:A:LYS:H	1:147:A:LYS:HG2	20	0.32
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	15	0.32
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	17	0.32
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	16	0.32
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	7	0.32
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	9	0.32
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	17	0.32
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	10	0.32
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	2	0.32
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	7	0.32
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	14	0.32
(2,323)	1:116:A:LEU:HD22	1:116:A:LEU:HB2	3	0.32
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	8	0.32
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	10	0.32
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	1	0.32
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	6	0.32
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	3	0.32
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	1	0.32
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	4	0.32
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	8	0.32
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	20	0.32
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	6	0.31
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	15	0.31
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	1	0.31
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	9	0.31
(2,2371)	1:7:A:LYS:H	1:6:A:LYS:HG2	20	0.31
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	10	0.31
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	6	0.31
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	3	0.31
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	19	0.31
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	11	0.31
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	17	0.31
(2,1177)	1:123:A:GLU:H	1:123:A:GLU:HB2	15	0.31
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	6	0.31
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	12	0.31
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	13	0.31
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	14	0.31
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	17	0.31
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	10	0.31
(2,800)	1:142:A:ASN:HB2	1:146:A:ILE:HD12	8	0.31
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	6	0.31
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	5	0.31
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	11	0.31
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	16	0.31
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	17	0.31
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	4	0.31
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	12	0.31
(2,328)	1:86:A:THR:HA	1:86:A:THR:HG21	9	0.31
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	5	0.31
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	8	0.31
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	1	0.31
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	3	0.31
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	13	0.31
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	17	0.31
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	19	0.31
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	2	0.31
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	9	0.31
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	10	0.31
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	11	0.31
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	15	0.31
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	16	0.31
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	17	0.31
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	3	0.31
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	14	0.31
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	2	0.3
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	2	0.3
(2,2157)	1:16:A:GLY:H	1:119:A:ASP:HB2	18	0.3
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	5	0.3
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	16	0.3
(2,2024)	1:95:A:TYR:H	1:14:A:VAL:HG22	6	0.3
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	6	0.3
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	17	0.3
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	5	0.3
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	11	0.3
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	19	0.3
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	8	0.3
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	2	0.3
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	5	0.3
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	11	0.3
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	19	0.3
(2,779)	1:9:A:LYS:HE2	1:11:A:ILE:HD12	20	0.3
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	8	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	17	0.3
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	15	0.3
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	14	0.3
(2,540)	1:60:A:ILE:HD12	1:56:A:LYS:HD3	14	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	2	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	7	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	9	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	10	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	11	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	12	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	13	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	18	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	19	0.3
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	20	0.3
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	19	0.3
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	5	0.3
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	5	0.3
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	10	0.3
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	9	0.3
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	15	0.3
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	16	0.3
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	20	0.3
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	8	0.3
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	10	0.3
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	14	0.3
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	15	0.3
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	20	0.3
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	4	0.3
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	13	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	2	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	4	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	5	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	8	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	10	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	12	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	14	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	15	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	16	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	18	0.3
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	20	0.3
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	1	0.3
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	20	0.3
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	16	0.29
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	16	0.29
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	6	0.29
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	18	0.29
(2,1774)	1:100:A:GLN:H	1:163:A:PHE:HB3	4	0.29
(2,1774)	1:100:A:GLN:H	1:163:A:PHE:HB3	14	0.29
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	3	0.29
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	9	0.29
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	13	0.29
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	2	0.29
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	19	0.29
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	2	0.29
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	12	0.29
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	20	0.29
(2,1336)	1:149:A:ARG:H	1:149:A:ARG:HD3	19	0.29
(2,1287)	1:163:A:PHE:H	1:163:A:PHE:HB3	20	0.29
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	7	0.29
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	1	0.29
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	2	0.29
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	3	0.29
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	4	0.29
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	6	0.29
(2,821)	1:151:A:GLU:HG2	1:148:A:LYS:HG2	10	0.29
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	14	0.29
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	11	0.29
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	18	0.29
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	5	0.29
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	13	0.29
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	2	0.29
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	13	0.29
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	18	0.29
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	2	0.29
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	13	0.29
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	1	0.29
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	3	0.29
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	5	0.29
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	6	0.29
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	15	0.29
(2,538)	1:169:A:ILE:HD12	1:167:A:ARG:HD2	17	0.29
(2,490)	1:76:A:LEU:HD22	1:39:A:THR:HG21	17	0.29
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	1	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	12	0.29
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	3	0.29
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	18	0.29
(2,392)	1:93:A:ASP:HA	1:91:A:LEU:HD13	20	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	1	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	3	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	5	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	6	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	8	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	9	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	13	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	14	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	19	0.29
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	20	0.29
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	9	0.29
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	6	0.29
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	7	0.29
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	9	0.29
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	7	0.29
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	14	0.29
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	18	0.29
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	19	0.29
(1,3)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	4	0.29
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	3	0.28
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	7	0.28
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	15	0.28
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	4	0.28
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	2	0.28
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	15	0.28
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	17	0.28
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	11	0.28
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	17	0.28
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	2	0.28
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	20	0.28
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	13	0.28
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	1	0.28
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	9	0.28
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	14	0.28
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	8	0.28
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	4	0.28
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	6	0.28
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	9	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1381)	1:30:A:GLN:H	1:27:A:LYS:HB2	17	0.28
(2,1336)	1:149:A:ARG:H	1:149:A:ARG:HD3	2	0.28
(2,1074)	1:143:A:GLU:H	1:143:A:GLU:HB2	20	0.28
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	2	0.28
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	4	0.28
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	8	0.28
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	2	0.28
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	6	0.28
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	10	0.28
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	15	0.28
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	3	0.28
(2,857)	1:31:A:LYS:HG3	1:30:A:GLN:HG2	3	0.28
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	20	0.28
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	1	0.28
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	2	0.28
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	8	0.28
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	1	0.28
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	9	0.28
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	10	0.28
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	3	0.28
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	16	0.28
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	20	0.28
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	7	0.28
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	11	0.28
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	18	0.28
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	16	0.28
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	4	0.28
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	7	0.28
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	16	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	1	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	2	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	3	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	4	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	6	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	7	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	8	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	10	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	12	0.28
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	19	0.28
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	7	0.28
(2,84)	1:83:A:LYS:HA	1:83:A:LYS:HG2	11	0.28
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	16	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:9:A:LYS:HE2	1:88:A:LYS:HG2	12	0.28
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	14	0.27
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	19	0.27
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	12	0.27
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	1	0.27
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	5	0.27
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	11	0.27
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	16	0.27
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	20	0.27
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	16	0.27
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	13	0.27
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	4	0.27
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	13	0.27
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	19	0.27
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	19	0.27
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	11	0.27
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	20	0.27
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	1	0.27
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	7	0.27
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	4	0.27
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	6	0.27
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	7	0.27
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	10	0.27
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	12	0.27
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	13	0.27
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	4	0.27
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	18	0.27
(2,1425)	1:44:A:ARG:H	1:44:A:ARG:HB3	11	0.27
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	3	0.27
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	11	0.27
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	14	0.27
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	18	0.27
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	1	0.27
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	17	0.27
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	12	0.27
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	16	0.27
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	20	0.27
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	2	0.27
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	5	0.27
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	1	0.27
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	6	0.27
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	15	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	17	0.27
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	19	0.27
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD11	5	0.27
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	11	0.27
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	8	0.27
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	17	0.27
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	19	0.27
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	20	0.27
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	8	0.27
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	19	0.27
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	7	0.27
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	2	0.27
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	5	0.27
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	15	0.27
(2,466)	1:190:A:LEU:HG	1:190:A:LEU:HD12	17	0.27
(2,457)	1:189:A:HIS:HB3	1:114:A:LEU:HD12	1	0.27
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	15	0.27
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	19	0.27
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	8	0.27
(2,406)	1:149:A:ARG:HD3	1:146:A:ILE:HA	14	0.27
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	2	0.27
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	19	0.27
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	9	0.27
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	11	0.27
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	13	0.27
(2,250)	1:141:A:ASP:HB3	1:141:A:ASP:HA	17	0.27
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	1	0.27
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	15	0.27
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	15	0.27
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	15	0.26
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	11	0.26
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	17	0.26
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	2	0.26
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	3	0.26
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	7	0.26
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	2	0.26
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	4	0.26
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	6	0.26
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	7	0.26
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	14	0.26
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	18	0.26
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	6	0.26
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	17	0.26
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	19	0.26
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	1	0.26
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	8	0.26
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	9	0.26
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	12	0.26
(2,1967)	1:20:A:GLY:H	1:21:A:LYS:HB2	19	0.26
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	1	0.26
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	6	0.26
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	20	0.26
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	18	0.26
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	7	0.26
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	11	0.26
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	12	0.26
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	15	0.26
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	16	0.26
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	17	0.26
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	5	0.26
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	20	0.26
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	5	0.26
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	5	0.26
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	5	0.26
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	20	0.26
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	11	0.26
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	4	0.26
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	5	0.26
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	6	0.26
(2,1382)	1:70:A:GLU:H	1:70:A:GLU:HB2	8	0.26
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	12	0.26
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	7	0.26
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	1	0.26
(2,1017)	1:171:A:ARG:HD3	1:171:A:ARG:HA	15	0.26
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	3	0.26
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	14	0.26
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	3	0.26
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	9	0.26
(2,903)	1:83:A:LYS:HB3	1:85:A:ASN:HD22	18	0.26
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	9	0.26
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	2	0.26
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	4	0.26
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	7	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	8	0.26
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	11	0.26
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	12	0.26
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	3	0.26
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	3	0.26
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	11	0.26
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	3	0.26
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	4	0.26
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	14	0.26
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	15	0.26
(2,553)	1:154:A:TYR:HE1	1:158:A:GLU:HG2	15	0.26
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	12	0.26
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	16	0.26
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	2	0.26
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	3	0.26
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	8	0.26
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	9	0.26
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	14	0.26
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	9	0.26
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	19	0.26
(2,466)	1:190:A:LEU:HG	1:190:A:LEU:HD12	16	0.26
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	2	0.26
(2,408)	1:44:A:ARG:HD2	1:44:A:ARG:HA	7	0.26
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	10	0.26
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	6	0.26
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	10	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	2	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	4	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	6	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	8	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	12	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	14	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	15	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	16	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	19	0.26
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	20	0.26
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	7	0.26
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	12	0.26
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	18	0.26
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	16	0.26
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	18	0.26
(1,3)	1:9:A:LYS:HE2	1:88:A:LYS:HG2	17	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	20	0.26
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	1	0.26
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	2	0.26
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	4	0.26
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	18	0.26
(2,2401)	1:8:A:THR:H	1:5:A:LEU:HD12	15	0.25
(2,2273)	1:12:A:PHE:H	1:116:A:LEU:HB3	20	0.25
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	20	0.25
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	1	0.25
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	12	0.25
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	3	0.25
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	5	0.25
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	15	0.25
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	15	0.25
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	3	0.25
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	14	0.25
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	9	0.25
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	13	0.25
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	20	0.25
(2,2101)	1:27:A:LYS:H	1:25:A:CYS:HB2	6	0.25
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	3	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	2	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	7	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	8	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	10	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	12	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	14	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	15	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	16	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	19	0.25
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	20	0.25
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	10	0.25
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	4	0.25
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	7	0.25
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	16	0.25
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	4	0.25
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	6	0.25
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	7	0.25
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	8	0.25
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	9	0.25
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	10	0.25
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	11	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	12	0.25
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	8	0.25
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	13	0.25
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	9	0.25
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	14	0.25
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	4	0.25
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	10	0.25
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	11	0.25
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	15	0.25
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	16	0.25
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	17	0.25
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	18	0.25
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	20	0.25
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	1	0.25
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	7	0.25
(2,868)	1:160:A:VAL:HG12	1:163:A:PHE:HB3	14	0.25
(2,842)	1:11:A:ILE:HG12	1:90:A:PHE:HD1	7	0.25
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	13	0.25
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	6	0.25
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	3	0.25
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	5	0.25
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	10	0.25
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	13	0.25
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	18	0.25
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	12	0.25
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	18	0.25
(2,742)	1:120:A:ALA:HA	1:176:A:GLU:HG3	19	0.25
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	5	0.25
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	12	0.25
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	15	0.25
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	18	0.25
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	5	0.25
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	6	0.25
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	16	0.25
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	5	0.25
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	6	0.25
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	18	0.25
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	1	0.25
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	6	0.25
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	12	0.25
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	15	0.25
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	11	0.25
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	18	0.25
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	5	0.25
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	12	0.25
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	3	0.25
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	6	0.25
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	13	0.25
(2,422)	1:41:A:ASP:HB2	1:44:A:ARG:HB2	11	0.25
(2,369)	1:32:A:TYR:HA	1:32:A:TYR:HD1	17	0.25
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	2	0.25
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	9	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	1	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	3	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	5	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	7	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	11	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	13	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	17	0.25
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	18	0.25
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	11	0.25
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	9	0.25
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	11	0.25
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	18	0.25
(2,223)	1:132:A:ARG:HA	1:132:A:ARG:HD2	12	0.25
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	10	0.25
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	16	0.25
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	2	0.25
(1,32)	1:50:A:GLY:H	1:51:A:SER:HB2	12	0.25
(1,3)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	5	0.25
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	9	0.25
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	10	0.25
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	13	0.25
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	17	0.25
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	19	0.25
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	20	0.25
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	3	0.24
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	19	0.24
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	6	0.24
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	11	0.24
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	2	0.24
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	6	0.24
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	9	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	13	0.24
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	15	0.24
(2,2214)	1:189:A:HIS:H	1:190:A:LEU:HG	17	0.24
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	16	0.24
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	1	0.24
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	8	0.24
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	10	0.24
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	17	0.24
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	12	0.24
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	20	0.24
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	1	0.24
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	2	0.24
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	5	0.24
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	10	0.24
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	13	0.24
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	15	0.24
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	2	0.24
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	10	0.24
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	15	0.24
(2,2098)	1:190:A:LEU:H	1:190:A:LEU:HG	16	0.24
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	7	0.24
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	10	0.24
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	14	0.24
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	3	0.24
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	5	0.24
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	9	0.24
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	15	0.24
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	10	0.24
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	2	0.24
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	8	0.24
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	18	0.24
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	4	0.24
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	13	0.24
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	17	0.24
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	20	0.24
(2,1773)	1:144:A:GLU:H	1:142:A:ASN:HB2	8	0.24
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	2	0.24
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	3	0.24
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	14	0.24
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	16	0.24
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	19	0.24
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	17	0.24
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	1	0.24
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	4	0.24
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	7	0.24
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	10	0.24
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	20	0.24
(2,1336)	1:149:A:ARG:H	1:149:A:ARG:HD3	15	0.24
(2,1287)	1:163:A:PHE:H	1:163:A:PHE:HB3	4	0.24
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	7	0.24
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	8	0.24
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	11	0.24
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	14	0.24
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	15	0.24
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	19	0.24
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	17	0.24
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	5	0.24
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	4	0.24
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	7	0.24
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	8	0.24
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	4	0.24
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	8	0.24
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	11	0.24
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	14	0.24
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	15	0.24
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	19	0.24
(2,930)	1:174:A:ASN:HB3	1:176:A:GLU:HB2	5	0.24
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	1	0.24
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	9	0.24
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	14	0.24
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	1	0.24
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	4	0.24
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD11	6	0.24
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	18	0.24
(2,636)	1:124:A:THR:HB	1:125:A:MET:HB3	13	0.24
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	11	0.24
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	12	0.24
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	6	0.24
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	4	0.24
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	10	0.24
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	17	0.24
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	19	0.24
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	4	0.24
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	10	0.24
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	3	0.24
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	4	0.24
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	1	0.24
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	10	0.24
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	14	0.24
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	19	0.24
(2,409)	1:107:A:ARG:HD2	1:106:A:GLU:HG2	14	0.24
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	11	0.24
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	20	0.24
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	13	0.24
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	19	0.24
(2,208)	1:52:A:ALA:HB2	1:52:A:ALA:HA	12	0.24
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	3	0.24
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	11	0.24
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	19	0.24
(1,25)	1:72:A:VAL:HB	1:69:A:LEU:HA	4	0.24
(1,22)	1:38:A:SER:HA	1:91:A:LEU:HD13	4	0.24
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	6	0.24
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	5	0.24
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	6	0.24
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	8	0.24
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	11	0.24
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	12	0.24
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	2	0.23
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	20	0.23
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	6	0.23
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	10	0.23
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	12	0.23
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	13	0.23
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	15	0.23
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	1	0.23
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	12	0.23
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	6	0.23
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	9	0.23
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	12	0.23
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	18	0.23
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	8	0.23
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	3	0.23
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	2	0.23
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	15	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	6	0.23
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	13	0.23
(2,1954)	1:137:A:GLY:H	1:135:A:THR:HG21	18	0.23
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	17	0.23
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	20	0.23
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	12	0.23
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	15	0.23
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	9	0.23
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	11	0.23
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	19	0.23
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	1	0.23
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	4	0.23
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	17	0.23
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	2	0.23
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	7	0.23
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	8	0.23
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	3	0.23
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	20	0.23
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	16	0.23
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	13	0.23
(2,1387)	1:85:A:ASN:H	1:85:A:ASN:HB3	7	0.23
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	16	0.23
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	5	0.23
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	19	0.23
(2,1107)	1:173:A:VAL:H	1:172:A:LYS:HB2	18	0.23
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	19	0.23
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	5	0.23
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	9	0.23
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	6	0.23
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	10	0.23
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	12	0.23
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	17	0.23
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	1	0.23
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	6	0.23
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	9	0.23
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	12	0.23
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	13	0.23
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	5	0.23
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	6	0.23
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	11	0.23
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	12	0.23
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	4	0.23
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	8	0.23
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	12	0.23
(2,804)	1:183:A:PHE:HB3	1:186:A:VAL:HG12	16	0.23
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	19	0.23
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	2	0.23
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	14	0.23
(2,671)	1:164:A:TYR:HA	1:167:A:ARG:HB3	17	0.23
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	16	0.23
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	8	0.23
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	3	0.23
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	4	0.23
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	5	0.23
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	20	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	2	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	3	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	8	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	10	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	12	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	16	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	17	0.23
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	19	0.23
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	17	0.23
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	4	0.23
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	2	0.23
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	8	0.23
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	17	0.23
(2,409)	1:107:A:ARG:HD2	1:106:A:GLU:HG2	2	0.23
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	3	0.23
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	17	0.23
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	3	0.23
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	4	0.23
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	17	0.23
(2,1)	1:85:A:ASN:HA	1:85:A:ASN:HB2	7	0.23
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	6	0.23
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	18	0.23
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	13	0.23
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	3	0.23
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	14	0.23
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	15	0.23
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	16	0.23
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	1	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	8	0.22
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	11	0.22
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	4	0.22
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	5	0.22
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	10	0.22
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	20	0.22
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	1	0.22
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	2	0.22
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	10	0.22
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	16	0.22
(2,2159)	1:54:A:GLY:H	1:55:A:LYS:HB3	9	0.22
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	7	0.22
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	8	0.22
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	12	0.22
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	14	0.22
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	19	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	3	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	8	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	9	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	10	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	12	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	14	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	18	0.22
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	19	0.22
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	4	0.22
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	11	0.22
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	10	0.22
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	4	0.22
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	7	0.22
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	12	0.22
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	17	0.22
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	3	0.22
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	8	0.22
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	7	0.22
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	1	0.22
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	3	0.22
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	1	0.22
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	2	0.22
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	8	0.22
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	16	0.22
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	3	0.22
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	15	0.22
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	6	0.22
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	4	0.22
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	1	0.22
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	10	0.22
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	17	0.22
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	16	0.22
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	7	0.22
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	10	0.22
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	14	0.22
(2,1431)	1:11:A:ILE:H	1:11:A:ILE:HG12	20	0.22
(2,1388)	1:30:A:GLN:H	1:30:A:GLN:HG2	20	0.22
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	1	0.22
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	8	0.22
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	13	0.22
(2,1302)	1:158:A:GLU:H	1:158:A:GLU:HG3	9	0.22
(2,1130)	1:65:A:GLN:H	1:65:A:GLN:HG2	3	0.22
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	16	0.22
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	19	0.22
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	11	0.22
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	5	0.22
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	19	0.22
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	10	0.22
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	15	0.22
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	16	0.22
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	17	0.22
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	18	0.22
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	3	0.22
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	10	0.22
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	13	0.22
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	17	0.22
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	7	0.22
(2,845)	1:44:A:ARG:HG2	1:41:A:ASP:HA	11	0.22
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	12	0.22
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	5	0.22
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	7	0.22
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	10	0.22
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	15	0.22
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	17	0.22
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	3	0.22
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	6	0.22
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	7	0.22
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	12	0.22
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	7	0.22
(2,613)	1:34:A:TYR:HE2	1:32:A:TYR:HD1	8	0.22
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	11	0.22
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	10	0.22
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	15	0.22
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	2	0.22
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	3	0.22
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	5	0.22
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	9	0.22
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	13	0.22
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	15	0.22
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	4	0.22
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	11	0.22
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	13	0.22
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	11	0.22
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	13	0.22
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	18	0.22
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	5	0.22
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	6	0.22
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	7	0.22
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	9	0.22
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	11	0.22
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	13	0.22
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	15	0.22
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	18	0.22
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	4	0.22
(2,462)	1:134:A:GLU:HG3	1:131:A:LYS:HE2	20	0.22
(2,457)	1:189:A:HIS:HB3	1:114:A:LEU:HD12	13	0.22
(2,452)	1:61:A:MET:HG3	1:60:A:ILE:HG13	13	0.22
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	2	0.22
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	5	0.22
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	7	0.22
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	18	0.22
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	20	0.22
(2,373)	1:189:A:HIS:HA	1:114:A:LEU:HD12	20	0.22
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	8	0.22
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	10	0.22
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	15	0.22
(2,273)	1:138:A:ARG:HA	1:138:A:ARG:HD2	17	0.22
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	13	0.22
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	16	0.22
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	7	0.22
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	12	0.22
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	13	0.22
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	2	0.22
(1,1)	1:88:A:LYS:HA	1:88:A:LYS:HB3	7	0.22
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	8	0.21
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	6	0.21
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	15	0.21
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	17	0.21
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	11	0.21
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	17	0.21
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	18	0.21
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	2	0.21
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	9	0.21
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	18	0.21
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	19	0.21
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	4	0.21
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	18	0.21
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	20	0.21
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	8	0.21
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	14	0.21
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	8	0.21
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	14	0.21
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	9	0.21
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	16	0.21
(2,2223)	1:166:A:LYS:H	1:167:A:ARG:HG2	17	0.21
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	16	0.21
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	4	0.21
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	5	0.21
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	9	0.21
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	13	0.21
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	14	0.21
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	19	0.21
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	5	0.21
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	20	0.21
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	19	0.21
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	1	0.21
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	5	0.21
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	11	0.21
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	15	0.21
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	5	0.21
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	6	0.21
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	9	0.21
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	13	0.21
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	14	0.21
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	20	0.21
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	11	0.21
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	1	0.21
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	5	0.21
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	18	0.21
(2,1698)	1:77:A:ARG:H	1:108:A:ARG:HD2	2	0.21
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	17	0.21
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	15	0.21
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	6	0.21
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	9	0.21
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	12	0.21
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	13	0.21
(2,1524)	1:174:A:ASN:H	1:174:A:ASN:HD22	7	0.21
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	20	0.21
(2,1388)	1:30:A:GLN:H	1:30:A:GLN:HG2	8	0.21
(2,1388)	1:30:A:GLN:H	1:30:A:GLN:HG2	17	0.21
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	2	0.21
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	4	0.21
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	5	0.21
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	11	0.21
(2,1336)	1:149:A:ARG:H	1:149:A:ARG:HD3	1	0.21
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	6	0.21
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	12	0.21
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	7	0.21
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	15	0.21
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	16	0.21
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	9	0.21
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	13	0.21
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	18	0.21
(2,978)	1:150:A:LEU:HB2	1:154:A:TYR:HE1	2	0.21
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	14	0.21
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	20	0.21
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	16	0.21
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	1	0.21
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	19	0.21
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	7	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	11	0.21
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	17	0.21
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	6	0.21
(2,815)	1:154:A:TYR:HB3	1:150:A:LEU:HD12	19	0.21
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	6	0.21
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	20	0.21
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	7	0.21
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	1	0.21
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	8	0.21
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	9	0.21
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	1	0.21
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	2	0.21
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	5	0.21
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	7	0.21
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	3	0.21
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	18	0.21
(2,607)	1:34:A:TYR:HE2	1:34:A:TYR:HA	7	0.21
(2,600)	1:117:A:TYR:HE1	1:172:A:LYS:HB2	4	0.21
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	14	0.21
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	1	0.21
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	14	0.21
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	9	0.21
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	20	0.21
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	1	0.21
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	6	0.21
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	1	0.21
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	4	0.21
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	9	0.21
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	12	0.21
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	15	0.21
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	19	0.21
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	5	0.21
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	9	0.21
(2,310)	1:73:A:LEU:HB2	1:73:A:LEU:HG	10	0.21
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	2	0.21
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	4	0.21
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	13	0.21
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	1	0.21
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	7	0.21
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	20	0.21
(2,130)	1:61:A:MET:HA	1:61:A:MET:HG2	11	0.21
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	14	0.21
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	2	0.21
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	5	0.21
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	9	0.21
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	11	0.21
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	2	0.21
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	15	0.21
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	3	0.21
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	7	0.21
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	8	0.21
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	5	0.21
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	15	0.21
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	7	0.21
(1,25)	1:72:A:VAL:HB	1:69:A:LEU:HA	2	0.21
(1,25)	1:72:A:VAL:HB	1:69:A:LEU:HA	9	0.21
(1,25)	1:72:A:VAL:HB	1:69:A:LEU:HA	11	0.21
(1,3)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	7	0.21
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	4	0.2
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	7	0.2
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	8	0.2
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	18	0.2
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	19	0.2
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	5	0.2
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	7	0.2
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	10	0.2
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	11	0.2
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	14	0.2
(2,2214)	1:189:A:HIS:H	1:190:A:LEU:HG	11	0.2
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	19	0.2
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	3	0.2
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	6	0.2
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	17	0.2
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	6	0.2
(2,2118)	1:193:A:LEU:H	1:191:A:ASP:HB2	11	0.2
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	12	0.2
(2,2040)	1:51:A:SER:H	1:52:A:ALA:HB2	13	0.2
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	13	0.2
(2,1973)	1:18:A:GLY:H	1:125:A:MET:HG2	19	0.2
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	3	0.2
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	6	0.2
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	19	0.2
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	6	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	12	0.2
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	2	0.2
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	6	0.2
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	20	0.2
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	12	0.2
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	16	0.2
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	18	0.2
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	8	0.2
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	3	0.2
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	5	0.2
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	6	0.2
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	7	0.2
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	10	0.2
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	18	0.2
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	20	0.2
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	2	0.2
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	11	0.2
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	9	0.2
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	13	0.2
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	18	0.2
(2,1657)	1:28:A:ILE:H	1:30:A:GLN:HG3	14	0.2
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	18	0.2
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	2	0.2
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	8	0.2
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	11	0.2
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	3	0.2
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	6	0.2
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	15	0.2
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	20	0.2
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	11	0.2
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	20	0.2
(2,1287)	1:163:A:PHE:H	1:163:A:PHE:HB3	14	0.2
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	8	0.2
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	20	0.2
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	11	0.2
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	20	0.2
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	2	0.2
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	20	0.2
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	13	0.2
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	8	0.2
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	9	0.2
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	18	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	2	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	5	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	6	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	7	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	9	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	10	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	12	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	14	0.2
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	15	0.2
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	5	0.2
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	5	0.2
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	8	0.2
(2,841)	1:60:A:ILE:HG12	1:56:A:LYS:HA	13	0.2
(2,836)	1:155:A:LYS:HD2	1:154:A:TYR:HB3	9	0.2
(2,836)	1:155:A:LYS:HD2	1:154:A:TYR:HB3	19	0.2
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	3	0.2
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	20	0.2
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	10	0.2
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	14	0.2
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	3	0.2
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	9	0.2
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	8	0.2
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	5	0.2
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	19	0.2
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	3	0.2
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	10	0.2
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	6	0.2
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	10	0.2
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	14	0.2
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	17	0.2
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	20	0.2
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	2	0.2
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	12	0.2
(2,516)	1:179:A:VAL:HG22	1:183:A:PHE:HB3	16	0.2
(2,512)	1:172:A:LYS:HA	1:173:A:VAL:HG12	18	0.2
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	10	0.2
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	13	0.2
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	14	0.2
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	11	0.2
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	8	0.2
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	1	0.2
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	12	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	1	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	3	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	5	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	8	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	9	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	12	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	16	0.2
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	20	0.2
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	7	0.2
(2,223)	1:132:A:ARG:HA	1:132:A:ARG:HD2	3	0.2
(2,223)	1:132:A:ARG:HA	1:132:A:ARG:HD2	15	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	1	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	2	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	8	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	9	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	11	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	13	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	18	0.2
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	19	0.2
(2,212)	1:169:A:ILE:HG22	1:169:A:ILE:HG13	15	0.2
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	18	0.2
(2,82)	1:29:A:VAL:HG12	1:33:A:GLY:HA3	18	0.2
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	1	0.2
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	10	0.2
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	14	0.2
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	20	0.2
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	8	0.2
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	13	0.2
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	18	0.2
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	12	0.2
(2,19)	1:76:A:LEU:HA	1:76:A:LEU:HG	17	0.2
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	2	0.2
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	3	0.2
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	11	0.2
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	14	0.2
(1,11)	1:58:A:SER:HA	1:61:A:MET:HG3	11	0.2
(1,3)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	18	0.2
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	11	0.19
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	7	0.19
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	4	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	7	0.19
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	14	0.19
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	16	0.19
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	19	0.19
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	15	0.19
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	14	0.19
(2,2268)	1:37:A:LEU:H	1:91:A:LEU:HG	18	0.19
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	2	0.19
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	3	0.19
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	10	0.19
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	20	0.19
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	17	0.19
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	11	0.19
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	8	0.19
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	11	0.19
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	4	0.19
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	20	0.19
(2,2133)	1:187:A:CYS:H	1:185:A:GLN:HB3	18	0.19
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	17	0.19
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	11	0.19
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	13	0.19
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	10	0.19
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	20	0.19
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	7	0.19
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	9	0.19
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	8	0.19
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	11	0.19
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	20	0.19
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	1	0.19
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	20	0.19
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	2	0.19
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	11	0.19
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	8	0.19
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	20	0.19
(2,1874)	1:8:A:THR:H	1:7:A:LYS:HB3	4	0.19
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	7	0.19
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	11	0.19
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	10	0.19
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	9	0.19
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	16	0.19
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	10	0.19
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	4	0.19
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	18	0.19
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	13	0.19
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	16	0.19
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	18	0.19
(2,1625)	1:79:A:ALA:H	1:76:A:LEU:HB2	17	0.19
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	1	0.19
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	15	0.19
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	17	0.19
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	1	0.19
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	4	0.19
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	5	0.19
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	8	0.19
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	9	0.19
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	17	0.19
(2,1287)	1:163:A:PHE:H	1:163:A:PHE:HB3	16	0.19
(2,1150)	1:106:A:GLU:H	1:106:A:GLU:HB2	13	0.19
(2,1150)	1:106:A:GLU:H	1:106:A:GLU:HB2	15	0.19
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	2	0.19
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	6	0.19
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	19	0.19
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	12	0.19
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	3	0.19
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	5	0.19
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	20	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	1	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	2	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	3	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	4	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	5	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	6	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	7	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	8	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	10	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	11	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	12	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	13	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	15	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	17	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	19	0.19
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	20	0.19
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	20	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	13	0.19
(2,970)	1:39:A:THR:HG22	1:72:A:VAL:HA	19	0.19
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	4	0.19
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	20	0.19
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	3	0.19
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	8	0.19
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	11	0.19
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	13	0.19
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	17	0.19
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	18	0.19
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	20	0.19
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	17	0.19
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	18	0.19
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	15	0.19
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	9	0.19
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	12	0.19
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	17	0.19
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	18	0.19
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	18	0.19
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	7	0.19
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	12	0.19
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	16	0.19
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	2	0.19
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	4	0.19
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	5	0.19
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	6	0.19
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	17	0.19
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	3	0.19
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	19	0.19
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	8	0.19
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	16	0.19
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	5	0.19
(2,554)	1:154:A:TYR:HE1	1:122:A:PRO:HG2	13	0.19
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	19	0.19
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	7	0.19
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	8	0.19
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	20	0.19
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	18	0.19
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	15	0.19
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	16	0.19
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	1	0.19
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,405)	1:122:A:PRO:HD2	1:121:A:GLY:HA3	19	0.19
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	15	0.19
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	13	0.19
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	16	0.19
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	6	0.19
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	7	0.19
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	14	0.19
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	19	0.19
(2,295)	1:68:A:PRO:HA	1:68:A:PRO:HB2	16	0.19
(2,295)	1:68:A:PRO:HA	1:68:A:PRO:HB2	17	0.19
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	3	0.19
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	13	0.19
(2,231)	1:161:A:ILE:HD12	1:161:A:ILE:HB	3	0.19
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	5	0.19
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	6	0.19
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	10	0.19
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	12	0.19
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	14	0.19
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	15	0.19
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	20	0.19
(2,166)	1:142:A:ASN:HB3	1:142:A:ASN:HA	8	0.19
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	2	0.19
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	17	0.19
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	6	0.19
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	8	0.19
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	12	0.19
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	13	0.19
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	16	0.19
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	14	0.19
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	1	0.19
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	13	0.19
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	16	0.19
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	18	0.19
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	9	0.19
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	12	0.19
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	17	0.19
(1,33)	1:49:A:SER:H	1:47:A:VAL:H	4	0.19
(1,3)	1:6:A:LYS:HE2	1:6:A:LYS:HG2	15	0.19
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	11	0.18
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	1	0.18
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	3	0.18
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	5	0.18
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	16	0.18
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	18	0.18
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	19	0.18
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	5	0.18
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	13	0.18
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	17	0.18
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	8	0.18
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	13	0.18
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	11	0.18
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	13	0.18
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	19	0.18
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	6	0.18
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	12	0.18
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	8	0.18
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	11	0.18
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	13	0.18
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	8	0.18
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	6	0.18
(2,2097)	1:190:A:LEU:H	1:189:A:HIS:HB2	16	0.18
(2,2026)	1:176:A:GLU:H	1:174:A:ASN:HD22	15	0.18
(2,2020)	1:110:A:GLY:H	1:111:A:GLN:HG2	1	0.18
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	10	0.18
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	4	0.18
(2,1951)	1:22:A:GLY:H	1:21:A:LYS:HG2	10	0.18
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	9	0.18
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	4	0.18
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	1	0.18
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	3	0.18
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	15	0.18
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	18	0.18
(2,1917)	1:167:A:ARG:H	1:169:A:ILE:HG22	17	0.18
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	9	0.18
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	20	0.18
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	10	0.18
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	14	0.18
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	1	0.18
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	2	0.18
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	5	0.18
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	10	0.18
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	10	0.18
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	9	0.18
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	14	0.18
(2,1800)	1:61:A:MET:H	1:60:A:ILE:HD12	19	0.18
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	3	0.18
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	5	0.18
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	6	0.18
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	10	0.18
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	17	0.18
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	12	0.18
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	14	0.18
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	16	0.18
(2,1770)	1:144:A:GLU:H	1:145:A:THR:HA	20	0.18
(2,1768)	1:148:A:LYS:H	1:146:A:ILE:HG22	10	0.18
(2,1758)	1:127:A:GLN:H	1:126:A:THR:HA	13	0.18
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	2	0.18
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	5	0.18
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	13	0.18
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	5	0.18
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	12	0.18
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	17	0.18
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	19	0.18
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	5	0.18
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	11	0.18
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	4	0.18
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	11	0.18
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	12	0.18
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	8	0.18
(2,1482)	1:117:A:TYR:H	1:172:A:LYS:HB2	18	0.18
(2,1358)	1:120:A:ALA:H	1:119:A:ASP:H	19	0.18
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	2	0.18
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	15	0.18
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	16	0.18
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	2	0.18
(2,1204)	1:51:A:SER:H	1:51:A:SER:HB2	13	0.18
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	18	0.18
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	7	0.18
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	4	0.18
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	8	0.18
(2,1044)	1:30:A:GLN:HG3	1:30:A:GLN:HA	17	0.18
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	9	0.18
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	9	0.18
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	14	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	16	0.18
(2,1026)	1:139:A:VAL:HA	1:139:A:VAL:HG22	18	0.18
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	7	0.18
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	12	0.18
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	13	0.18
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	6	0.18
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	12	0.18
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	19	0.18
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	11	0.18
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	4	0.18
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	19	0.18
(2,937)	1:6:A:LYS:HG3	1:6:A:LYS:HB3	4	0.18
(2,937)	1:6:A:LYS:HG3	1:6:A:LYS:HB3	5	0.18
(2,937)	1:6:A:LYS:HG3	1:6:A:LYS:HB3	11	0.18
(2,937)	1:6:A:LYS:HG3	1:6:A:LYS:HB3	17	0.18
(2,937)	1:6:A:LYS:HG3	1:6:A:LYS:HB3	20	0.18
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	6	0.18
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	10	0.18
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	16	0.18
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	8	0.18
(2,904)	1:194:A:LYS:HB3	1:192:A:ALA:H	6	0.18
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	15	0.18
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	19	0.18
(2,844)	1:68:A:PRO:HG2	1:43:A:LEU:HD22	7	0.18
(2,841)	1:60:A:ILE:HG12	1:56:A:LYS:HA	4	0.18
(2,836)	1:155:A:LYS:HD2	1:154:A:TYR:HB3	5	0.18
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	4	0.18
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	17	0.18
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	17	0.18
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	14	0.18
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	4	0.18
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	12	0.18
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	13	0.18
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	17	0.18
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	6	0.18
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	9	0.18
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	12	0.18
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	9	0.18
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	4	0.18
(2,541)	1:11:A:ILE:HD12	1:34:A:TYR:HE2	11	0.18
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	1	0.18
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	2	0.18
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	3	0.18
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	6	0.18
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	10	0.18
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	12	0.18
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	15	0.18
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	16	0.18
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	19	0.18
(2,492)	1:170:A:VAL:HG11	1:172:A:LYS:H	4	0.18
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	4	0.18
(2,486)	1:37:A:LEU:HD12	1:90:A:PHE:HB3	8	0.18
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	5	0.18
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	18	0.18
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	6	0.18
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	7	0.18
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	9	0.18
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	3	0.18
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	4	0.18
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	13	0.18
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	15	0.18
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	18	0.18
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	8	0.18
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	10	0.18
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	17	0.18
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	19	0.18
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	14	0.18
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	15	0.18
(2,333)	1:35:A:THR:HB	1:37:A:LEU:HG	16	0.18
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	18	0.18
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	19	0.18
(2,297)	1:44:A:ARG:HG2	1:44:A:ARG:HA	4	0.18
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	2	0.18
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	4	0.18
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	13	0.18
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	6	0.18
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	12	0.18
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	19	0.18
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	3	0.18
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	7	0.18
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	15	0.18
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	19	0.18
(2,54)	1:76:A:LEU:HD12	1:76:A:LEU:HB2	17	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	4	0.18
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	6	0.18
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	10	0.18
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	10	0.18
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	16	0.18
(2,44)	1:30:A:GLN:HB2	1:30:A:GLN:HG2	14	0.18
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	20	0.18
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	6	0.18
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	8	0.18
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	9	0.18
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	14	0.18
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	20	0.18
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	4	0.17
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	7	0.17
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	13	0.17
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	16	0.17
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	1	0.17
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	7	0.17
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	14	0.17
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	1	0.17
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	17	0.17
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	9	0.17
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	11	0.17
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	1	0.17
(2,2278)	1:115:A:LEU:H	1:114:A:LEU:HD12	1	0.17
(2,2268)	1:37:A:LEU:H	1:91:A:LEU:HG	3	0.17
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	4	0.17
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	1	0.17
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	4	0.17
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	8	0.17
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	18	0.17
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	5	0.17
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	11	0.17
(2,2205)	1:26:A:GLU:H	1:29:A:VAL:HG22	13	0.17
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	18	0.17
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	20	0.17
(2,2168)	1:133:A:GLY:H	1:141:A:ASP:HB3	20	0.17
(2,2151)	1:15:A:GLY:H	1:16:A:GLY:H	18	0.17
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	6	0.17
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	7	0.17
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	17	0.17
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	4	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	9	0.17
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	8	0.17
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	2	0.17
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	19	0.17
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	16	0.17
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	1	0.17
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	14	0.17
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	11	0.17
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	9	0.17
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	14	0.17
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	16	0.17
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	4	0.17
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	18	0.17
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	3	0.17
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	6	0.17
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	17	0.17
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	19	0.17
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	14	0.17
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	12	0.17
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	16	0.17
(2,1878)	1:87:A:SER:H	1:90:A:PHE:HD2	19	0.17
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	4	0.17
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	8	0.17
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	15	0.17
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	7	0.17
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	13	0.17
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	14	0.17
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	3	0.17
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	9	0.17
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	11	0.17
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	1	0.17
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	4	0.17
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	12	0.17
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	13	0.17
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	4	0.17
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	6	0.17
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	15	0.17
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	17	0.17
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	18	0.17
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	4	0.17
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	14	0.17
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	18	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	7	0.17
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	8	0.17
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	20	0.17
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	6	0.17
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	5	0.17
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	3	0.17
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	4	0.17
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	19	0.17
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	20	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	1	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	2	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	3	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	5	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	6	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	8	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	9	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	10	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	13	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	14	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	15	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	16	0.17
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	20	0.17
(2,1583)	1:13:A:VAL:H	1:92:A:ILE:HA	19	0.17
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	5	0.17
(2,1511)	1:93:A:ASP:H	1:37:A:LEU:HB2	16	0.17
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	2	0.17
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	10	0.17
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	3	0.17
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	13	0.17
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	16	0.17
(2,1204)	1:51:A:SER:H	1:51:A:SER:HB2	4	0.17
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	15	0.17
(2,1150)	1:106:A:GLU:H	1:106:A:GLU:HB2	14	0.17
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	8	0.17
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	9	0.17
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	17	0.17
(2,1072)	1:143:A:GLU:H	1:143:A:GLU:HG3	13	0.17
(2,1049)	1:26:A:GLU:HB2	1:29:A:VAL:HG21	3	0.17
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	5	0.17
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	17	0.17
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	1	0.17
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	7	0.17
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	8	0.17
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	9	0.17
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	15	0.17
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	16	0.17
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	17	0.17
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	18	0.17
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	10	0.17
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	17	0.17
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	2	0.17
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	5	0.17
(2,943)	1:179:A:VAL:HG12	1:179:A:VAL:HA	16	0.17
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	2	0.17
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	9	0.17
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	11	0.17
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	12	0.17
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	3	0.17
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	12	0.17
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	11	0.17
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	13	0.17
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	20	0.17
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	13	0.17
(2,848)	1:5:A:LEU:HG	1:2:A:GLU:HG2	15	0.17
(2,841)	1:60:A:ILE:HG12	1:56:A:LYS:HA	12	0.17
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	10	0.17
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	13	0.17
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	16	0.17
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	20	0.17
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	10	0.17
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	13	0.17
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	14	0.17
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	15	0.17
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	16	0.17
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	9	0.17
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	17	0.17
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	8	0.17
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	13	0.17
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	15	0.17
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	19	0.17
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	8	0.17
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	18	0.17
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	19	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,661)	1:87:A:SER:HB3	1:88:A:LYS:HE3	16	0.17
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	1	0.17
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	15	0.17
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	19	0.17
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	1	0.17
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	12	0.17
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	13	0.17
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	20	0.17
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	14	0.17
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	2	0.17
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	19	0.17
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	7	0.17
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	17	0.17
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	20	0.17
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	14	0.17
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	1	0.17
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	3	0.17
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	9	0.17
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	1	0.17
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	15	0.17
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	5	0.17
(2,464)	1:11:A:ILE:HG12	1:113:A:THR:HB	20	0.17
(2,462)	1:134:A:GLU:HG3	1:131:A:LYS:HE2	6	0.17
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	12	0.17
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	19	0.17
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	16	0.17
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	2	0.17
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	6	0.17
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	7	0.17
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	8	0.17
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	11	0.17
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	20	0.17
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	9	0.17
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	1	0.17
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	5	0.17
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	9	0.17
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	16	0.17
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	17	0.17
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	18	0.17
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	1	0.17
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	3	0.17
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,307)	1:44:A:ARG:HD2	1:44:A:ARG:HG3	11	0.17
(2,297)	1:44:A:ARG:HG2	1:44:A:ARG:HA	19	0.17
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	14	0.17
(2,231)	1:161:A:ILE:HD12	1:161:A:ILE:HB	11	0.17
(2,218)	1:167:A:ARG:HD2	1:167:A:ARG:HB3	3	0.17
(2,212)	1:169:A:ILE:HG22	1:169:A:ILE:HG13	10	0.17
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	4	0.17
(2,207)	1:169:A:ILE:HA	1:169:A:ILE:HG22	17	0.17
(2,80)	1:186:A:VAL:HG12	1:186:A:VAL:HA	18	0.17
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	12	0.17
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	14	0.17
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	17	0.17
(2,51)	1:6:A:LYS:HG2	1:6:A:LYS:HE3	19	0.17
(2,44)	1:30:A:GLN:HB2	1:30:A:GLN:HG2	17	0.17
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	17	0.17
(1,18)	1:130:A:LEU:HD22	1:129:A:LEU:HB2	17	0.17
(1,18)	1:130:A:LEU:HD22	1:129:A:LEU:HB3	20	0.17
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	9	0.16
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	16	0.16
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	9	0.16
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	13	0.16
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	7	0.16
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	14	0.16
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	9	0.16
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	16	0.16
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	7	0.16
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	15	0.16
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	18	0.16
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	2	0.16
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	3	0.16
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	5	0.16
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	6	0.16
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	18	0.16
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	5	0.16
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	16	0.16
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	17	0.16
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	20	0.16
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	19	0.16
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	2	0.16
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	9	0.16
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	10	0.16
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	15	0.16
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	16	0.16
(2,2193)	1:85:A:ASN:HD22	1:86:A:THR:H	11	0.16
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	17	0.16
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	9	0.16
(2,2160)	1:102:A:GLY:H	1:105:A:PHE:H	9	0.16
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	12	0.16
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	18	0.16
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	3	0.16
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	7	0.16
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	12	0.16
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	16	0.16
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	7	0.16
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	8	0.16
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	9	0.16
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	11	0.16
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	4	0.16
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	5	0.16
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	7	0.16
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	14	0.16
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	2	0.16
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	3	0.16
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	20	0.16
(2,1923)	1:126:A:THR:H	1:124:A:THR:HG21	5	0.16
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	6	0.16
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	7	0.16
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	12	0.16
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	19	0.16
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	13	0.16
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	4	0.16
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	9	0.16
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	4	0.16
(2,1898)	1:25:A:CYS:H	1:28:A:ILE:HD12	17	0.16
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	18	0.16
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	14	0.16
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	5	0.16
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	12	0.16
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	16	0.16
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	17	0.16
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	20	0.16
(2,1869)	1:31:A:LYS:H	1:28:A:ILE:HG22	17	0.16
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1863)	1:136:A:SER:H	1:134:A:GLU:HG2	4	0.16
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	5	0.16
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	8	0.16
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	15	0.16
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	18	0.16
(2,1835)	1:111:A:GLN:H	1:6:A:LYS:HA	9	0.16
(2,1830)	1:34:A:TYR:H	1:90:A:PHE:HA	19	0.16
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	7	0.16
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	20	0.16
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	2	0.16
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	8	0.16
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	14	0.16
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	15	0.16
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	18	0.16
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	7	0.16
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	17	0.16
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	2	0.16
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	15	0.16
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	19	0.16
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	17	0.16
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	8	0.16
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	10	0.16
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	14	0.16
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	16	0.16
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	20	0.16
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	5	0.16
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	2	0.16
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	3	0.16
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	7	0.16
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	16	0.16
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	2	0.16
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	7	0.16
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	19	0.16
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	3	0.16
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	6	0.16
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	14	0.16
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	15	0.16
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	7	0.16
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	17	0.16
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	18	0.16
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	1	0.16
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	6	0.16
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	8	0.16
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	9	0.16
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	12	0.16
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	3	0.16
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	13	0.16
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	1	0.16
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	2	0.16
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	3	0.16
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	1	0.16
(2,1336)	1:149:A:ARG:H	1:149:A:ARG:HD3	3	0.16
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	10	0.16
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	12	0.16
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	14	0.16
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	15	0.16
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	20	0.16
(2,1204)	1:51:A:SER:H	1:51:A:SER:HB2	17	0.16
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	6	0.16
(2,1152)	1:47:A:VAL:H	1:47:A:VAL:HB	18	0.16
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	3	0.16
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	5	0.16
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	14	0.16
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	16	0.16
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	14	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	1	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	2	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	3	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	6	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	7	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	12	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	16	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	18	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	19	0.16
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	20	0.16
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	2	0.16
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	14	0.16
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	4	0.16
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	18	0.16
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	1	0.16
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	1	0.16
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	3	0.16
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	8	0.16
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	19	0.16
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	2	0.16
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	6	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	1	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	3	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	6	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	7	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	8	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	10	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	16	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	18	0.16
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	19	0.16
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	5	0.16
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	10	0.16
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	1	0.16
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	11	0.16
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	13	0.16
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	16	0.16
(2,841)	1:60:A:ILE:HG12	1:56:A:LYS:HA	11	0.16
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	11	0.16
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	12	0.16
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	15	0.16
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	17	0.16
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	1	0.16
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	2	0.16
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	9	0.16
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	16	0.16
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	19	0.16
(2,714)	1:36:A:HIS:HA	1:91:A:LEU:HB2	3	0.16
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	15	0.16
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	9	0.16
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	16	0.16
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	20	0.16
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	14	0.16
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	10	0.16
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	16	0.16
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	20	0.16
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	6	0.16
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	2	0.16
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	5	0.16
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	17	0.16
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	18	0.16
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	4	0.16
(2,515)	1:182:A:VAL:HG22	1:118:A:VAL:HA	19	0.16
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	8	0.16
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	16	0.16
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	17	0.16
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	19	0.16
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	1	0.16
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	7	0.16
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	13	0.16
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	3	0.16
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	14	0.16
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	4	0.16
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	11	0.16
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	3	0.16
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	2	0.16
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	5	0.16
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	6	0.16
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	14	0.16
(2,435)	1:123:A:GLU:HG3	1:124:A:THR:HA	10	0.16
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	5	0.16
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	12	0.16
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	13	0.16
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	14	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	2	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	3	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	6	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	7	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	8	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	10	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	12	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	14	0.16
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	15	0.16
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	1	0.16
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	12	0.16
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	18	0.16
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	19	0.16
(2,362)	1:77:A:ARG:HA	1:1:A:MET:HB3	15	0.16
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	11	0.16
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	20	0.16
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	2	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	6	0.16
(2,306)	1:44:A:ARG:HD2	1:44:A:ARG:HG2	7	0.16
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	15	0.16
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	10	0.16
(2,255)	1:155:A:LYS:HB2	1:155:A:LYS:HD2	12	0.16
(2,231)	1:161:A:ILE:HD12	1:161:A:ILE:HB	15	0.16
(2,212)	1:169:A:ILE:HG22	1:169:A:ILE:HG13	12	0.16
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	12	0.16
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	11	0.16
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	17	0.16
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	5	0.16
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	5	0.16
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	4	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	2	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	3	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	4	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	6	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	11	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	12	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	17	0.16
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	18	0.16
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	4	0.16
(2,11)	1:146:A:ILE:HG22	1:150:A:LEU:HG	10	0.16
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	6	0.16
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	9	0.16
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	16	0.16
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	18	0.16
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	20	0.16
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	9	0.16
(1,21)	1:90:A:PHE:HA	1:91:A:LEU:HD12	3	0.16
(2,2423)	1:175:A:ALA:H	1:19:A:SER:HB2	10	0.15
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	3	0.15
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	6	0.15
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	10	0.15
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	14	0.15
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	8	0.15
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	11	0.15
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	8	0.15
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	13	0.15
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	17	0.15
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	6	0.15
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	19	0.15
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	14	0.15
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	15	0.15
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	12	0.15
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	9	0.15
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	12	0.15
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	16	0.15
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	20	0.15
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	8	0.15
(2,2278)	1:115:A:LEU:H	1:114:A:LEU:HD12	13	0.15
(2,2278)	1:115:A:LEU:H	1:114:A:LEU:HD12	20	0.15
(2,2259)	1:91:A:LEU:H	1:34:A:TYR:HB2	1	0.15
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	7	0.15
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	13	0.15
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	1	0.15
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	8	0.15
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	3	0.15
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	6	0.15
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	14	0.15
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	8	0.15
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	11	0.15
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	14	0.15
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	18	0.15
(2,2154)	1:135:A:THR:H	1:131:A:LYS:HD3	4	0.15
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	17	0.15
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	9	0.15
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	11	0.15
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	16	0.15
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	11	0.15
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	20	0.15
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	2	0.15
(2,2032)	1:93:A:ASP:H	1:12:A:PHE:HA	20	0.15
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	20	0.15
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	8	0.15
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	6	0.15
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	18	0.15
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	5	0.15
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	7	0.15
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	16	0.15
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	19	0.15
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	1	0.15
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	9	0.15
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	4	0.15
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	16	0.15
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	18	0.15
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	3	0.15
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	8	0.15
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	11	0.15
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	14	0.15
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	15	0.15
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	19	0.15
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	13	0.15
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	15	0.15
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	4	0.15
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	15	0.15
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	2	0.15
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	6	0.15
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	18	0.15
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	1	0.15
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	10	0.15
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	16	0.15
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	17	0.15
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	20	0.15
(2,1801)	1:44:A:ARG:H	1:43:A:LEU:HD22	16	0.15
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	19	0.15
(2,1798)	1:61:A:MET:H	1:57:A:LEU:HA	11	0.15
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	7	0.15
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	11	0.15
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	19	0.15
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	3	0.15
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	13	0.15
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	20	0.15
(2,1774)	1:100:A:GLN:H	1:163:A:PHE:HB3	20	0.15
(2,1742)	1:57:A:LEU:H	1:54:A:GLY:HA3	12	0.15
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	9	0.15
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	12	0.15
(2,1721)	1:53:A:ARG:H	1:52:A:ALA:HB2	12	0.15
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	11	0.15
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	1	0.15
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	4	0.15
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	14	0.15
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	20	0.15
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	4	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	10	0.15
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	6	0.15
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	17	0.15
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	9	0.15
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	12	0.15
(2,1631)	1:62:A:GLU:H	1:61:A:MET:HA	19	0.15
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	2	0.15
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	5	0.15
(2,1621)	1:154:A:TYR:H	1:151:A:GLU:HB2	19	0.15
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	3	0.15
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	11	0.15
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	17	0.15
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	3	0.15
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	17	0.15
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	9	0.15
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	7	0.15
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	3	0.15
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	9	0.15
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	14	0.15
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	17	0.15
(2,1473)	1:175:A:ALA:H	1:174:A:ASN:HB2	13	0.15
(2,1471)	1:118:A:VAL:H	1:21:A:LYS:HB2	5	0.15
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	8	0.15
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	9	0.15
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	14	0.15
(2,1417)	1:58:A:SER:H	1:58:A:SER:HB3	2	0.15
(2,1392)	1:79:A:ALA:H	1:81:A:VAL:H	10	0.15
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	13	0.15
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	10	0.15
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	14	0.15
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	15	0.15
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	19	0.15
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	6	0.15
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	8	0.15
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	11	0.15
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	16	0.15
(2,1204)	1:51:A:SER:H	1:51:A:SER:HB2	7	0.15
(2,1204)	1:51:A:SER:H	1:51:A:SER:HB2	8	0.15
(2,1204)	1:51:A:SER:H	1:51:A:SER:HB2	9	0.15
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	19	0.15
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	20	0.15
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1150)	1:106:A:GLU:H	1:106:A:GLU:HB2	19	0.15
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	4	0.15
(2,1115)	1:194:A:LYS:H	1:194:A:LYS:HB3	15	0.15
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	4	0.15
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	20	0.15
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	8	0.15
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	9	0.15
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	10	0.15
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	13	0.15
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	14	0.15
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	16	0.15
(2,1041)	1:138:A:ARG:HG2	1:138:A:ARG:HD2	16	0.15
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	3	0.15
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	8	0.15
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	9	0.15
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	10	0.15
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	1	0.15
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	14	0.15
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	1	0.15
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	4	0.15
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	9	0.15
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	13	0.15
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	20	0.15
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	12	0.15
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	14	0.15
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	20	0.15
(2,930)	1:174:A:ASN:HB3	1:176:A:GLU:HB2	20	0.15
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	14	0.15
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	15	0.15
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	9	0.15
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	2	0.15
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	5	0.15
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	9	0.15
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	12	0.15
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	14	0.15
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	17	0.15
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	14	0.15
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	2	0.15
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	3	0.15
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	7	0.15
(2,848)	1:5:A:LEU:HG	1:2:A:GLU:HG2	14	0.15
(2,848)	1:5:A:LEU:HG	1:2:A:GLU:HG2	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	10	0.15
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	1	0.15
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	17	0.15
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	11	0.15
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	1	0.15
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD11	13	0.15
(2,770)	1:93:A:ASP:HB2	1:91:A:LEU:HD13	16	0.15
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	3	0.15
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	9	0.15
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	5	0.15
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	10	0.15
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	12	0.15
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	14	0.15
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	11	0.15
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	6	0.15
(2,663)	1:87:A:SER:HB3	1:83:A:LYS:HG3	20	0.15
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	12	0.15
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	14	0.15
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	1	0.15
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	17	0.15
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	14	0.15
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	3	0.15
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	9	0.15
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	10	0.15
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	11	0.15
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	12	0.15
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	13	0.15
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	19	0.15
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	17	0.15
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	2	0.15
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	5	0.15
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	12	0.15
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	13	0.15
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	15	0.15
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	5	0.15
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	11	0.15
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	14	0.15
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	18	0.15
(2,492)	1:170:A:VAL:HG11	1:172:A:LYS:H	6	0.15
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	2	0.15
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	6	0.15
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	13	0.15
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	16	0.15
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	18	0.15
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	19	0.15
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	12	0.15
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	12	0.15
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	3	0.15
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	6	0.15
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	7	0.15
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	18	0.15
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	7	0.15
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	8	0.15
(2,422)	1:41:A:ASP:HB2	1:44:A:ARG:HB2	17	0.15
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	4	0.15
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	13	0.15
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	18	0.15
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	16	0.15
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	20	0.15
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	14	0.15
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	20	0.15
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	10	0.15
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	18	0.15
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	7	0.15
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	9	0.15
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	14	0.15
(2,330)	1:173:A:VAL:HG12	1:118:A:VAL:HG22	15	0.15
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	11	0.15
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	13	0.15
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	16	0.15
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	18	0.15
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	8	0.15
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	8	0.15
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	14	0.15
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	17	0.15
(2,231)	1:161:A:ILE:HD12	1:161:A:ILE:HB	4	0.15
(2,212)	1:169:A:ILE:HG22	1:169:A:ILE:HG13	3	0.15
(2,212)	1:169:A:ILE:HG22	1:169:A:ILE:HG13	5	0.15
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	5	0.15
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	13	0.15
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	19	0.15
(2,139)	1:143:A:GLU:HA	1:143:A:GLU:HG3	20	0.15
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	9	0.15
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	12	0.15
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	18	0.15
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	20	0.15
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	20	0.15
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	20	0.15
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	1	0.15
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	19	0.15
(2,44)	1:30:A:GLN:HB2	1:30:A:GLN:HG2	8	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	1	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	5	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	7	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	8	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	9	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	10	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	14	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	15	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	16	0.15
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	19	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	1	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	2	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	3	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	4	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	5	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	7	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	8	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	10	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	12	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	13	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	14	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	17	0.15
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	19	0.15
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	16	0.15
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	15	0.14
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	16	0.14
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	4	0.14
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	6	0.14
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	19	0.14
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	20	0.14
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	17	0.14
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	10	0.14
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	8	0.14
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	5	0.14
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	13	0.14
(2,2311)	1:75:A:MET:H	1:78:A:ASP:HB2	11	0.14
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	14	0.14
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	2	0.14
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	3	0.14
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	4	0.14
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	6	0.14
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	20	0.14
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	5	0.14
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	17	0.14
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	8	0.14
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	9	0.14
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	10	0.14
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	20	0.14
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	17	0.14
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	7	0.14
(2,2221)	1:57:A:LEU:H	1:56:A:LYS:HB3	18	0.14
(2,2215)	1:147:A:LYS:H	1:148:A:LYS:HD2	14	0.14
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	7	0.14
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	3	0.14
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	4	0.14
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	6	0.14
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	12	0.14
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	17	0.14
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	6	0.14
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	11	0.14
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	14	0.14
(2,2142)	1:71:A:THR:H	1:69:A:LEU:H	5	0.14
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	5	0.14
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	18	0.14
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	19	0.14
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	6	0.14
(2,2101)	1:27:A:LYS:H	1:25:A:CYS:HB2	9	0.14
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	4	0.14
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	15	0.14
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	17	0.14
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	20	0.14
(2,2047)	1:118:A:VAL:H	1:175:A:ALA:HB2	19	0.14
(2,2044)	1:16:A:GLY:H	1:21:A:LYS:HA	7	0.14
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	9	0.14
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	13	0.14
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	1	0.14
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	3	0.14
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	4	0.14
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	9	0.14
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	16	0.14
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	19	0.14
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	2	0.14
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	3	0.14
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	12	0.14
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	2	0.14
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	6	0.14
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	17	0.14
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	18	0.14
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	14	0.14
(2,1947)	1:135:A:THR:H	1:134:A:GLU:HG2	4	0.14
(2,1927)	1:108:A:ARG:H	1:108:A:ARG:HD2	8	0.14
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	7	0.14
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	19	0.14
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	8	0.14
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	13	0.14
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	14	0.14
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	16	0.14
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	17	0.14
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	19	0.14
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	11	0.14
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	1	0.14
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	2	0.14
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	5	0.14
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	13	0.14
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	16	0.14
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	17	0.14
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	1	0.14
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	16	0.14
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	5	0.14
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	3	0.14
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	12	0.14
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	14	0.14
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	9	0.14
(2,1878)	1:87:A:SER:H	1:90:A:PHE:HD2	14	0.14
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1845)	1:107:A:ARG:H	1:106:A:GLU:HG3	7	0.14
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	4	0.14
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	12	0.14
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	4	0.14
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	5	0.14
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	16	0.14
(2,1801)	1:44:A:ARG:H	1:43:A:LEU:HD22	10	0.14
(2,1799)	1:61:A:MET:H	1:63:A:LYS:HB3	7	0.14
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	4	0.14
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	5	0.14
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	6	0.14
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	6	0.14
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	8	0.14
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	17	0.14
(2,1779)	1:155:A:LYS:H	1:155:A:LYS:HB3	10	0.14
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	15	0.14
(2,1716)	1:5:A:LEU:H	1:6:A:LYS:HE3	4	0.14
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	8	0.14
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	10	0.14
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	6	0.14
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	8	0.14
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	11	0.14
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	20	0.14
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	18	0.14
(2,1636)	1:72:A:VAL:H	1:75:A:MET:HB2	2	0.14
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	14	0.14
(2,1545)	1:192:A:ALA:H	1:194:A:LYS:HE2	16	0.14
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	18	0.14
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	18	0.14
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	9	0.14
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	14	0.14
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	18	0.14
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	6	0.14
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	16	0.14
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	7	0.14
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	12	0.14
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	18	0.14
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	19	0.14
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	5	0.14
(2,1417)	1:58:A:SER:H	1:58:A:SER:HB3	18	0.14
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	5	0.14
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	7	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	1	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	2	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	3	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	10	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	12	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	13	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	15	0.14
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	18	0.14
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	4	0.14
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	12	0.14
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	4	0.14
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	7	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	1	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	2	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	3	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	4	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	5	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	6	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	7	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	8	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	9	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	10	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	11	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	12	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	13	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	14	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	15	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	16	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	17	0.14
(2,1178)	1:179:A:VAL:H	1:179:A:VAL:HB	18	0.14
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	1	0.14
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	13	0.14
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	18	0.14
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	19	0.14
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	1	0.14
(2,1095)	1:174:A:ASN:H	1:174:A:ASN:HB2	12	0.14
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	5	0.14
(2,1045)	1:84:A:VAL:HA	1:84:A:VAL:HG22	15	0.14
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	3	0.14
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	15	0.14
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	15	0.14
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	19	0.14
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	17	0.14
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	18	0.14
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	2	0.14
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	5	0.14
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	10	0.14
(2,1000)	1:28:A:ILE:HB	1:28:A:ILE:HG22	11	0.14
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	10	0.14
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	19	0.14
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	16	0.14
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	2	0.14
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	3	0.14
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	5	0.14
(2,946)	1:138:A:ARG:HG3	1:138:A:ARG:HA	17	0.14
(2,930)	1:174:A:ASN:HB3	1:176:A:GLU:HB2	19	0.14
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	13	0.14
(2,908)	1:81:A:VAL:HG22	1:81:A:VAL:HB	4	0.14
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	1	0.14
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	14	0.14
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	18	0.14
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	20	0.14
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	14	0.14
(2,848)	1:5:A:LEU:HG	1:2:A:GLU:HG2	12	0.14
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	18	0.14
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	12	0.14
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	20	0.14
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	6	0.14
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	7	0.14
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	15	0.14
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	4	0.14
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	7	0.14
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	15	0.14
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	5	0.14
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	1	0.14
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	2	0.14
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	16	0.14
(2,758)	1:137:A:GLY:HA3	1:138:A:ARG:HG2	19	0.14
(2,755)	1:15:A:GLY:HA3	1:21:A:LYS:HE2	5	0.14
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	2	0.14
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	13	0.14
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	4	0.14
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	13	0.14
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	6	0.14
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	11	0.14
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	17	0.14
(2,714)	1:36:A:HIS:HA	1:91:A:LEU:HB2	18	0.14
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	18	0.14
(2,625)	1:164:A:TYR:HE1	1:112:A:PRO:HB3	15	0.14
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	7	0.14
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	17	0.14
(2,594)	1:180:A:ASP:HB3	1:183:A:PHE:HD1	12	0.14
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	17	0.14
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	18	0.14
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	7	0.14
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	9	0.14
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	15	0.14
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	16	0.14
(2,528)	1:192:A:ALA:HB2	1:188:A:THR:HG21	20	0.14
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	5	0.14
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	15	0.14
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	5	0.14
(2,517)	1:179:A:VAL:HG22	1:180:A:ASP:HB2	20	0.14
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	9	0.14
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	18	0.14
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	4	0.14
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	8	0.14
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	11	0.14
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	12	0.14
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	20	0.14
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	2	0.14
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	7	0.14
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	20	0.14
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	3	0.14
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	8	0.14
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	12	0.14
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	9	0.14
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	10	0.14
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	7	0.14
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	19	0.14
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	3	0.14
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	5	0.14
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	11	0.14
(2,388)	1:114:A:LEU:HA	1:113:A:THR:HB	20	0.14
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	15	0.14
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	2	0.14
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	7	0.14
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	9	0.14
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	10	0.14
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	11	0.14
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	15	0.14
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	16	0.14
(2,350)	1:84:A:VAL:HA	1:87:A:SER:HB2	11	0.14
(2,329)	1:179:A:VAL:HG22	1:180:A:ASP:HB3	20	0.14
(2,319)	1:66:A:LEU:HD21	1:66:A:LEU:HA	18	0.14
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	10	0.14
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	18	0.14
(2,297)	1:44:A:ARG:HG2	1:44:A:ARG:HA	10	0.14
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	20	0.14
(2,231)	1:161:A:ILE:HD12	1:161:A:ILE:HB	2	0.14
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	7	0.14
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	18	0.14
(2,192)	1:65:A:GLN:HG2	1:65:A:GLN:HA	7	0.14
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	3	0.14
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	12	0.14
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	20	0.14
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	7	0.14
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	16	0.14
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	2	0.14
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	8	0.14
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	10	0.14
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	12	0.14
(2,81)	1:57:A:LEU:HD22	1:43:A:LEU:HB3	11	0.14
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	11	0.14
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	16	0.14
(2,38)	1:144:A:GLU:HB2	1:144:A:GLU:HA	13	0.14
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	15	0.14
(2,9)	1:84:A:VAL:HG22	1:84:A:VAL:HB	15	0.14
(1,22)	1:38:A:SER:HA	1:91:A:LEU:HD13	5	0.14
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	7	0.13
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	18	0.13
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	5	0.13
(2,2417)	1:121:A:GLY:H	1:124:A:THR:HB	10	0.13
(2,2402)	1:45:A:SER:H	1:44:A:ARG:HB2	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2388)	1:131:A:LYS:H	1:130:A:LEU:HB3	13	0.13
(2,2385)	1:170:A:VAL:H	1:164:A:TYR:HA	20	0.13
(2,2381)	1:177:A:GLY:H	1:177:A:GLY:HA3	7	0.13
(2,2381)	1:177:A:GLY:H	1:177:A:GLY:HA3	19	0.13
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	7	0.13
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	9	0.13
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	11	0.13
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	18	0.13
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	20	0.13
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	4	0.13
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	18	0.13
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	7	0.13
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	9	0.13
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	11	0.13
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	12	0.13
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	15	0.13
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	18	0.13
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	19	0.13
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	9	0.13
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	14	0.13
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	20	0.13
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	3	0.13
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	6	0.13
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	8	0.13
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	11	0.13
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	2	0.13
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	13	0.13
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	17	0.13
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	19	0.13
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	5	0.13
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	11	0.13
(2,2256)	1:7:A:LYS:H	1:3:A:GLU:HA	17	0.13
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	4	0.13
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	10	0.13
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	14	0.13
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	4	0.13
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	8	0.13
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	14	0.13
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	19	0.13
(2,2154)	1:135:A:THR:H	1:131:A:LYS:HD3	14	0.13
(2,2153)	1:15:A:GLY:H	1:94:A:GLY:H	6	0.13
(2,2150)	1:15:A:GLY:H	1:93:A:ASP:HA	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	1	0.13
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	9	0.13
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	20	0.13
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	1	0.13
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	8	0.13
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	16	0.13
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	1	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	1	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	2	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	5	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	9	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	10	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	11	0.13
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	19	0.13
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	9	0.13
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	3	0.13
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	6	0.13
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	10	0.13
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	12	0.13
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	20	0.13
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	10	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	1	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	2	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	10	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	12	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	18	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	19	0.13
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	20	0.13
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	4	0.13
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	5	0.13
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	10	0.13
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	11	0.13
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	14	0.13
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	16	0.13
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	17	0.13
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	15	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	2	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	5	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	7	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	8	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	10	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	13	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	14	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	15	0.13
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	20	0.13
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	1	0.13
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	6	0.13
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	8	0.13
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	10	0.13
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	15	0.13
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	11	0.13
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	11	0.13
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	18	0.13
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	11	0.13
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	2	0.13
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	5	0.13
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	5	0.13
(2,1922)	1:126:A:THR:H	1:125:A:MET:HB3	9	0.13
(2,1907)	1:184:A:SER:H	1:185:A:GLN:HG2	10	0.13
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	9	0.13
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	10	0.13
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	15	0.13
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	14	0.13
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	2	0.13
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	8	0.13
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	9	0.13
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	13	0.13
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	16	0.13
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	2	0.13
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	3	0.13
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	8	0.13
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	19	0.13
(2,1882)	1:87:A:SER:H	1:83:A:LYS:HG2	6	0.13
(2,1878)	1:87:A:SER:H	1:90:A:PHE:HD2	10	0.13
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	1	0.13
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	13	0.13
(2,1869)	1:31:A:LYS:H	1:28:A:ILE:HG22	8	0.13
(2,1845)	1:107:A:ARG:H	1:106:A:GLU:HG3	11	0.13
(2,1843)	1:111:A:GLN:H	1:106:A:GLU:HG2	17	0.13
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	2	0.13
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	6	0.13
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	9	0.13
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	19	0.13
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	6	0.13
(2,1801)	1:44:A:ARG:H	1:43:A:LEU:HD22	4	0.13
(2,1801)	1:44:A:ARG:H	1:43:A:LEU:HD22	20	0.13
(2,1792)	1:142:A:ASN:H	1:146:A:ILE:HA	13	0.13
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	10	0.13
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	16	0.13
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	1	0.13
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	10	0.13
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	12	0.13
(2,1779)	1:155:A:LYS:H	1:155:A:LYS:HB3	12	0.13
(2,1779)	1:155:A:LYS:H	1:155:A:LYS:HB3	14	0.13
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	6	0.13
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	18	0.13
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	5	0.13
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	17	0.13
(2,1708)	1:143:A:GLU:H	1:130:A:LEU:HD12	2	0.13
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	2	0.13
(2,1678)	1:141:A:ASP:H	1:138:A:ARG:HB2	17	0.13
(2,1678)	1:141:A:ASP:H	1:138:A:ARG:HB2	18	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	1	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	2	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	3	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	7	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	9	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	13	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	14	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	15	0.13
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	16	0.13
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	11	0.13
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	13	0.13
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	10	0.13
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	16	0.13
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	4	0.13
(2,1558)	1:188:A:THR:H	1:189:A:HIS:HB2	6	0.13
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	13	0.13
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	20	0.13
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	3	0.13
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	10	0.13
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	12	0.13
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	15	0.13
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	19	0.13
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	15	0.13
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	4	0.13
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	6	0.13
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	11	0.13
(2,1417)	1:58:A:SER:H	1:58:A:SER:HB3	20	0.13
(2,1392)	1:79:A:ALA:H	1:81:A:VAL:H	16	0.13
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	3	0.13
(2,1307)	1:9:A:LYS:H	1:9:A:LYS:HD3	13	0.13
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	18	0.13
(2,1297)	1:9:A:LYS:H	1:90:A:PHE:HD2	19	0.13
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	7	0.13
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	17	0.13
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	19	0.13
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	13	0.13
(2,1227)	1:48:A:SER:H	1:48:A:SER:HB3	20	0.13
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	4	0.13
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	9	0.13
(2,1096)	1:174:A:ASN:H	1:174:A:ASN:HB3	10	0.13
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	9	0.13
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	10	0.13
(2,1077)	1:132:A:ARG:H	1:131:A:LYS:HB2	15	0.13
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	9	0.13
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	10	0.13
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	13	0.13
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	10	0.13
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	14	0.13
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	10	0.13
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	12	0.13
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	13	0.13
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	14	0.13
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	18	0.13
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	3	0.13
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	8	0.13
(2,989)	1:11:A:ILE:HB	1:11:A:ILE:HG22	13	0.13
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	20	0.13
(2,979)	1:34:A:TYR:HD1	1:88:A:LYS:HE3	2	0.13
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	8	0.13
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	5	0.13
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	20	0.13
(2,946)	1:138:A:ARG:HG3	1:138:A:ARG:HA	5	0.13
(2,932)	1:5:A:LEU:HA	1:7:A:LYS:HB3	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,930)	1:174:A:ASN:HB3	1:176:A:GLU:HB2	8	0.13
(2,921)	1:72:A:VAL:HA	1:73:A:LEU:HG	15	0.13
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	2	0.13
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	6	0.13
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	9	0.13
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	12	0.13
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	4	0.13
(2,848)	1:5:A:LEU:HG	1:2:A:GLU:HG2	10	0.13
(2,841)	1:60:A:ILE:HG12	1:56:A:LYS:HA	1	0.13
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	14	0.13
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	4	0.13
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	10	0.13
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	19	0.13
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	11	0.13
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	18	0.13
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	5	0.13
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	6	0.13
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	8	0.13
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	18	0.13
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	19	0.13
(2,748)	1:122:A:PRO:HD2	1:120:A:ALA:HA	19	0.13
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	1	0.13
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	3	0.13
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	7	0.13
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	12	0.13
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	3	0.13
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	4	0.13
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	6	0.13
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	6	0.13
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	2	0.13
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	20	0.13
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	10	0.13
(2,609)	1:34:A:TYR:HE2	1:88:A:LYS:HB2	13	0.13
(2,602)	1:154:A:TYR:HE1	1:122:A:PRO:HD2	19	0.13
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	3	0.13
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	10	0.13
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	14	0.13
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	16	0.13
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	7	0.13
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	15	0.13
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	17	0.13
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	9	0.13
(2,530)	1:60:A:ILE:HG22	1:66:A:LEU:HA	15	0.13
(2,528)	1:192:A:ALA:HB2	1:188:A:THR:HG21	7	0.13
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	4	0.13
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	8	0.13
(2,517)	1:179:A:VAL:HG22	1:180:A:ASP:HB2	11	0.13
(2,517)	1:179:A:VAL:HG22	1:180:A:ASP:HB2	18	0.13
(2,515)	1:182:A:VAL:HG22	1:118:A:VAL:HA	13	0.13
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	4	0.13
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	5	0.13
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	10	0.13
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	2	0.13
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	8	0.13
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	10	0.13
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	20	0.13
(2,462)	1:134:A:GLU:HG3	1:131:A:LYS:HE2	16	0.13
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	2	0.13
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	4	0.13
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	7	0.13
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	9	0.13
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	14	0.13
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	16	0.13
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	4	0.13
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	15	0.13
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	16	0.13
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	20	0.13
(2,444)	1:83:A:LYS:HB3	1:84:A:VAL:HA	11	0.13
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	6	0.13
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	12	0.13
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	8	0.13
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	20	0.13
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	8	0.13
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	12	0.13
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	17	0.13
(2,376)	1:176:A:GLU:HA	1:124:A:THR:HG21	19	0.13
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	1	0.13
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	3	0.13
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	8	0.13
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	16	0.13
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	4	0.13
(2,361)	1:125:A:MET:HA	1:125:A:MET:HG2	19	0.13
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	14	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,302)	1:2:A:GLU:HA	1:2:A:GLU:HG2	4	0.13
(2,297)	1:44:A:ARG:HG2	1:44:A:ARG:HA	8	0.13
(2,295)	1:68:A:PRO:HA	1:68:A:PRO:HB2	11	0.13
(2,292)	1:72:A:VAL:HB	1:72:A:VAL:HG22	7	0.13
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	10	0.13
(2,285)	1:109:A:ILE:HD12	1:109:A:ILE:HB	11	0.13
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	17	0.13
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	17	0.13
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	6	0.13
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	17	0.13
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	1	0.13
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	8	0.13
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	10	0.13
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	14	0.13
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	11	0.13
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	15	0.13
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	20	0.13
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	8	0.13
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	13	0.13
(2,165)	1:112:A:PRO:HA	1:10:A:ILE:HG22	9	0.13
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	4	0.13
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	6	0.13
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	11	0.13
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	13	0.13
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	4	0.13
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	14	0.13
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	15	0.13
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	17	0.13
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	18	0.13
(2,44)	1:30:A:GLN:HB2	1:30:A:GLN:HG2	20	0.13
(2,26)	1:194:A:LYS:HB2	1:194:A:LYS:HA	4	0.13
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	15	0.13
(1,8)	1:47:A:VAL:HG21	1:47:A:VAL:HA	5	0.13
(1,8)	1:47:A:VAL:HG21	1:47:A:VAL:HA	14	0.13
(2,2419)	1:56:A:LYS:H	1:56:A:LYS:HB3	14	0.12
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	1	0.12
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	2	0.12
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	20	0.12
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	5	0.12
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	10	0.12
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	15	0.12
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	8	0.12
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	10	0.12
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	5	0.12
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	9	0.12
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	11	0.12
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	1	0.12
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	2	0.12
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	5	0.12
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	13	0.12
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	3	0.12
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	5	0.12
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	10	0.12
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	18	0.12
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	1	0.12
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	7	0.12
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	8	0.12
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	3	0.12
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	9	0.12
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	18	0.12
(2,2300)	1:176:A:GLU:H	1:175:A:ALA:HB2	14	0.12
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	4	0.12
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	6	0.12
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	10	0.12
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	12	0.12
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	19	0.12
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	3	0.12
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	6	0.12
(2,2290)	1:72:A:VAL:H	1:70:A:GLU:HG2	7	0.12
(2,2270)	1:120:A:ALA:H	1:125:A:MET:HG2	10	0.12
(2,2264)	1:175:A:ALA:H	1:176:A:GLU:HB2	18	0.12
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	13	0.12
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	15	0.12
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	16	0.12
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	5	0.12
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	10	0.12
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	9	0.12
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	19	0.12
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	5	0.12
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	7	0.12
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	13	0.12
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	18	0.12
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	5	0.12
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	7	0.12
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	16	0.12
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	18	0.12
(2,2142)	1:71:A:THR:H	1:69:A:LEU:H	16	0.12
(2,2142)	1:71:A:THR:H	1:69:A:LEU:H	19	0.12
(2,2139)	1:45:A:SER:H	1:48:A:SER:H	16	0.12
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	1	0.12
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	3	0.12
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	8	0.12
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	14	0.12
(2,2116)	1:78:A:ASP:H	1:109:A:ILE:HG22	10	0.12
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	2	0.12
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	20	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	3	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	4	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	6	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	7	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	8	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	12	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	13	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	14	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	15	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	16	0.12
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	20	0.12
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	8	0.12
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	12	0.12
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	20	0.12
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	11	0.12
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	16	0.12
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	18	0.12
(2,2020)	1:110:A:GLY:H	1:111:A:GLN:HG2	5	0.12
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	4	0.12
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	13	0.12
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	19	0.12
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	4	0.12
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	5	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	1	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	2	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	3	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	6	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	9	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	12	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	18	0.12
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	20	0.12
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	2	0.12
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	4	0.12
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	13	0.12
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	18	0.12
(2,1994)	1:86:A:THR:H	1:84:A:VAL:H	17	0.12
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	9	0.12
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	3	0.12
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	12	0.12
(2,1984)	1:177:A:GLY:H	1:120:A:ALA:HA	15	0.12
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	2	0.12
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	9	0.12
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	15	0.12
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	19	0.12
(2,1967)	1:20:A:GLY:H	1:21:A:LYS:HB2	15	0.12
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	11	0.12
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	20	0.12
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	5	0.12
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	8	0.12
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	13	0.12
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	15	0.12
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	20	0.12
(2,1933)	1:58:A:SER:H	1:57:A:LEU:HD22	12	0.12
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	4	0.12
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	15	0.12
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	20	0.12
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	6	0.12
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	18	0.12
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	1	0.12
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	5	0.12
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	17	0.12
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	1	0.12
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	6	0.12
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	18	0.12
(2,1878)	1:87:A:SER:H	1:90:A:PHE:HD2	11	0.12
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	10	0.12
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	14	0.12
(2,1845)	1:107:A:ARG:H	1:106:A:GLU:HG3	16	0.12
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	8	0.12
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	18	0.12
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	11	0.12
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	18	0.12
(2,1746)	1:156:A:ALA:H	1:155:A:LYS:HB2	8	0.12
(2,1746)	1:156:A:ALA:H	1:155:A:LYS:HB2	20	0.12
(2,1736)	1:81:A:VAL:H	1:5:A:LEU:HD22	3	0.12
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	1	0.12
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	3	0.12
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	4	0.12
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	9	0.12
(2,1733)	1:4:A:LYS:H	1:4:A:LYS:HG2	19	0.12
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	1	0.12
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	4	0.12
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	6	0.12
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	7	0.12
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	13	0.12
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	18	0.12
(2,1708)	1:143:A:GLU:H	1:130:A:LEU:HD12	1	0.12
(2,1700)	1:77:A:ARG:H	1:74:A:ASP:HB2	15	0.12
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	1	0.12
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	5	0.12
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	6	0.12
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	9	0.12
(2,1672)	1:39:A:THR:H	1:93:A:ASP:HA	4	0.12
(2,1669)	1:21:A:LYS:H	1:19:A:SER:HB2	7	0.12
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	19	0.12
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	1	0.12
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	12	0.12
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	10	0.12
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	15	0.12
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	18	0.12
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	8	0.12
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	13	0.12
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	17	0.12
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	20	0.12
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	15	0.12
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	11	0.12
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	14	0.12
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	4	0.12
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	7	0.12
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	4	0.12
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	11	0.12
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	15	0.12
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	16	0.12
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	8	0.12
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	5	0.12
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	8	0.12
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	12	0.12
(2,1473)	1:175:A:ALA:H	1:174:A:ASN:HB2	7	0.12
(2,1473)	1:175:A:ALA:H	1:174:A:ASN:HB2	15	0.12
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	8	0.12
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	17	0.12
(2,1424)	1:44:A:ARG:H	1:44:A:ARG:HD3	18	0.12
(2,1392)	1:79:A:ALA:H	1:81:A:VAL:H	19	0.12
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	11	0.12
(2,1337)	1:62:A:GLU:H	1:62:A:GLU:HG3	13	0.12
(2,1242)	1:121:A:GLY:H	1:120:A:ALA:H	18	0.12
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	4	0.12
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	5	0.12
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	9	0.12
(2,1240)	1:182:A:VAL:H	1:182:A:VAL:HB	14	0.12
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	1	0.12
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	2	0.12
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	17	0.12
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	14	0.12
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	7	0.12
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	2	0.12
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	7	0.12
(2,1153)	1:4:A:LYS:H	1:4:A:LYS:HB2	8	0.12
(2,1152)	1:47:A:VAL:H	1:47:A:VAL:HB	8	0.12
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	20	0.12
(2,1047)	1:9:A:LYS:HD2	1:88:A:LYS:HB2	15	0.12
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	9	0.12
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	13	0.12
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	11	0.12
(2,1030)	1:124:A:THR:HB	1:127:A:GLN:HG3	20	0.12
(2,1018)	1:171:A:ARG:HA	1:114:A:LEU:HD12	20	0.12
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	4	0.12
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	2	0.12
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	4	0.12
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	5	0.12
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	14	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	20	0.12
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	15	0.12
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	7	0.12
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	16	0.12
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	18	0.12
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	4	0.12
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	6	0.12
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	4	0.12
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	11	0.12
(2,951)	1:11:A:ILE:HD12	1:193:A:LEU:HB2	7	0.12
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	4	0.12
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	12	0.12
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	13	0.12
(2,916)	1:34:A:TYR:HE2	1:32:A:TYR:HB2	8	0.12
(2,916)	1:34:A:TYR:HE2	1:32:A:TYR:HB2	12	0.12
(2,912)	1:73:A:LEU:HG	1:105:A:PHE:H	2	0.12
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	11	0.12
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	3	0.12
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	6	0.12
(2,889)	1:109:A:ILE:HD12	1:108:A:ARG:HD2	12	0.12
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	2	0.12
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	4	0.12
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	6	0.12
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	7	0.12
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	8	0.12
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	15	0.12
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	16	0.12
(2,869)	1:160:A:VAL:HG12	1:157:A:THR:HA	20	0.12
(2,861)	1:76:A:LEU:HD12	1:76:A:LEU:H	17	0.12
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	10	0.12
(2,848)	1:5:A:LEU:HG	1:2:A:GLU:HG2	16	0.12
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	11	0.12
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	15	0.12
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	16	0.12
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	11	0.12
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	11	0.12
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	20	0.12
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	5	0.12
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	12	0.12
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	16	0.12
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	18	0.12
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	17	0.12
(2,607)	1:34:A:TYR:HE2	1:34:A:TYR:HA	8	0.12
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	7	0.12
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	11	0.12
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	13	0.12
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	18	0.12
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	20	0.12
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	13	0.12
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	4	0.12
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	6	0.12
(2,546)	1:109:A:ILE:HD12	1:77:A:ARG:HA	18	0.12
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	15	0.12
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	3	0.12
(2,530)	1:60:A:ILE:HG22	1:66:A:LEU:HA	10	0.12
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	1	0.12
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	2	0.12
(2,527)	1:79:A:ALA:HB2	1:37:A:LEU:HB2	20	0.12
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	19	0.12
(2,517)	1:179:A:VAL:HG22	1:180:A:ASP:HB2	13	0.12
(2,517)	1:179:A:VAL:HG22	1:180:A:ASP:HB2	16	0.12
(2,515)	1:182:A:VAL:HG22	1:118:A:VAL:HA	8	0.12
(2,515)	1:182:A:VAL:HG22	1:118:A:VAL:HA	10	0.12
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	1	0.12
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	12	0.12
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	6	0.12
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	11	0.12
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	14	0.12
(2,506)	1:118:A:VAL:HG12	1:21:A:LYS:HA	20	0.12
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	10	0.12
(2,495)	1:170:A:VAL:HA	1:170:A:VAL:HG12	17	0.12
(2,492)	1:170:A:VAL:HG11	1:172:A:LYS:H	11	0.12
(2,489)	1:76:A:LEU:HD22	1:76:A:LEU:HB2	7	0.12
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	15	0.12
(2,465)	1:167:A:ARG:HG2	1:164:A:TYR:HA	17	0.12
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	5	0.12
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	13	0.12
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	20	0.12
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	13	0.12
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	17	0.12
(2,446)	1:75:A:MET:HB3	1:78:A:ASP:HB2	18	0.12
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	3	0.12
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	18	0.12
(2,433)	1:106:A:GLU:HG3	1:111:A:GLN:HA	6	0.12
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	9	0.12
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	14	0.12
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	19	0.12
(2,422)	1:41:A:ASP:HB2	1:44:A:ARG:HB2	1	0.12
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	13	0.12
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	6	0.12
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	10	0.12
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	17	0.12
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	18	0.12
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	19	0.12
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	3	0.12
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	7	0.12
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	10	0.12
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	11	0.12
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	18	0.12
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	6	0.12
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	16	0.12
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	3	0.12
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	7	0.12
(2,354)	1:153:A:TYR:HA	1:153:A:TYR:HD1	20	0.12
(2,319)	1:66:A:LEU:HD23	1:66:A:LEU:HA	2	0.12
(2,305)	1:149:A:ARG:HD3	1:149:A:ARG:HB3	10	0.12
(2,302)	1:2:A:GLU:HA	1:2:A:GLU:HG2	17	0.12
(2,295)	1:68:A:PRO:HA	1:68:A:PRO:HB2	10	0.12
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	18	0.12
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	20	0.12
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	6	0.12
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	7	0.12
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	12	0.12
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	14	0.12
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	16	0.12
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	4	0.12
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	8	0.12
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	10	0.12
(2,189)	1:21:A:LYS:HB2	1:21:A:LYS:HA	13	0.12
(2,187)	1:27:A:LYS:HA	1:30:A:GLN:HG3	20	0.12
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	12	0.12
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	16	0.12
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	17	0.12
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	5	0.12
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	12	0.12
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	1	0.12
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	14	0.12
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	17	0.12
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	19	0.12
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	6	0.12
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	7	0.12
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	9	0.12
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	11	0.12
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	13	0.12
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	16	0.12
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	15	0.12
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	5	0.12
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	9	0.12
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	17	0.12
(2,87)	1:171:A:ARG:HA	1:117:A:TYR:HB2	9	0.12
(2,78)	1:150:A:LEU:HD22	1:150:A:LEU:HA	19	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	1	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	2	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	5	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	7	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	8	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	9	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	13	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	14	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	16	0.12
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	19	0.12
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	10	0.12
(2,7)	1:79:A:ALA:HA	1:79:A:ALA:HB2	19	0.12
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	17	0.12
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	19	0.12
(1,14)	1:149:A:ARG:HD2	1:146:A:ILE:HD13	20	0.12
(1,8)	1:81:A:VAL:HA	1:81:A:VAL:HG22	1	0.12
(1,8)	1:47:A:VAL:HG21	1:47:A:VAL:HA	10	0.12
(1,8)	1:47:A:VAL:HG21	1:47:A:VAL:HA	16	0.12
(1,8)	1:81:A:VAL:HA	1:81:A:VAL:HG22	17	0.12
(1,8)	1:47:A:VAL:HG21	1:47:A:VAL:HA	19	0.12
(1,5)	1:151:A:GLU:HG3	1:148:A:LYS:HA	19	0.12
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	4	0.11
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	12	0.11
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	9	0.11
(2,2381)	1:177:A:GLY:H	1:177:A:GLY:HA3	10	0.11
(2,2381)	1:177:A:GLY:H	1:177:A:GLY:HA3	18	0.11
(2,2381)	1:177:A:GLY:H	1:177:A:GLY:HA3	20	0.11
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	3	0.11
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	12	0.11
(2,2353)	1:30:A:GLN:H	1:29:A:VAL:HB	18	0.11
(2,2349)	1:194:A:LYS:H	1:9:A:LYS:HE2	2	0.11
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	1	0.11
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	6	0.11
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	13	0.11
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	14	0.11
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	16	0.11
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	7	0.11
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	14	0.11
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	17	0.11
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	6	0.11
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	10	0.11
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	14	0.11
(2,2331)	1:28:A:ILE:H	1:30:A:GLN:HB2	16	0.11
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	2	0.11
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	15	0.11
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	17	0.11
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	17	0.11
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	20	0.11
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	15	0.11
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	17	0.11
(2,2309)	1:78:A:ASP:H	1:79:A:ALA:HB2	20	0.11
(2,2308)	1:73:A:LEU:H	1:73:A:LEU:HB3	10	0.11
(2,2291)	1:149:A:ARG:H	1:148:A:LYS:HD3	13	0.11
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	18	0.11
(2,2264)	1:175:A:ALA:H	1:176:A:GLU:HB2	15	0.11
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	6	0.11
(2,2226)	1:29:A:VAL:H	1:29:A:VAL:HB	5	0.11
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	2	0.11
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	12	0.11
(2,2184)	1:134:A:GLU:H	1:131:A:LYS:HE2	20	0.11
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	2	0.11
(2,2182)	1:173:A:VAL:H	1:186:A:VAL:HA	15	0.11
(2,2157)	1:16:A:GLY:H	1:119:A:ASP:HB2	7	0.11
(2,2153)	1:15:A:GLY:H	1:94:A:GLY:H	7	0.11
(2,2151)	1:15:A:GLY:H	1:16:A:GLY:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	2	0.11
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	4	0.11
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	10	0.11
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	12	0.11
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	13	0.11
(2,2142)	1:71:A:THR:H	1:69:A:LEU:H	17	0.11
(2,2139)	1:45:A:SER:H	1:48:A:SER:H	5	0.11
(2,2135)	1:145:A:THR:H	1:148:A:LYS:H	15	0.11
(2,2130)	1:25:A:CYS:H	1:21:A:LYS:HA	12	0.11
(2,2130)	1:25:A:CYS:H	1:21:A:LYS:HA	19	0.11
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	13	0.11
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	17	0.11
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	17	0.11
(2,2086)	1:39:A:THR:H	1:37:A:LEU:HA	18	0.11
(2,2083)	1:138:A:ARG:H	1:138:A:ARG:HD2	16	0.11
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	11	0.11
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	17	0.11
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	1	0.11
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	14	0.11
(2,2072)	1:153:A:TYR:H	1:151:A:GLU:HB2	19	0.11
(2,2047)	1:118:A:VAL:H	1:175:A:ALA:HB2	13	0.11
(2,2041)	1:46:A:GLU:H	1:43:A:LEU:HD12	5	0.11
(2,2032)	1:93:A:ASP:H	1:12:A:PHE:HA	16	0.11
(2,2029)	1:142:A:ASN:H	1:145:A:THR:HG21	8	0.11
(2,2029)	1:142:A:ASN:H	1:145:A:THR:HG21	15	0.11
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	10	0.11
(2,2022)	1:110:A:GLY:H	1:5:A:LEU:HB3	12	0.11
(2,2019)	1:110:A:GLY:H	1:106:A:GLU:HA	2	0.11
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	1	0.11
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	7	0.11
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	3	0.11
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	6	0.11
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	17	0.11
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	7	0.11
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	13	0.11
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	15	0.11
(2,2009)	1:168:A:GLY:H	1:166:A:LYS:HB2	19	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	1	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	3	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	5	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	8	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	10	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	12	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	14	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	16	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	17	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	19	0.11
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	20	0.11
(2,1993)	1:133:A:GLY:H	1:131:A:LYS:HD3	20	0.11
(2,1974)	1:18:A:GLY:H	1:17:A:PRO:HB2	4	0.11
(2,1974)	1:18:A:GLY:H	1:17:A:PRO:HB2	17	0.11
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	3	0.11
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	10	0.11
(2,1966)	1:18:A:GLY:H	1:21:A:LYS:HE2	17	0.11
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	10	0.11
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	17	0.11
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	20	0.11
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	1	0.11
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	3	0.11
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	7	0.11
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	9	0.11
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	10	0.11
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	16	0.11
(2,1933)	1:58:A:SER:H	1:57:A:LEU:HD22	11	0.11
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	1	0.11
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	9	0.11
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	16	0.11
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	20	0.11
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	15	0.11
(2,1901)	1:45:A:SER:H	1:41:A:ASP:HB2	4	0.11
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	12	0.11
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	15	0.11
(2,1899)	1:114:A:LEU:H	1:11:A:ILE:HD12	7	0.11
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	10	0.11
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	11	0.11
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	4	0.11
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	5	0.11
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	17	0.11
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	16	0.11
(2,1878)	1:87:A:SER:H	1:90:A:PHE:HD2	13	0.11
(2,1873)	1:87:A:SER:H	1:83:A:LYS:HB2	19	0.11
(2,1869)	1:31:A:LYS:H	1:28:A:ILE:HG22	20	0.11
(2,1865)	1:136:A:SER:H	1:134:A:GLU:HB3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1859)	1:136:A:SER:H	1:135:A:THR:HA	4	0.11
(2,1837)	1:111:A:GLN:H	1:110:A:GLY:HA3	3	0.11
(2,1835)	1:111:A:GLN:H	1:6:A:LYS:HA	16	0.11
(2,1835)	1:111:A:GLN:H	1:6:A:LYS:HA	19	0.11
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	1	0.11
(2,1826)	1:107:A:ARG:H	1:109:A:ILE:HB	12	0.11
(2,1801)	1:44:A:ARG:H	1:43:A:LEU:HD22	11	0.11
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	1	0.11
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	16	0.11
(2,1770)	1:144:A:GLU:H	1:145:A:THR:HA	10	0.11
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	11	0.11
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	19	0.11
(2,1708)	1:143:A:GLU:H	1:130:A:LEU:HD12	19	0.11
(2,1707)	1:125:A:MET:H	1:126:A:THR:HG21	20	0.11
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	4	0.11
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	12	0.11
(2,1678)	1:141:A:ASP:H	1:138:A:ARG:HB2	11	0.11
(2,1672)	1:39:A:THR:H	1:93:A:ASP:HA	16	0.11
(2,1666)	1:183:A:PHE:H	1:185:A:GLN:HE21	12	0.11
(2,1661)	1:139:A:VAL:H	1:141:A:ASP:HB3	10	0.11
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	2	0.11
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	3	0.11
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	8	0.11
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	13	0.11
(2,1576)	1:158:A:GLU:H	1:156:A:ALA:HB2	12	0.11
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	1	0.11
(2,1575)	1:9:A:LYS:H	1:9:A:LYS:HD2	16	0.11
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	1	0.11
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	2	0.11
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	16	0.11
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	18	0.11
(2,1539)	1:119:A:ASP:H	1:173:A:VAL:HG12	5	0.11
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	7	0.11
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	10	0.11
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	13	0.11
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	14	0.11
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	15	0.11
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	6	0.11
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	12	0.11
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	2	0.11
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	5	0.11
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1499)	1:165:A:GLU:H	1:167:A:ARG:H	19	0.11
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	1	0.11
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	2	0.11
(2,1496)	1:12:A:PHE:H	1:190:A:LEU:HD22	5	0.11
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	15	0.11
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	18	0.11
(2,1476)	1:175:A:ALA:H	1:118:A:VAL:HG12	20	0.11
(2,1473)	1:175:A:ALA:H	1:174:A:ASN:HB2	4	0.11
(2,1473)	1:175:A:ALA:H	1:174:A:ASN:HB2	11	0.11
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	1	0.11
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	2	0.11
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	7	0.11
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	17	0.11
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	18	0.11
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	20	0.11
(2,1453)	1:187:A:CYS:H	1:189:A:HIS:H	16	0.11
(2,1432)	1:37:A:LEU:H	1:37:A:LEU:HB3	7	0.11
(2,1424)	1:44:A:ARG:H	1:44:A:ARG:HD3	15	0.11
(2,1417)	1:58:A:SER:H	1:58:A:SER:HB3	10	0.11
(2,1417)	1:58:A:SER:H	1:58:A:SER:HB3	13	0.11
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	9	0.11
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	14	0.11
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	18	0.11
(2,1337)	1:62:A:GLU:H	1:62:A:GLU:HG3	1	0.11
(2,1337)	1:62:A:GLU:H	1:62:A:GLU:HG3	9	0.11
(2,1337)	1:62:A:GLU:H	1:62:A:GLU:HG3	12	0.11
(2,1281)	1:127:A:GLN:H	1:128:A:ARG:H	20	0.11
(2,1242)	1:121:A:GLY:H	1:120:A:ALA:H	13	0.11
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	5	0.11
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	19	0.11
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	2	0.11
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	5	0.11
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	8	0.11
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	10	0.11
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	15	0.11
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	16	0.11
(2,1218)	1:185:A:GLN:H	1:185:A:GLN:HG2	18	0.11
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	3	0.11
(2,1087)	1:141:A:ASP:H	1:141:A:ASP:HB2	8	0.11
(2,1072)	1:143:A:GLU:H	1:143:A:GLU:HG3	8	0.11
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	2	0.11
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	7	0.11
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	15	0.11
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	18	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	7	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	8	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	11	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	12	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	15	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	18	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	19	0.11
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	20	0.11
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	2	0.11
(2,1037)	1:10:A:ILE:HB	1:112:A:PRO:HA	20	0.11
(2,1029)	1:169:A:ILE:HD12	1:164:A:TYR:HB2	20	0.11
(2,1012)	1:87:A:SER:HA	1:8:A:THR:HG21	20	0.11
(2,1010)	1:188:A:THR:HB	1:185:A:GLN:HG2	16	0.11
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	1	0.11
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	6	0.11
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	12	0.11
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	15	0.11
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	16	0.11
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	1	0.11
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	9	0.11
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	16	0.11
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	20	0.11
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	2	0.11
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	9	0.11
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	10	0.11
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	12	0.11
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	14	0.11
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	3	0.11
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	1	0.11
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	8	0.11
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	9	0.11
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	10	0.11
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	13	0.11
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	14	0.11
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	15	0.11
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	5	0.11
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	10	0.11
(2,961)	1:151:A:GLU:HG3	1:148:A:LYS:HE2	16	0.11
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	12	0.11
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	14	0.11
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	8	0.11
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	10	0.11
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	15	0.11
(2,930)	1:174:A:ASN:HB3	1:176:A:GLU:HB2	6	0.11
(2,919)	1:39:A:THR:HB	1:76:A:LEU:HG	20	0.11
(2,912)	1:73:A:LEU:HG	1:105:A:PHE:H	17	0.11
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	4	0.11
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	19	0.11
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	1	0.11
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	3	0.11
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	17	0.11
(2,869)	1:160:A:VAL:HG12	1:157:A:THR:HA	6	0.11
(2,835)	1:141:A:ASP:HB3	1:138:A:ARG:HB3	14	0.11
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	16	0.11
(2,828)	1:56:A:LYS:HB2	1:56:A:LYS:HE2	8	0.11
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	3	0.11
(2,792)	1:180:A:ASP:HB3	1:183:A:PHE:HA	13	0.11
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	6	0.11
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	8	0.11
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	19	0.11
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	12	0.11
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	3	0.11
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	5	0.11
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	1	0.11
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	5	0.11
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	8	0.11
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	9	0.11
(2,686)	1:44:A:ARG:HA	1:47:A:VAL:H	13	0.11
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	1	0.11
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	3	0.11
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	8	0.11
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	10	0.11
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	14	0.11
(2,666)	1:87:A:SER:HB2	1:83:A:LYS:HG2	1	0.11
(2,666)	1:87:A:SER:HB2	1:83:A:LYS:HG2	2	0.11
(2,666)	1:87:A:SER:HB2	1:83:A:LYS:HG2	17	0.11
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	7	0.11
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	14	0.11
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	19	0.11
(2,630)	1:8:A:THR:HB	1:7:A:LYS:HB3	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,607)	1:34:A:TYR:HE2	1:34:A:TYR:HA	6	0.11
(2,607)	1:34:A:TYR:HE2	1:34:A:TYR:HA	14	0.11
(2,596)	1:154:A:TYR:HB3	1:154:A:TYR:HE1	15	0.11
(2,581)	1:32:A:TYR:HB2	1:190:A:LEU:HB3	2	0.11
(2,573)	1:153:A:TYR:HD1	1:15:A:GLY:HA3	12	0.11
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	9	0.11
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	11	0.11
(2,565)	1:154:A:TYR:HD1	1:154:A:TYR:HB2	12	0.11
(2,556)	1:34:A:TYR:HD1	1:29:A:VAL:HG12	4	0.11
(2,556)	1:34:A:TYR:HD1	1:29:A:VAL:HG12	9	0.11
(2,556)	1:34:A:TYR:HD1	1:29:A:VAL:HG12	10	0.11
(2,556)	1:34:A:TYR:HD1	1:29:A:VAL:HG12	14	0.11
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	4	0.11
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	18	0.11
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	9	0.11
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	10	0.11
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	18	0.11
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	8	0.11
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	10	0.11
(2,539)	1:60:A:ILE:HD12	1:56:A:LYS:HA	18	0.11
(2,530)	1:60:A:ILE:HG22	1:66:A:LEU:HA	12	0.11
(2,530)	1:60:A:ILE:HG22	1:66:A:LEU:HA	18	0.11
(2,528)	1:192:A:ALA:HB2	1:188:A:THR:HG21	12	0.11
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	1	0.11
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	2	0.11
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	3	0.11
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	6	0.11
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	9	0.11
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	18	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	3	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	8	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	11	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	13	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	15	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	16	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	17	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	18	0.11
(2,508)	1:120:A:ALA:HB2	1:19:A:SER:HB2	20	0.11
(2,505)	1:118:A:VAL:H	1:118:A:VAL:HG12	2	0.11
(2,505)	1:118:A:VAL:H	1:118:A:VAL:HG12	5	0.11
(2,505)	1:118:A:VAL:H	1:118:A:VAL:HG12	15	0.11
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	14	0.11
(2,497)	1:150:A:LEU:HD22	1:122:A:PRO:HD3	19	0.11
(2,485)	1:37:A:LEU:HD12	1:83:A:LYS:HE2	8	0.11
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	3	0.11
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	7	0.11
(2,483)	1:37:A:LEU:HD12	1:91:A:LEU:HA	9	0.11
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	16	0.11
(2,462)	1:134:A:GLU:HG3	1:131:A:LYS:HE2	3	0.11
(2,459)	1:149:A:ARG:HB2	1:146:A:ILE:HA	1	0.11
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	1	0.11
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	15	0.11
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	19	0.11
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	4	0.11
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	1	0.11
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	10	0.11
(2,426)	1:163:A:PHE:HB3	1:161:A:ILE:HG13	1	0.11
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	5	0.11
(2,424)	1:78:A:ASP:HB3	1:75:A:MET:HG2	15	0.11
(2,417)	1:129:A:LEU:HB2	1:146:A:ILE:HD12	17	0.11
(2,410)	1:107:A:ARG:HD2	1:106:A:GLU:HB2	19	0.11
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	9	0.11
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	12	0.11
(2,389)	1:114:A:LEU:HA	1:169:A:ILE:HB	16	0.11
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	4	0.11
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	11	0.11
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	13	0.11
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	14	0.11
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	19	0.11
(2,376)	1:176:A:GLU:HA	1:124:A:THR:HG21	10	0.11
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	2	0.11
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	10	0.11
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	12	0.11
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	13	0.11
(2,371)	1:127:A:GLN:HA	1:143:A:GLU:HG2	17	0.11
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	14	0.11
(2,367)	1:21:A:LYS:HA	1:118:A:VAL:HB	17	0.11
(2,360)	1:151:A:GLU:HA	1:154:A:TYR:HB3	17	0.11
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	6	0.11
(2,317)	1:43:A:LEU:HD12	1:46:A:GLU:HB2	19	0.11
(2,311)	1:143:A:GLU:HG3	1:130:A:LEU:HD12	6	0.11
(2,311)	1:143:A:GLU:HG3	1:130:A:LEU:HD12	15	0.11
(2,302)	1:2:A:GLU:HA	1:2:A:GLU:HG2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,302)	1:2:A:GLU:HA	1:2:A:GLU:HG2	11	0.11
(2,302)	1:2:A:GLU:HA	1:2:A:GLU:HG2	18	0.11
(2,302)	1:2:A:GLU:HA	1:2:A:GLU:HG2	19	0.11
(2,298)	1:41:A:ASP:HB2	1:41:A:ASP:HA	8	0.11
(2,295)	1:68:A:PRO:HA	1:68:A:PRO:HB2	3	0.11
(2,295)	1:68:A:PRO:HA	1:68:A:PRO:HB2	8	0.11
(2,292)	1:72:A:VAL:HB	1:72:A:VAL:HG22	13	0.11
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	15	0.11
(2,243)	1:127:A:GLN:HB2	1:124:A:THR:HA	16	0.11
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	3	0.11
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	9	0.11
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	3	0.11
(2,190)	1:147:A:LYS:HA	1:147:A:LYS:HG2	9	0.11
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	3	0.11
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	4	0.11
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	15	0.11
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	18	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	1	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	2	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	3	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	9	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	10	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	14	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	15	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	16	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	19	0.11
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	20	0.11
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	2	0.11
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	5	0.11
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	8	0.11
(2,127)	1:186:A:VAL:HG22	1:186:A:VAL:HA	15	0.11
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	3	0.11
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	5	0.11
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	5	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	2	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	3	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	7	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	11	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	12	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	13	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	14	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	16	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	18	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	19	0.11
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	20	0.11
(2,97)	1:63:A:LYS:HA	1:63:A:LYS:HG3	7	0.11
(2,81)	1:57:A:LEU:HD22	1:43:A:LEU:HB3	12	0.11
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	3	0.11
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	7	0.11
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	9	0.11
(2,53)	1:63:A:LYS:HG2	1:63:A:LYS:HB2	20	0.11
(2,50)	1:31:A:LYS:HG3	1:31:A:LYS:HA	6	0.11
(2,23)	1:7:A:LYS:HA	1:7:A:LYS:HB2	16	0.11
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	3	0.11
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	6	0.11
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	10	0.11
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	12	0.11
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	15	0.11
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	17	0.11
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	20	0.11
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	7	0.11
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	10	0.11
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	14	0.11
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	6	0.11
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	7	0.11
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	8	0.11
(1,22)	1:38:A:SER:HA	1:91:A:LEU:HD13	6	0.11
(1,22)	1:38:A:SER:HA	1:91:A:LEU:HD13	11	0.11
(1,5)	1:151:A:GLU:HG3	1:148:A:LYS:HA	5	0.11
(2,2412)	1:76:A:LEU:H	1:43:A:LEU:HD22	9	0.1
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	5	0.1
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	6	0.1
(2,2404)	1:65:A:GLN:H	1:64:A:GLY:H	16	0.1
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	5	0.1
(2,2334)	1:169:A:ILE:H	1:170:A:VAL:HG12	12	0.1
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	1	0.1
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	8	0.1
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	16	0.1
(2,2332)	1:121:A:GLY:H	1:176:A:GLU:HA	20	0.1
(2,2330)	1:153:A:TYR:H	1:150:A:LEU:HA	1	0.1
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	4	0.1
(2,2314)	1:111:A:GLN:H	1:109:A:ILE:HB	12	0.1
(2,2287)	1:189:A:HIS:H	1:116:A:LEU:HD12	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2264)	1:175:A:ALA:H	1:176:A:GLU:HB2	7	0.1
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	1	0.1
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	3	0.1
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	12	0.1
(2,2243)	1:133:A:GLY:H	1:131:A:LYS:HA	19	0.1
(2,2207)	1:131:A:LYS:H	1:131:A:LYS:HB2	9	0.1
(2,2204)	1:174:A:ASN:H	1:119:A:ASP:HB3	18	0.1
(2,2185)	1:134:A:GLU:H	1:140:A:ASP:HB2	8	0.1
(2,2160)	1:102:A:GLY:H	1:105:A:PHE:H	6	0.1
(2,2144)	1:108:A:ARG:H	1:109:A:ILE:HA	19	0.1
(2,2142)	1:71:A:THR:H	1:69:A:LEU:H	1	0.1
(2,2140)	1:188:A:THR:H	1:190:A:LEU:HB2	16	0.1
(2,2139)	1:45:A:SER:H	1:48:A:SER:H	4	0.1
(2,2139)	1:45:A:SER:H	1:48:A:SER:H	14	0.1
(2,2139)	1:45:A:SER:H	1:48:A:SER:H	15	0.1
(2,2130)	1:25:A:CYS:H	1:21:A:LYS:HA	18	0.1
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	3	0.1
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	7	0.1
(2,2110)	1:192:A:ALA:H	1:194:A:LYS:HA	14	0.1
(2,2079)	1:72:A:VAL:H	1:73:A:LEU:HG	4	0.1
(2,2078)	1:62:A:GLU:H	1:60:A:ILE:HG22	7	0.1
(2,2029)	1:142:A:ASN:H	1:145:A:THR:HG21	1	0.1
(2,2029)	1:142:A:ASN:H	1:145:A:THR:HG21	13	0.1
(2,2029)	1:142:A:ASN:H	1:145:A:THR:HG21	14	0.1
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	2	0.1
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	8	0.1
(2,2017)	1:33:A:GLY:H	1:29:A:VAL:HG22	17	0.1
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	14	0.1
(2,2014)	1:33:A:GLY:H	1:32:A:TYR:HD1	15	0.1
(2,2006)	1:86:A:THR:H	1:85:A:ASN:HB3	6	0.1
(2,1974)	1:18:A:GLY:H	1:17:A:PRO:HB2	10	0.1
(2,1973)	1:18:A:GLY:H	1:125:A:MET:HG2	13	0.1
(2,1972)	1:40:A:GLY:H	1:41:A:ASP:HB2	5	0.1
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	7	0.1
(2,1962)	1:54:A:GLY:H	1:47:A:VAL:HB	9	0.1
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	6	0.1
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	14	0.1
(2,1936)	1:83:A:LYS:H	1:81:A:VAL:HG22	18	0.1
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	3	0.1
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	10	0.1
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	14	0.1
(2,1926)	1:48:A:SER:H	1:47:A:VAL:HG22	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1925)	1:126:A:THR:H	1:146:A:ILE:HG22	1	0.1
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	2	0.1
(2,1900)	1:45:A:SER:H	1:44:A:ARG:HD2	9	0.1
(2,1895)	1:114:A:LEU:H	1:11:A:ILE:HB	6	0.1
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	7	0.1
(2,1888)	1:6:A:LYS:H	1:5:A:LEU:HD22	11	0.1
(2,1887)	1:6:A:LYS:H	1:6:A:LYS:HD3	9	0.1
(2,1875)	1:164:A:TYR:H	1:170:A:VAL:HG12	20	0.1
(2,1845)	1:107:A:ARG:H	1:106:A:GLU:HG3	12	0.1
(2,1845)	1:107:A:ARG:H	1:106:A:GLU:HG3	17	0.1
(2,1798)	1:61:A:MET:H	1:57:A:LEU:HA	12	0.1
(2,1781)	1:144:A:GLU:H	1:146:A:ILE:HD12	9	0.1
(2,1780)	1:73:A:LEU:H	1:76:A:LEU:HB3	5	0.1
(2,1749)	1:113:A:THR:H	1:114:A:LEU:HD22	5	0.1
(2,1746)	1:156:A:ALA:H	1:155:A:LYS:HB2	16	0.1
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	2	0.1
(2,1730)	1:160:A:VAL:H	1:158:A:GLU:HA	15	0.1
(2,1708)	1:143:A:GLU:H	1:130:A:LEU:HD12	7	0.1
(2,1681)	1:151:A:GLU:H	1:150:A:LEU:HD12	8	0.1
(2,1678)	1:141:A:ASP:H	1:138:A:ARG:HB2	13	0.1
(2,1672)	1:39:A:THR:H	1:93:A:ASP:HA	17	0.1
(2,1646)	1:149:A:ARG:H	1:150:A:LEU:HB3	17	0.1
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	7	0.1
(2,1643)	1:140:A:ASP:H	1:139:A:VAL:HB	19	0.1
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	12	0.1
(2,1612)	1:79:A:ALA:H	1:75:A:MET:HB3	14	0.1
(2,1609)	1:84:A:VAL:H	1:85:A:ASN:HB3	11	0.1
(2,1604)	1:95:A:TYR:H	1:39:A:THR:HA	1	0.1
(2,1574)	1:146:A:ILE:H	1:143:A:GLU:HG2	14	0.1
(2,1539)	1:119:A:ASP:H	1:173:A:VAL:HG12	4	0.1
(2,1539)	1:119:A:ASP:H	1:173:A:VAL:HG12	18	0.1
(2,1535)	1:173:A:VAL:H	1:119:A:ASP:HB3	4	0.1
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	2	0.1
(2,1512)	1:93:A:ASP:H	1:37:A:LEU:HG	19	0.1
(2,1511)	1:93:A:ASP:H	1:37:A:LEU:HB2	14	0.1
(2,1511)	1:93:A:ASP:H	1:37:A:LEU:HB2	15	0.1
(2,1510)	1:92:A:ILE:H	1:37:A:LEU:HD12	12	0.1
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	3	0.1
(2,1503)	1:165:A:GLU:H	1:162:A:ALA:HB2	14	0.1
(2,1472)	1:36:A:HIS:H	1:37:A:LEU:HD12	3	0.1
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	5	0.1
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	8	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	9	0.1
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	10	0.1
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	11	0.1
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	13	0.1
(2,1464)	1:169:A:ILE:H	1:168:A:GLY:HA3	14	0.1
(2,1442)	1:194:A:LYS:H	1:193:A:LEU:HD22	3	0.1
(2,1432)	1:37:A:LEU:H	1:37:A:LEU:HB3	18	0.1
(2,1424)	1:44:A:ARG:H	1:44:A:ARG:HD3	5	0.1
(2,1424)	1:44:A:ARG:H	1:44:A:ARG:HD3	14	0.1
(2,1392)	1:79:A:ALA:H	1:81:A:VAL:H	9	0.1
(2,1392)	1:79:A:ALA:H	1:81:A:VAL:H	12	0.1
(2,1365)	1:111:A:GLN:H	1:111:A:GLN:HG2	15	0.1
(2,1346)	1:146:A:ILE:H	1:146:A:ILE:HG12	19	0.1
(2,1260)	1:169:A:ILE:H	1:169:A:ILE:HG13	16	0.1
(2,1242)	1:121:A:GLY:H	1:120:A:ALA:H	15	0.1
(2,1238)	1:56:A:LYS:H	1:55:A:LYS:HB3	9	0.1
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	7	0.1
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	9	0.1
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	12	0.1
(2,1220)	1:185:A:GLN:H	1:185:A:GLN:HB2	13	0.1
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	2	0.1
(2,1194)	1:45:A:SER:H	1:45:A:SER:HB3	20	0.1
(2,1156)	1:131:A:LYS:H	1:131:A:LYS:HD3	1	0.1
(2,1096)	1:174:A:ASN:H	1:174:A:ASN:HB3	18	0.1
(2,1072)	1:143:A:GLU:H	1:143:A:GLU:HG3	1	0.1
(2,1070)	1:125:A:MET:H	1:125:A:MET:HG2	4	0.1
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	1	0.1
(2,1042)	1:161:A:ILE:HD12	1:157:A:THR:HB	5	0.1
(2,1027)	1:10:A:ILE:HA	1:10:A:ILE:HG22	10	0.1
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	7	0.1
(2,1002)	1:29:A:VAL:HG12	1:29:A:VAL:HB	19	0.1
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	4	0.1
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	8	0.1
(2,1001)	1:135:A:THR:HG21	1:135:A:THR:HA	10	0.1
(2,989)	1:11:A:ILE:HB	1:11:A:ILE:HG22	1	0.1
(2,989)	1:11:A:ILE:HB	1:11:A:ILE:HG22	14	0.1
(2,988)	1:149:A:ARG:HB2	1:149:A:ARG:HA	14	0.1
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	1	0.1
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	3	0.1
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	8	0.1
(2,985)	1:188:A:THR:HB	1:188:A:THR:HG21	17	0.1
(2,975)	1:161:A:ILE:HG22	1:117:A:TYR:HE1	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	2	0.1
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	3	0.1
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	18	0.1
(2,971)	1:189:A:HIS:HA	1:188:A:THR:HG21	19	0.1
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	13	0.1
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	15	0.1
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	18	0.1
(2,953)	1:43:A:LEU:HD12	1:71:A:THR:HG21	19	0.1
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	2	0.1
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	3	0.1
(2,934)	1:63:A:LYS:HG2	1:65:A:GLN:HB3	18	0.1
(2,921)	1:72:A:VAL:HA	1:73:A:LEU:HG	14	0.1
(2,910)	1:72:A:VAL:HA	1:75:A:MET:HB3	20	0.1
(2,899)	1:76:A:LEU:HD12	1:75:A:MET:HB2	8	0.1
(2,899)	1:76:A:LEU:HD12	1:75:A:MET:HB2	20	0.1
(2,897)	1:32:A:TYR:HE1	1:186:A:VAL:HG21	10	0.1
(2,875)	1:118:A:VAL:HG22	1:21:A:LYS:HE2	18	0.1
(2,874)	1:117:A:TYR:HD1	1:118:A:VAL:HG22	19	0.1
(2,869)	1:160:A:VAL:HG12	1:157:A:THR:HA	3	0.1
(2,856)	1:172:A:LYS:HG2	1:117:A:TYR:HB3	20	0.1
(2,834)	1:84:A:VAL:HB	1:5:A:LEU:HD22	17	0.1
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	2	0.1
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	8	0.1
(2,818)	1:146:A:ILE:HB	1:126:A:THR:HG21	14	0.1
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	6	0.1
(2,808)	1:174:A:ASN:HB2	1:119:A:ASP:HB3	13	0.1
(2,799)	1:190:A:LEU:HB3	1:187:A:CYS:HA	12	0.1
(2,759)	1:89:A:GLY:HA3	1:9:A:LYS:HB2	17	0.1
(2,724)	1:141:A:ASP:HA	1:143:A:GLU:HB2	10	0.1
(2,720)	1:60:A:ILE:HA	1:65:A:GLN:HA	2	0.1
(2,715)	1:36:A:HIS:HA	1:91:A:LEU:HB3	4	0.1
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	3	0.1
(2,702)	1:5:A:LEU:HA	1:84:A:VAL:HB	17	0.1
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	4	0.1
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	6	0.1
(2,680)	1:10:A:ILE:HA	1:8:A:THR:HG21	11	0.1
(2,666)	1:87:A:SER:HB2	1:83:A:LYS:HG2	6	0.1
(2,666)	1:87:A:SER:HB2	1:83:A:LYS:HG2	12	0.1
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	3	0.1
(2,664)	1:87:A:SER:HB2	1:84:A:VAL:HG22	13	0.1
(2,607)	1:34:A:TYR:HE2	1:34:A:TYR:HA	5	0.1
(2,607)	1:34:A:TYR:HE2	1:34:A:TYR:HA	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,605)	1:34:A:TYR:HE2	1:88:A:LYS:HE2	19	0.1
(2,572)	1:153:A:TYR:HD1	1:149:A:ARG:HD2	20	0.1
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	2	0.1
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	4	0.1
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	18	0.1
(2,568)	1:154:A:TYR:HD1	1:157:A:THR:HG21	19	0.1
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	3	0.1
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	8	0.1
(2,547)	1:109:A:ILE:HD12	1:76:A:LEU:HB2	13	0.1
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	1	0.1
(2,544)	1:11:A:ILE:H	1:11:A:ILE:HD12	16	0.1
(2,530)	1:60:A:ILE:HG22	1:66:A:LEU:HA	2	0.1
(2,528)	1:192:A:ALA:HB2	1:188:A:THR:HG21	4	0.1
(2,528)	1:192:A:ALA:HB2	1:188:A:THR:HG21	10	0.1
(2,523)	1:84:A:VAL:HG22	1:4:A:LYS:HG2	7	0.1
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	4	0.1
(2,503)	1:36:A:HIS:HB3	1:29:A:VAL:HG12	11	0.1
(2,469)	1:158:A:GLU:HB3	1:154:A:TYR:HA	12	0.1
(2,451)	1:61:A:MET:HG2	1:60:A:ILE:HB	10	0.1
(2,437)	1:2:A:GLU:HG2	1:6:A:LYS:HE3	20	0.1
(2,436)	1:2:A:GLU:HG2	1:109:A:ILE:HA	14	0.1
(2,387)	1:117:A:TYR:HA	1:117:A:TYR:HD1	1	0.1
(2,368)	1:21:A:LYS:HG2	1:21:A:LYS:HA	7	0.1
(2,344)	1:84:A:VAL:HA	1:90:A:PHE:HD2	11	0.1
(2,311)	1:143:A:GLU:HG3	1:130:A:LEU:HD12	16	0.1
(2,298)	1:41:A:ASP:HB2	1:41:A:ASP:HA	14	0.1
(2,296)	1:61:A:MET:HA	1:61:A:MET:HG3	11	0.1
(2,292)	1:72:A:VAL:HB	1:72:A:VAL:HG22	15	0.1
(2,274)	1:136:A:SER:HB2	1:136:A:SER:HA	14	0.1
(2,231)	1:161:A:ILE:HD12	1:161:A:ILE:HB	10	0.1
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	11	0.1
(2,219)	1:138:A:ARG:HD2	1:138:A:ARG:HB2	13	0.1
(2,212)	1:169:A:ILE:HG22	1:169:A:ILE:HG13	16	0.1
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	11	0.1
(2,211)	1:11:A:ILE:HG22	1:11:A:ILE:HG12	18	0.1
(2,204)	1:57:A:LEU:HG	1:53:A:ARG:HG3	20	0.1
(2,181)	1:120:A:ALA:HB2	1:120:A:ALA:HA	11	0.1
(2,165)	1:112:A:PRO:HA	1:10:A:ILE:HG22	17	0.1
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	4	0.1
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	6	0.1
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	13	0.1
(2,140)	1:142:A:ASN:HA	1:142:A:ASN:HB2	17	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,123)	1:47:A:VAL:HB	1:47:A:VAL:HG12	6	0.1
(2,123)	1:47:A:VAL:HB	1:47:A:VAL:HG12	13	0.1
(2,112)	1:161:A:ILE:HA	1:161:A:ILE:HG22	1	0.1
(2,101)	1:107:A:ARG:HB3	1:107:A:ARG:HD2	2	0.1
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	1	0.1
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	6	0.1
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	8	0.1
(2,98)	1:138:A:ARG:HB2	1:138:A:ARG:HA	10	0.1
(2,59)	1:140:A:ASP:HB3	1:140:A:ASP:HA	13	0.1
(2,44)	1:30:A:GLN:HB2	1:30:A:GLN:HG2	15	0.1
(2,23)	1:7:A:LYS:HA	1:7:A:LYS:HB2	9	0.1
(2,23)	1:7:A:LYS:HA	1:7:A:LYS:HB2	10	0.1
(2,23)	1:7:A:LYS:HA	1:7:A:LYS:HB2	11	0.1
(2,23)	1:7:A:LYS:HA	1:7:A:LYS:HB2	15	0.1
(2,23)	1:7:A:LYS:HA	1:7:A:LYS:HB2	19	0.1
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	4	0.1
(2,21)	1:172:A:LYS:HB2	1:172:A:LYS:HA	11	0.1
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	5	0.1
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	9	0.1
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	16	0.1
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	18	0.1
(2,5)	1:175:A:ALA:HB2	1:175:A:ALA:HA	20	0.1
(1,32)	1:102:A:GLY:H	1:99:A:VAL:HA	10	0.1
(1,7)	1:194:A:LYS:HB2	1:194:A:LYS:HG2	20	0.1

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

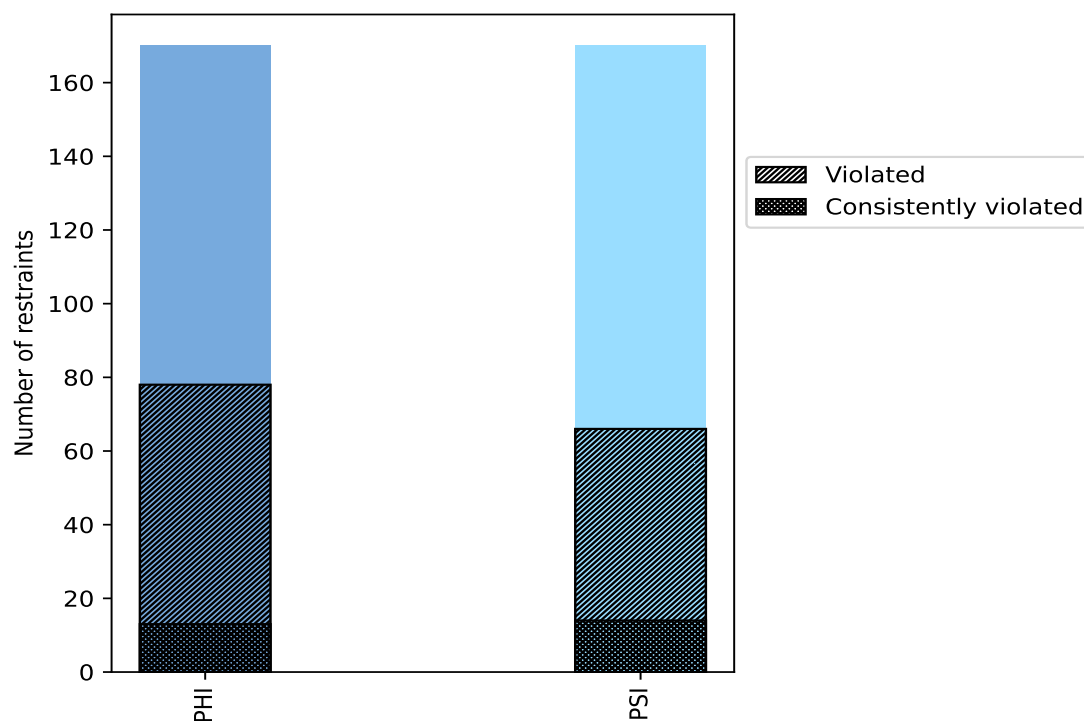
### 10.1 Summary of dihedral-angle violations [i](#)

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	170	50.0	78	45.9	22.9	13	7.6	3.8
PSI	170	50.0	66	38.8	19.4	14	8.2	4.1
Total	340	100.0	144	42.4	42.4	27	7.9	7.9

<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](#)



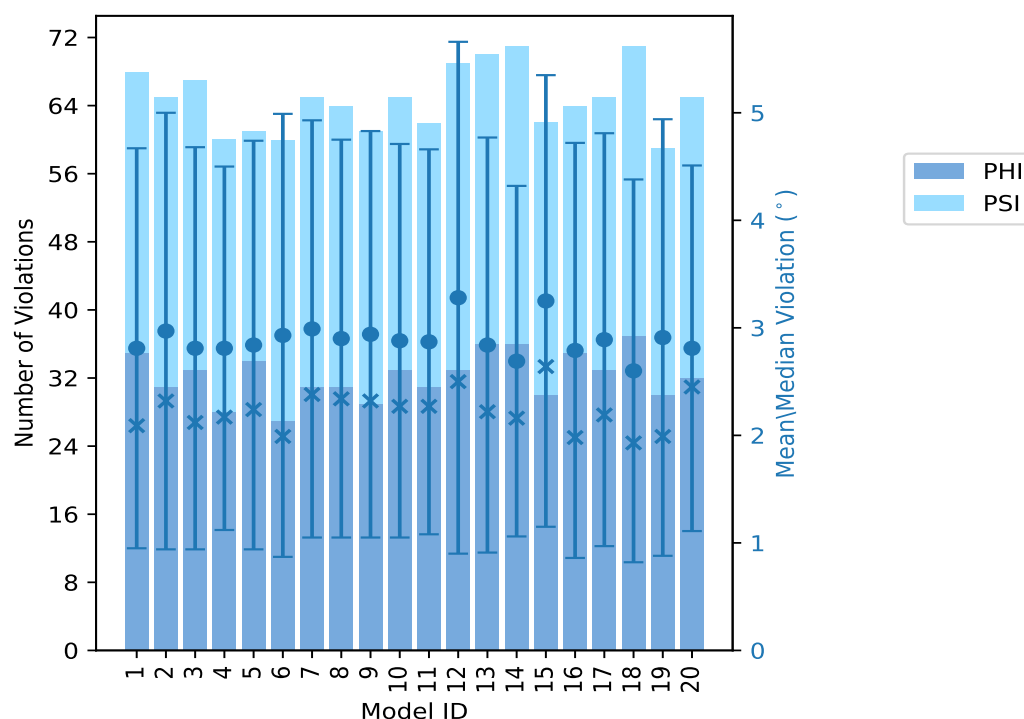
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model

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	35	33	68	2.81	8.85	1.86	2.09
2	31	34	65	2.97	9.44	2.03	2.32
3	33	34	67	2.81	8.81	1.87	2.12
4	28	32	60	2.81	8.95	1.69	2.17
5	34	27	61	2.84	9.38	1.9	2.24
6	27	33	60	2.93	9.74	2.06	1.99
7	31	34	65	2.99	9.63	1.94	2.38
8	31	33	64	2.9	9.13	1.85	2.34
9	29	32	61	2.94	9.6	1.89	2.32
10	33	32	65	2.88	9.07	1.83	2.27
11	31	31	62	2.87	9.48	1.79	2.27
12	33	36	69	3.28	11.25	2.38	2.5
13	36	34	70	2.84	10.39	1.93	2.22
14	36	35	71	2.69	8.86	1.63	2.16
15	30	32	62	3.25	9.38	2.1	2.64
16	35	29	64	2.79	9.22	1.93	1.98
17	33	32	65	2.89	10.71	1.92	2.19
18	37	34	71	2.6	9.92	1.78	1.93
19	30	29	59	2.91	8.9	2.03	1.99
20	32	33	65	2.81	8.43	1.7	2.45

### 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>	%
23	11	34	1	5.0
9	7	16	2	10.0
4	5	9	3	15.0
3	3	6	4	20.0
2	2	4	5	25.0
5	2	7	6	30.0
1	2	3	7	35.0
0	0	0	8	40.0
3	3	6	9	45.0
0	1	1	10	50.0
1	2	3	11	55.0

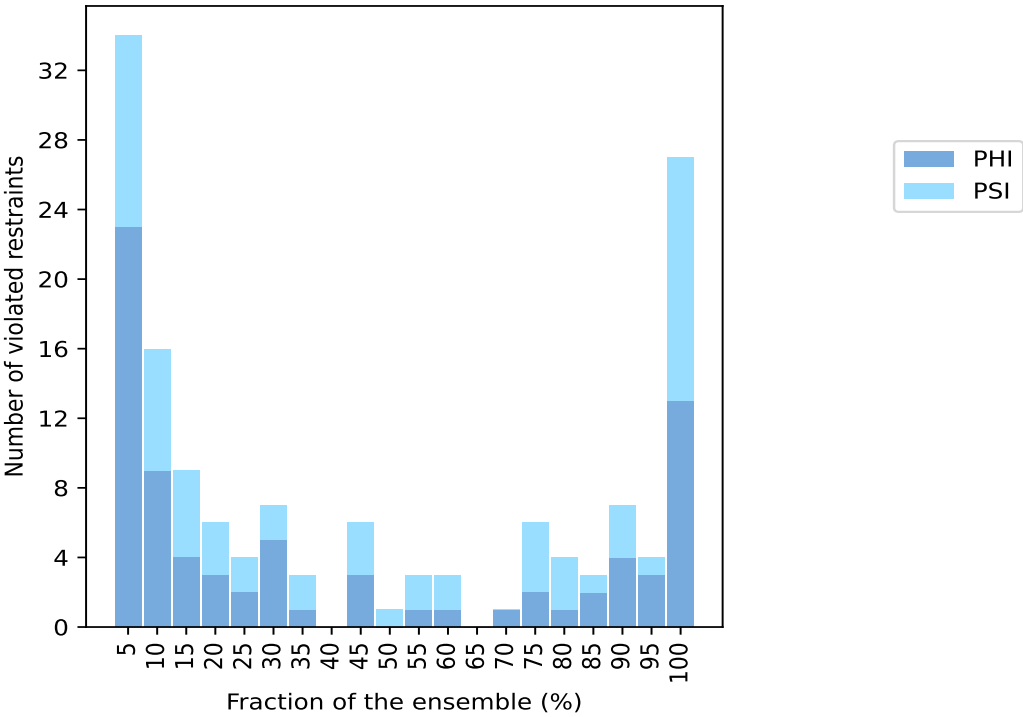
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count <sup>1</sup>	%
1	2	3	12	60.0
0	0	0	13	65.0
1	0	1	14	70.0
2	4	6	15	75.0
1	3	4	16	80.0
2	1	3	17	85.0
4	3	7	18	90.0
3	1	4	19	95.0
13	14	27	20	100.0

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

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



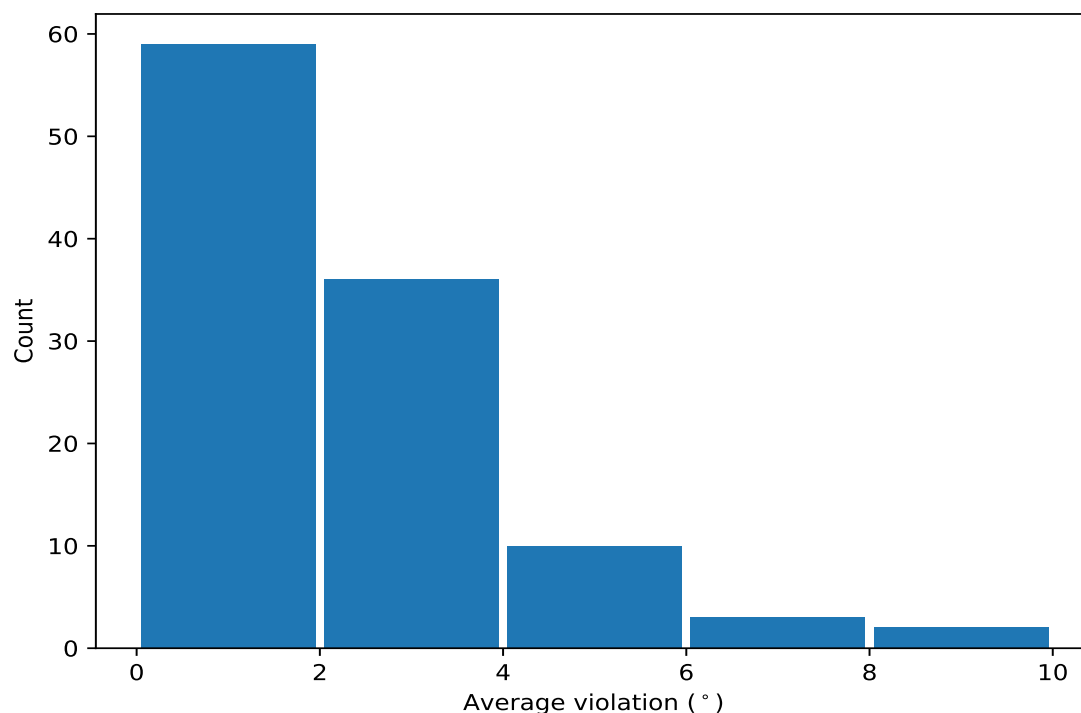
10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	20	9.22	0.79	9.18
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	20	6.76	1.29	7.37
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	20	6.45	0.55	6.51
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	20	5.76	1.08	5.76
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	20	5.15	1.12	4.75
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	20	4.89	0.98	5.14
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	20	4.84	0.46	4.92
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	20	4.31	1.35	4.65
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	20	4.09	0.84	4.2
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	20	4.06	0.61	3.94
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	20	4.0	1.02	3.84
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	20	3.86	0.88	4.01
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	20	3.75	0.39	3.66
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	20	3.68	1.29	3.58
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	20	3.65	0.5	3.72
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	20	3.24	0.39	3.16
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	20	3.14	0.81	3.06
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	20	3.02	0.89	2.93
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	20	2.84	0.56	2.76
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	20	2.8	1.7	2.42

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	20	2.54	0.41	2.65
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	20	2.41	0.64	2.41
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	20	2.26	0.52	2.36
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	20	2.23	1.06	1.82
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	20	2.11	0.53	2.08
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	20	2.02	0.43	1.98
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	20	1.85	0.53	1.78
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	19	8.59	0.77	8.68
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	19	6.51	0.55	6.45
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	19	2.66	1.14	2.43
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	19	1.83	0.73	1.62
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	18	2.37	0.81	2.22
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	18	2.23	0.63	2.32
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	18	2.16	0.38	2.17
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	18	2.05	0.38	1.98
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	18	1.86	0.53	1.72
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	18	1.74	0.49	1.69
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	18	1.57	0.43	1.48
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	17	3.06	0.55	2.92
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	17	1.99	0.54	1.75
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	17	1.7	0.38	1.58
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	16	2.92	0.56	3.0
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	16	1.61	0.47	1.57
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	16	1.45	0.4	1.31
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	16	1.41	0.27	1.44
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	15	2.16	0.66	2.01
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	15	2.15	0.28	2.08
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	15	1.74	0.48	1.77
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	15	1.56	0.47	1.39
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	15	1.5	0.39	1.4
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	15	1.37	0.21	1.37
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	14	1.74	0.41	1.65
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	12	2.55	1.01	2.62
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	12	1.37	0.26	1.32
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	12	1.28	0.19	1.29
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	11	4.04	1.59	4.04
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	11	1.99	0.63	1.9
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	11	1.12	0.08	1.12
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	10	1.36	0.2	1.36
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	9	2.05	0.73	1.76
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	9	1.65	0.51	1.42
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	9	1.51	0.51	1.37
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	9	1.48	0.39	1.63
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	9	1.44	0.26	1.37
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	9	1.39	0.53	1.19
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	7	3.86	2.45	3.18
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	7	2.44	0.72	2.6
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	7	1.31	0.17	1.35
(1,197)	1:115:A:LEU:C	1:116:A:LEU:N	1:116:A:LEU:CA	1:116:A:LEU:C	6	1.89	1.13	1.38
(1,129)	1:69:A:LEU:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	6	1.48	0.27	1.42
(1,83)	1:45:A:SER:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	6	1.38	0.22	1.36

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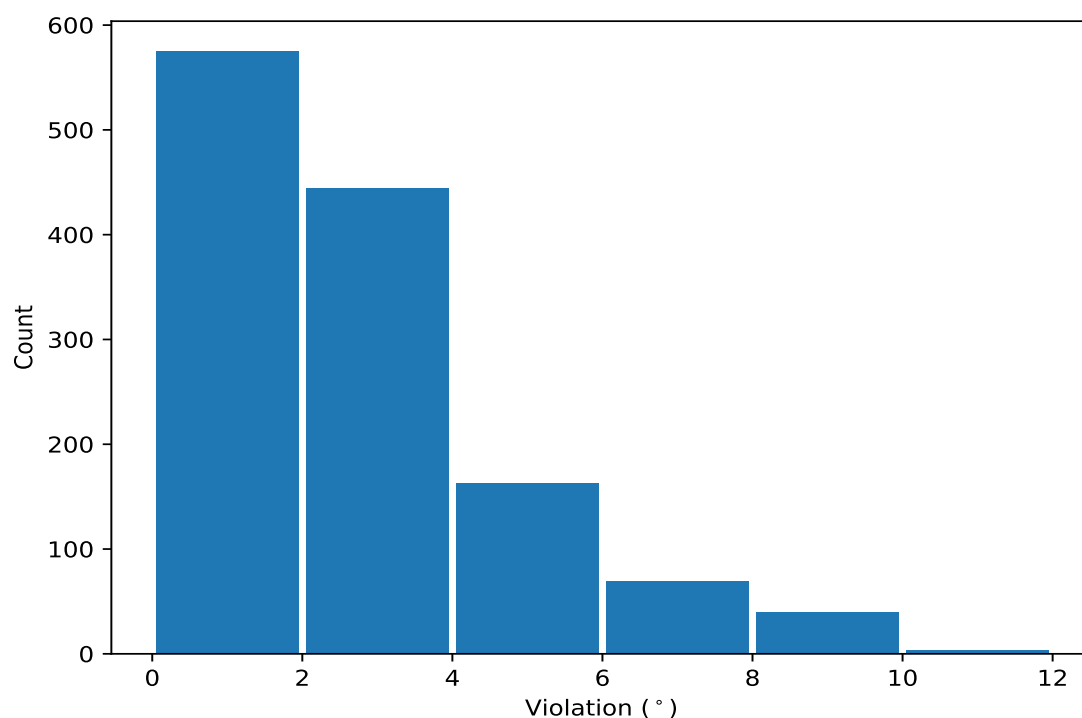
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,82)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:GLU:N	6	1.33	0.27	1.26
(1,64)	1:36:A:HIS:N	1:36:A:HIS:CA	1:36:A:HIS:C	1:37:A:LEU:N	6	1.31	0.18	1.24
(1,77)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	6	1.18	0.11	1.2
(1,133)	1:71:A:THR:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	6	1.18	0.11	1.19
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:LEU:N	5	2.02	0.44	1.87
(1,225)	1:131:A:LYS:C	1:132:A:ARG:N	1:132:A:ARG:CA	1:132:A:ARG:C	5	1.97	1.1	1.63
(1,178)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:ARG:N	5	1.95	0.32	1.9
(1,33)	1:20:A:GLY:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	5	1.56	0.31	1.46
(1,95)	1:51:A:SER:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	4	3.3	2.1	2.12
(1,98)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:GLY:N	4	3.26	3.26	1.6
(1,91)	1:49:A:SER:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	4	3.05	2.96	1.38
(1,13)	1:7:A:LYS:C	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	4	1.52	0.67	1.18
(1,100)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:LYS:N	4	1.42	0.41	1.25
(1,22)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:VAL:N	4	1.3	0.14	1.28
(1,278)	1:159:A:PRO:N	1:159:A:PRO:CA	1:159:A:PRO:C	1:160:A:VAL:N	3	1.54	0.25	1.64
(1,66)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:SER:N	3	1.52	0.09	1.5
(1,334)	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	1:190:A:LEU:N	3	1.41	0.36	1.27
(1,67)	1:37:A:LEU:C	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	3	1.39	0.26	1.3
(1,176)	1:105:A:PHE:N	1:105:A:PHE:CA	1:105:A:PHE:C	1:106:A:GLU:N	3	1.29	0.17	1.26
(1,8)	1:5:A:LEU:N	1:5:A:LEU:CA	1:5:A:LEU:C	1:6:A:LYS:N	3	1.29	0.18	1.24
(1,125)	1:67:A:VAL:C	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	3	1.26	0.05	1.24
(1,9)	1:5:A:LEU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	3	1.12	0.09	1.11
(1,71)	1:39:A:THR:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	3	1.08	0.09	1.04
(1,174)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:TYR:N	2	4.56	0.36	4.56
(1,121)	1:65:A:GLN:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	2	3.21	0.19	3.21
(1,99)	1:53:A:ARG:C	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	2	2.74	1.52	2.74
(1,330)	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	1:188:A:THR:N	2	2.14	0.0	2.14
(1,230)	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	1:135:A:THR:N	2	2.13	0.11	2.13
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:GLY:N	2	1.72	0.03	1.72
(1,31)	1:19:A:SER:C	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	2	1.46	0.06	1.46
(1,122)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:VAL:N	2	1.44	0.43	1.44
(1,229)	1:133:A:GLY:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	2	1.39	0.11	1.39
(1,340)	1:192:A:ALA:N	1:192:A:ALA:CA	1:192:A:ALA:C	1:193:A:LEU:N	2	1.2	0.03	1.2
(1,103)	1:55:A:LYS:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	2	1.18	0.01	1.18
(1,195)	1:114:A:LEU:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	2	1.15	0.02	1.15
(1,219)	1:128:A:ARG:C	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	2	1.14	0.13	1.14
(1,149)	1:79:A:ALA:C	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	2	1.08	0.04	1.08
(1,217)	1:127:A:GLN:C	1:128:A:ARG:N	1:128:A:ARG:CA	1:128:A:ARG:C	2	1.04	0.04	1.04
(1,312)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	2	1.02	0.03	1.02

<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 ⓘ

### 10.5.1 Histogram : Distribution of violations ⓘ

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 (°)
(1,94)	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	1:52:A:ALA:N	12	11.25
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	17	10.71
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	13	10.39
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	18	9.92
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	6	9.74
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	12	9.68
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	7	9.63
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	9	9.6
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	11	9.48
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	2	9.44
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	13	9.42
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	5	9.38
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	15	9.38
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	16	9.22
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	2	9.14
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	8	9.13
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	12	9.08
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	10	9.07
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	6	9.03
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	4	8.95
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	7	8.94

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	19	8.9
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	14	8.86
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	15	8.86
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	1	8.85
(1,98)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:GLY:N	12	8.85
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	11	8.85
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	3	8.81
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	8	8.79
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	19	8.76
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	1	8.72
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	10	8.68
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	3	8.67
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	9	8.59
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	16	8.55
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	17	8.51
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	15	8.47
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	20	8.43
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	5	8.4
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	14	8.29
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	15	8.24
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	18	8.22
(1,91)	1:49:A:SER:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	12	8.18
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	8	7.98
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	12	7.93
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	6	7.9
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1	7.82
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	6	7.81
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	16	7.69
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	3	7.62
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	5	7.59
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	19	7.55
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	20	7.5
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	13	7.49
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	10	7.45
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	20	7.4
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	2	7.34
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	13	7.33
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	3	7.28
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	7	7.08
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	16	7.04
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	18	7.04
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	1	7.03
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	19	6.96
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	2	6.95
(1,95)	1:51:A:SER:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	12	6.94
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	2	6.91
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	7	6.85
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	8	6.81
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	5	6.8
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	17	6.76
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	10	6.72

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	19	6.7
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	2	6.66
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	15	6.64
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	7	6.63
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	15	6.61
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	1	6.56
(1,244)	1:142:A:ASN:N	1:142:A:ASN:CA	1:142:A:ASN:C	1:143:A:GLU:N	20	6.53
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	17	6.52
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	14	6.51
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	15	6.51
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	2	6.49
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	9	6.49
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	16	6.47
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	7	6.47
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	13	6.46
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	6	6.45
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	8	6.45
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	11	6.45
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	15	6.44
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	3	6.44
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	12	6.43
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	20	6.32
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	3	6.3
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	19	6.3
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	18	6.29
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	8	6.27
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	16	6.27
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	12	6.25
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	10	6.23
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	9	6.22
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	17	6.2
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	4	6.18
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	14	6.17
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	13	6.08
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	9	6.07
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	15	6.06
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	5	6.05
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	18	6.03
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	4	6.0
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	14	6.0
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	17	5.98
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	9	5.97
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	2	5.94
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	4	5.91
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	12	5.87
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	18	5.83
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	7	5.82
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	14	5.78
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	11	5.71
(1,92)	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	1:51:A:SER:N	4	5.71
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	6	5.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	1	5.67
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	13	5.66
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	10	5.66
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	9	5.65
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	19	5.63
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	5	5.58
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	12	5.58
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	13	5.57
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	11	5.55
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	1	5.55
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	14	5.51
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	3	5.5
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	5	5.5
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	15	5.49
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	19	5.47
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	4	5.46
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	4	5.45
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	2	5.44
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	9	5.44
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	19	5.44
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	11	5.41
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	1	5.4
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	3	5.36
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	4	5.32
(1,192)	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1:114:A:LEU:N	6	5.32
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	7	5.31
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	12	5.28
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	17	5.28
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	8	5.27
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	2	5.24
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	12	5.24
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	19	5.22
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	17	5.21
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	3	5.2
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	7	5.2
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	6	5.2
(1,93)	1:50:A:GLY:C	1:51:A:SER:N	1:51:A:SER:CA	1:51:A:SER:C	4	5.19
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	20	5.15
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	2	5.14
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	7	5.14
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	9	5.12
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	19	5.12
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	1	5.12
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1	5.11
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	10	5.07
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	20	5.07
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	6	5.05
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	19	5.05
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	9	5.03
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	10	5.01
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	6	5.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	16	4.98
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	16	4.97
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	15	4.96
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	11	4.96
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	5	4.93
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	20	4.93
(1,174)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:TYR:N	2	4.92
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	12	4.91
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	10	4.9
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	1	4.9
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	16	4.89
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	11	4.87
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	3	4.86
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	9	4.8
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	12	4.8
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	8	4.78
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	11	4.77
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	10	4.76
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	17	4.75
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	15	4.73
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	5	4.72
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	13	4.72
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	14	4.71
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	11	4.68
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	16	4.68
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	11	4.65
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	11	4.63
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	18	4.63
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	6	4.62
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	14	4.62
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	17	4.61
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	5	4.6
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	20	4.6
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	3	4.57
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	10	4.56
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	16	4.56
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	8	4.54
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	11	4.53
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	18	4.51
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	20	4.51
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	10	4.51
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	5	4.5
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	11	4.49
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	4	4.48
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	12	4.48
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	15	4.48
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	18	4.47
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	7	4.46
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	8	4.46
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	15	4.45
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	10	4.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	19	4.44
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	7	4.43
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	17	4.42
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	2	4.4
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	17	4.4
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	14	4.39
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	12	4.39
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	7	4.39
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	10	4.38
(1,197)	1:115:A:LEU:C	1:116:A:LEU:N	1:116:A:LEU:CA	1:116:A:LEU:C	20	4.37
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	8	4.37
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	17	4.35
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	20	4.35
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	8	4.35
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	4	4.3
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	3	4.27
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	2	4.27
(1,99)	1:53:A:ARG:C	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	12	4.27
(1,227)	1:132:A:ARG:C	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	17	4.25
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	12	4.24
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	20	4.24
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	7	4.23
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	16	4.2
(1,174)	1:94:A:GLY:N	1:94:A:GLY:CA	1:94:A:GLY:C	1:95:A:TYR:N	1	4.19
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	13	4.18
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	18	4.17
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	13	4.16
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	15	4.13
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	6	4.12
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	7	4.11
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	11	4.1
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	16	4.1
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	15	4.09
(1,225)	1:131:A:LYS:C	1:132:A:ARG:N	1:132:A:ARG:CA	1:132:A:ARG:C	9	4.09
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	14	4.09
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	13	4.08
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	7	4.07
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	16	4.07
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	7	4.07
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	6	4.06
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	2	4.05
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	4	4.05
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	12	4.05
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	12	4.05
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	9	4.04
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	4	4.04
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	6	4.02
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	18	4.02
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	4	4.02
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	18	4.01
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	10	3.99

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	20	3.99
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	6	3.99
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	15	3.98
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	9	3.98
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	12	3.98
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	16	3.98
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	9	3.98
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	17	3.97
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	18	3.95
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	8	3.95
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	17	3.94
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	8	3.94
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	1	3.91
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	4	3.91
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	6	3.9
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	6	3.9
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	17	3.88
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	12	3.87
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	7	3.86
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	3	3.86
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	13	3.85
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	9	3.85
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	15	3.85
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	7	3.84
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	15	3.83
(1,325)	1:184:A:SER:C	1:185:A:GLN:N	1:185:A:GLN:CA	1:185:A:GLN:C	18	3.82
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	6	3.81
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1	3.81
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	4	3.78
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	20	3.78
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	2	3.77
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	20	3.77
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	1	3.76
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	18	3.76
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	17	3.75
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	2	3.75
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	5	3.75
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	9	3.74
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	5	3.74
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	1	3.74
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	14	3.71
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	17	3.71
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	15	3.71
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	16	3.71
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	5	3.7
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	8	3.7
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	10	3.69
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	5	3.68
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	15	3.68
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	19	3.65
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	6	3.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	7	3.64
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	3	3.64
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	16	3.63
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	4	3.63
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	5	3.63
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	17	3.63
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	8	3.62
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	9	3.62
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	5	3.6
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	3	3.59
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	2	3.58
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	14	3.58
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	14	3.58
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	16	3.58
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	3	3.57
(1,186)	1:110:A:GLY:N	1:110:A:GLY:CA	1:110:A:GLY:C	1:111:A:GLN:N	7	3.57
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	13	3.56
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	12	3.55
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	9	3.55
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	8	3.54
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	9	3.54
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	11	3.54
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	13	3.54
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	15	3.54
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	14	3.53
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	19	3.51
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	13	3.51
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	4	3.51
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	2	3.51
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	10	3.5
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	8	3.5
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	18	3.5
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	4	3.49
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	10	3.49
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	11	3.47
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	13	3.47
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	18	3.47
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	16	3.47
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	13	3.46
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	11	3.46
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	18	3.44
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	11	3.43
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	5	3.42
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	15	3.41
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	19	3.41
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	8	3.41
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	1	3.41
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	13	3.4
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	13	3.4
(1,121)	1:65:A:GLN:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	19	3.4
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	15	3.39

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	12	3.39
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	7	3.39
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	5	3.38
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	3	3.38
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	20	3.37
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	6	3.34
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	13	3.33
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	18	3.32
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	14	3.32
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	5	3.32
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	3	3.31
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	3	3.31
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	16	3.31
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	17	3.28
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	10	3.27
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	1	3.27
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	15	3.26
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	8	3.26
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	6	3.24
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	4	3.24
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	14	3.24
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	2	3.23
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	12	3.22
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	15	3.22
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	2	3.22
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	10	3.21
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	1	3.21
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	16	3.2
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	3	3.2
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	12	3.2
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	17	3.18
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	9	3.18
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	1	3.18
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	5	3.18
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	19	3.17
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	13	3.16
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	11	3.15
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	3	3.15
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	17	3.15
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	10	3.14
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	15	3.14
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	3	3.14
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	13	3.13
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	10	3.12
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	19	3.11
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	8	3.11
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	14	3.1
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	8	3.09
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	2	3.09
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	19	3.08
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	18	3.07

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	1	3.07
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	4	3.06
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	16	3.06
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	11	3.06
(1,272)	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1:157:A:THR:N	18	3.05
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	14	3.05
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	7	3.05
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	15	3.05
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	20	3.04
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	10	3.04
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	16	3.03
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	5	3.03
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	4	3.03
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	9	3.02
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	1	3.02
(1,121)	1:65:A:GLN:C	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	7	3.02
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	5	3.01
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	19	3.01
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	9	3.01
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	11	3.01
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	20	3.0
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	20	2.99
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	19	2.98
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	7	2.98
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	18	2.98
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	6	2.98
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	10	2.97
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	18	2.96
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	6	2.95
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	13	2.94
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	3	2.94
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	20	2.93
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	13	2.92
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	18	2.92
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	19	2.91
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	1	2.91
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	15	2.91
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	1	2.9
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	14	2.9
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	13	2.87
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	5	2.87
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	9	2.87
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	10	2.87
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	13	2.86
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	6	2.85
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	4	2.85
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	3	2.85
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	18	2.85
(1,319)	1:181:A:SER:C	1:182:A:VAL:N	1:182:A:VAL:CA	1:182:A:VAL:C	20	2.84
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	15	2.84
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	20	2.84

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	5	2.82
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	3	2.81
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	20	2.81
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	17	2.81
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	2	2.81
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	17	2.81
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	12	2.8
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	6	2.79
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	19	2.79
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	10	2.79
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	20	2.79
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	7	2.79
(1,202)	1:118:A:VAL:N	1:118:A:VAL:CA	1:118:A:VAL:C	1:119:A:ASP:N	19	2.78
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	20	2.78
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	20	2.77
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	14	2.77
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	1	2.77
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	8	2.77
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	20	2.76
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	10	2.76
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	13	2.75
(1,215)	1:126:A:THR:C	1:127:A:GLN:N	1:127:A:GLN:CA	1:127:A:GLN:C	13	2.75
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	16	2.75
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1	2.75
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	14	2.74
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	14	2.72
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	20	2.72
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	2	2.72
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	13	2.71
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	17	2.71
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	12	2.71
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	12	2.71
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	12	2.7
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	17	2.69
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	1	2.69
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	18	2.68
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	15	2.68
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	18	2.68
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:LEU:N	20	2.68
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	14	2.67
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	5	2.67
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	17	2.67
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	1	2.67
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	3	2.66
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	2	2.66
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	7	2.66
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	2	2.66
(1,13)	1:7:A:LYS:C	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	11	2.66
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	2	2.65
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	9	2.65
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	7	2.65

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	19	2.65
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	14	2.64
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	2	2.64
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	20	2.63
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	1	2.63
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	19	2.63
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	4	2.63
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	3	2.61
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	12	2.61
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	10	2.61
(1,68)	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	1:39:A:THR:N	8	2.61
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	7	2.6
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	14	2.6
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	2	2.6
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	6	2.6
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	4	2.59
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	8	2.59
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	15	2.59
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	9	2.59
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	14	2.59
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	18	2.59
(1,57)	1:32:A:TYR:C	1:33:A:GLY:N	1:33:A:GLY:CA	1:33:A:GLY:C	3	2.58
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	14	2.58
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	4	2.57
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	11	2.57
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	2	2.57
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	5	2.57
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	5	2.56
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	9	2.56
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	16	2.55
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	9	2.55
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	13	2.55
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	12	2.55
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	1	2.54
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	12	2.54
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	10	2.53
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	11	2.53
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	8	2.52
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	8	2.51
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	3	2.5
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	12	2.5
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	14	2.49
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	10	2.49
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	18	2.49
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	9	2.49
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	5	2.48
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	4	2.47
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	2	2.46
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	20	2.46
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	2	2.45
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	14	2.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	5	2.45
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	7	2.45
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	8	2.45
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	20	2.45
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	8	2.44
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	4	2.44
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	14	2.43
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	13	2.43
(1,159)	1:85:A:ASN:C	1:86:A:THR:N	1:86:A:THR:CA	1:86:A:THR:C	11	2.43
(1,89)	1:48:A:SER:C	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	11	2.43
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	10	2.43
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	11	2.42
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	7	2.42
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	17	2.41
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	8	2.41
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	12	2.41
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	13	2.4
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	18	2.4
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	15	2.4
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	6	2.4
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	7	2.39
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	7	2.38
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	8	2.38
(1,29)	1:18:A:GLY:C	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	13	2.38
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	15	2.38
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	9	2.37
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	20	2.36
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	3	2.36
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	11	2.36
(1,178)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:ARG:N	3	2.36
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	16	2.35
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	4	2.35
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	8	2.34
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	20	2.34
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	14	2.33
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	15	2.33
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	17	2.33
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	8	2.33
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	11	2.32
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	2	2.32
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	10	2.32
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	12	2.32
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	9	2.32
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	17	2.31
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	12	2.3
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	11	2.3
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:LEU:N	14	2.3
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	9	2.28
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	10	2.27
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	3	2.27
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	7	2.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	16	2.26
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	9	2.25
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	13	2.25
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	8	2.25
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	12	2.24
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	8	2.24
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	11	2.24
(1,230)	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	1:135:A:THR:N	14	2.24
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	5	2.24
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1	2.22
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	18	2.22
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	1	2.22
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	11	2.22
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	12	2.21
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	17	2.21
(1,178)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:ARG:N	6	2.21
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	15	2.2
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	14	2.2
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	11	2.2
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	9	2.2
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	13	2.19
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	2	2.19
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	17	2.19
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	7	2.18
(1,95)	1:51:A:SER:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	4	2.18
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	8	2.17
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	4	2.17
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	13	2.17
(1,33)	1:20:A:GLY:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	9	2.17
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	3	2.16
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	14	2.16
(1,98)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:GLY:N	18	2.16
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	20	2.16
(1,330)	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	1:188:A:THR:N	13	2.15
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	12	2.15
(1,330)	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	1:188:A:THR:N	1	2.14
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	14	2.14
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	4	2.13
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	14	2.13
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	2	2.13
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	19	2.12
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	8	2.12
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	3	2.12
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	13	2.12
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1	2.12
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	18	2.11
(1,100)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:LYS:N	7	2.11
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	14	2.1
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	19	2.09
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	9	2.09
(1,123)	1:66:A:LEU:C	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	7	2.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	20	2.09
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	10	2.08
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	6	2.08
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	13	2.08
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	16	2.07
(1,175)	1:104:A:GLU:C	1:105:A:PHE:N	1:105:A:PHE:CA	1:105:A:PHE:C	17	2.07
(1,95)	1:51:A:SER:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	6	2.07
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	16	2.07
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	20	2.07
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	8	2.06
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	9	2.06
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	18	2.06
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	1	2.06
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	8	2.05
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	17	2.05
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	10	2.04
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	20	2.04
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	11	2.04
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	4	2.03
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	20	2.03
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	15	2.03
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	2	2.03
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	3	2.02
(1,230)	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	1:135:A:THR:N	4	2.02
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	11	2.02
(1,95)	1:51:A:SER:C	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	13	2.02
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	14	2.02
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	3	2.02
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	18	2.01
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	14	2.01
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	16	2.01
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	17	2.01
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	16	2.0
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	8	2.0
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	3	2.0
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	5	1.99
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	15	1.99
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	2	1.99
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	1	1.99
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	19	1.99
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	15	1.98
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	16	1.98
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	10	1.98
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	14	1.97
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	15	1.97
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	16	1.97
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	14	1.97
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	16	1.96
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	16	1.96
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	17	1.96
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	8	1.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	5	1.96
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	1	1.96
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	4	1.95
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	4	1.95
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	19	1.94
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	2	1.94
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	15	1.93
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	16	1.93
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	15	1.93
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	18	1.93
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	9	1.93
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	10	1.92
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	16	1.92
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	11	1.91
(1,225)	1:131:A:LYS:C	1:132:A:ARG:N	1:132:A:ARG:CA	1:132:A:ARG:C	20	1.91
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	6	1.91
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	9	1.91
(1,334)	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	1:190:A:LEU:N	20	1.9
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	4	1.9
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	9	1.9
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	3	1.9
(1,250)	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1:146:A:ILE:N	1	1.9
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	1	1.9
(1,178)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:ARG:N	9	1.9
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	16	1.9
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	19	1.9
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	6	1.89
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	14	1.89
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	3	1.89
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	11	1.89
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	5	1.89
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	18	1.89
(1,329)	1:186:A:VAL:C	1:187:A:CYS:N	1:187:A:CYS:CA	1:187:A:CYS:C	1	1.88
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	17	1.88
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	7	1.88
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	2	1.88
(1,129)	1:69:A:LEU:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	10	1.88
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	19	1.88
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	14	1.88
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	3	1.87
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	3	1.87
(1,82)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:GLU:N	7	1.87
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	13	1.87
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	6	1.87
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:LEU:N	10	1.87
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	2	1.86
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	3	1.86
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	1	1.86
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	6	1.86
(1,197)	1:115:A:LEU:C	1:116:A:LEU:N	1:116:A:LEU:CA	1:116:A:LEU:C	3	1.86
(1,122)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:VAL:N	7	1.86

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:49:A:SER:N	1:49:A:SER:CA	1:49:A:SER:C	1:50:A:GLY:N	6	1.86
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	6	1.86
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	10	1.86
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	4	1.86
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:LEU:N	12	1.86
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	5	1.85
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	11	1.85
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	18	1.85
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	11	1.85
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	1	1.85
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	14	1.84
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	7	1.84
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	12	1.84
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	15	1.84
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	1	1.83
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	17	1.83
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	10	1.82
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	15	1.82
(1,178)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:ARG:N	8	1.82
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	6	1.82
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	8	1.81
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	2	1.81
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	10	1.81
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	2	1.8
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	18	1.8
(1,233)	1:135:A:THR:C	1:136:A:SER:N	1:136:A:SER:CA	1:136:A:SER:C	14	1.8
(1,83)	1:45:A:SER:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	18	1.8
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	15	1.8
(1,278)	1:159:A:PRO:N	1:159:A:PRO:CA	1:159:A:PRO:C	1:160:A:VAL:N	4	1.79
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	17	1.79
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	16	1.79
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	20	1.79
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	12	1.78
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	12	1.78
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	11	1.78
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	14	1.78
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	5	1.78
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	7	1.77
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	10	1.77
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	15	1.77
(1,126)	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	1:69:A:LEU:N	1	1.77
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	20	1.77
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	14	1.77
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	13	1.76
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	12	1.76
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	1	1.76
(1,129)	1:69:A:LEU:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	13	1.76
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	14	1.76
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	15	1.75
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	16	1.75
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	15	1.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	7	1.75
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	8	1.75
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	6	1.75
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	13	1.74
(1,67)	1:37:A:LEU:C	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	3	1.74
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:GLY:N	10	1.74
(1,321)	1:182:A:VAL:C	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	20	1.73
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	5	1.73
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	6	1.73
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	7	1.73
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	12	1.72
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	8	1.72
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	16	1.72
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	20	1.72
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	14	1.72
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	2	1.72
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	2	1.72
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	6	1.71
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	9	1.71
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	19	1.71
(1,155)	1:83:A:LYS:C	1:84:A:VAL:N	1:84:A:VAL:CA	1:84:A:VAL:C	11	1.71
(1,127)	1:68:A:PRO:C	1:69:A:LEU:N	1:69:A:LEU:CA	1:69:A:LEU:C	11	1.7
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	10	1.7
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	18	1.69
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	9	1.69
(1,207)	1:122:A:PRO:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	19	1.69
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	10	1.69
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	3	1.69
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:GLY:N	16	1.69
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	17	1.68
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	19	1.68
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	3	1.68
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	7	1.68
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	7	1.67
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	17	1.67
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	13	1.67
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	1	1.67
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	17	1.67
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	8	1.67
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	8	1.67
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	5	1.67
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	11	1.66
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	4	1.66
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	17	1.66
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	13	1.65
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	1	1.65
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	10	1.65
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	5	1.65
(1,64)	1:36:A:HIS:N	1:36:A:HIS:CA	1:36:A:HIS:C	1:37:A:LEU:N	18	1.65
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	13	1.65
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	13	1.64

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,278)	1:159:A:PRO:N	1:159:A:PRO:CA	1:159:A:PRO:C	1:160:A:VAL:N	2	1.64
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	2	1.64
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	7	1.64
(1,66)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:SER:N	8	1.64
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	14	1.64
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	5	1.64
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	11	1.63
(1,225)	1:131:A:LYS:C	1:132:A:ARG:N	1:132:A:ARG:CA	1:132:A:ARG:C	5	1.63
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	1	1.63
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	6	1.63
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	19	1.63
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	8	1.62
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	14	1.62
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	5	1.62
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	14	1.62
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	4	1.6
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	17	1.6
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	11	1.6
(1,115)	1:61:A:MET:C	1:62:A:GLU:N	1:62:A:GLU:CA	1:62:A:GLU:C	17	1.6
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	9	1.6
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	11	1.6
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	2	1.6
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	10	1.59
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	11	1.58
(1,302)	1:171:A:ARG:N	1:171:A:ARG:CA	1:171:A:ARG:C	1:172:A:LYS:N	9	1.58
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	4	1.58
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	13	1.58
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	17	1.58
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	8	1.58
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	19	1.58
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	5	1.58
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	19	1.57
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	8	1.57
(1,337)	1:190:A:LEU:C	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	12	1.55
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	7	1.55
(1,245)	1:142:A:ASN:C	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	20	1.55
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	18	1.55
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	5	1.55
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	7	1.55
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	4	1.55
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	1	1.54
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	12	1.54
(1,210)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:MET:N	19	1.54
(1,139)	1:74:A:ASP:C	1:75:A:MET:N	1:75:A:MET:CA	1:75:A:MET:C	11	1.54
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	8	1.54
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	7	1.54
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	14	1.53
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	1	1.53
(1,8)	1:5:A:LEU:N	1:5:A:LEU:CA	1:5:A:LEU:C	1:6:A:LYS:N	11	1.53
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	3	1.52
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	11	1.52

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	11	1.52
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	16	1.52
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	11	1.52
(1,31)	1:19:A:SER:C	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	17	1.52
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	13	1.52
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	12	1.52
(1,176)	1:105:A:PHE:N	1:105:A:PHE:CA	1:105:A:PHE:C	1:106:A:GLU:N	14	1.51
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	3	1.51
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	11	1.51
(1,22)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:VAL:N	15	1.51
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	7	1.51
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	19	1.5
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	20	1.5
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	5	1.5
(1,229)	1:133:A:GLY:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	4	1.5
(1,170)	1:92:A:ILE:N	1:92:A:ILE:CA	1:92:A:ILE:C	1:93:A:ASP:N	7	1.5
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	10	1.5
(1,66)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:SER:N	2	1.5
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	6	1.5
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	16	1.49
(1,33)	1:20:A:GLY:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	14	1.49
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	18	1.48
(1,228)	1:133:A:GLY:N	1:133:A:GLY:CA	1:133:A:GLY:C	1:134:A:GLU:N	4	1.48
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	3	1.48
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	2	1.48
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	4	1.48
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	12	1.48
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	17	1.47
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	12	1.47
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	19	1.47
(1,129)	1:69:A:LEU:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	18	1.47
(1,28)	1:18:A:GLY:N	1:18:A:GLY:CA	1:18:A:GLY:C	1:19:A:SER:N	13	1.47
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1	1.46
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	6	1.46
(1,96)	1:52:A:ALA:N	1:52:A:ALA:CA	1:52:A:ALA:C	1:53:A:ARG:N	4	1.46
(1,91)	1:49:A:SER:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	14	1.46
(1,33)	1:20:A:GLY:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	2	1.46
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	12	1.46
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	12	1.45
(1,178)	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	1:107:A:ARG:N	20	1.45
(1,64)	1:36:A:HIS:N	1:36:A:HIS:CA	1:36:A:HIS:C	1:37:A:LEU:N	3	1.45
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	1	1.45
(1,17)	1:10:A:ILE:C	1:11:A:ILE:N	1:11:A:ILE:CA	1:11:A:ILE:C	7	1.45
(1,252)	1:146:A:ILE:N	1:146:A:ILE:CA	1:146:A:ILE:C	1:147:A:LYS:N	20	1.44
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	18	1.44
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	10	1.44
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	3	1.44
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	17	1.44
(1,83)	1:45:A:SER:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	14	1.44
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	13	1.43
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	20	1.43

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,83)	1:45:A:SER:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	1	1.43
(1,82)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:GLU:N	9	1.43
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	7	1.43
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	13	1.42
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	19	1.42
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	2	1.42
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	5	1.42
(1,33)	1:20:A:GLY:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	10	1.42
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	12	1.42
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	4	1.42
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	4	1.41
(1,66)	1:37:A:LEU:N	1:37:A:LEU:CA	1:37:A:LEU:C	1:38:A:SER:N	3	1.41
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	2	1.41
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	17	1.41
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	5	1.4
(1,197)	1:115:A:LEU:C	1:116:A:LEU:N	1:116:A:LEU:CA	1:116:A:LEU:C	10	1.4
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	12	1.4
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	3	1.4
(1,31)	1:19:A:SER:C	1:20:A:GLY:N	1:20:A:GLY:CA	1:20:A:GLY:C	10	1.4
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	16	1.39
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	16	1.39
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	18	1.39
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	16	1.39
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	9	1.39
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	1	1.38
(1,6)	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	1:5:A:LEU:N	16	1.38
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	8	1.37
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	20	1.37
(1,246)	1:143:A:GLU:N	1:143:A:GLU:CA	1:143:A:GLU:C	1:144:A:GLU:N	10	1.37
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	7	1.37
(1,197)	1:115:A:LEU:C	1:116:A:LEU:N	1:116:A:LEU:CA	1:116:A:LEU:C	18	1.37
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	1	1.37
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	9	1.37
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	10	1.37
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	7	1.37
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	1	1.36
(1,129)	1:69:A:LEU:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	14	1.36
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	13	1.36
(1,81)	1:44:A:ARG:C	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	16	1.36
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	4	1.36
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	13	1.36
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	20	1.35
(1,187)	1:110:A:GLY:C	1:111:A:GLN:N	1:111:A:GLN:CA	1:111:A:GLN:C	14	1.35
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	17	1.35
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	14	1.35
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	6	1.35
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	18	1.35
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	3	1.35
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	10	1.34
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	3	1.34
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	8	1.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	18	1.34
(1,298)	1:169:A:ILE:N	1:169:A:ILE:CA	1:169:A:ILE:C	1:170:A:VAL:N	16	1.33
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	2	1.33
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	15	1.33
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	12	1.33
(1,125)	1:67:A:VAL:C	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	10	1.33
(1,77)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	1	1.33
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	17	1.33
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	20	1.33
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	18	1.33
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	6	1.32
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	9	1.32
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	4	1.32
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	7	1.32
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	15	1.32
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1	1.32
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	19	1.32
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	1	1.32
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	10	1.32
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	14	1.31
(1,133)	1:71:A:THR:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	1	1.31
(1,91)	1:49:A:SER:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	18	1.31
(1,22)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:VAL:N	19	1.31
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	13	1.31
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	17	1.3
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	5	1.3
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	9	1.3
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	19	1.3
(1,83)	1:45:A:SER:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	5	1.3
(1,67)	1:37:A:LEU:C	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	18	1.3
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	13	1.3
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	13	1.3
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	3	1.3
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	19	1.29
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	18	1.29
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	18	1.29
(1,100)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:LYS:N	17	1.29
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	2	1.29
(1,271)	1:155:A:LYS:C	1:156:A:ALA:N	1:156:A:ALA:CA	1:156:A:ALA:C	16	1.28
(1,229)	1:133:A:GLY:C	1:134:A:GLU:N	1:134:A:GLU:CA	1:134:A:GLU:C	14	1.28
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	6	1.28
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	6	1.28
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	19	1.28
(1,82)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:GLU:N	4	1.28
(1,13)	1:7:A:LYS:C	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	17	1.28
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	17	1.28
(1,334)	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	1:190:A:LEU:N	15	1.27
(1,219)	1:128:A:ARG:C	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	13	1.27
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	14	1.27
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	8	1.27
(1,133)	1:71:A:THR:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	13	1.27

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,33)	1:20:A:GLY:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	6	1.27
(1,335)	1:189:A:HIS:C	1:190:A:LEU:N	1:190:A:LEU:CA	1:190:A:LEU:C	17	1.26
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	16	1.26
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	13	1.26
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	9	1.26
(1,176)	1:105:A:PHE:N	1:105:A:PHE:CA	1:105:A:PHE:C	1:106:A:GLU:N	20	1.26
(1,133)	1:71:A:THR:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	19	1.26
(1,129)	1:69:A:LEU:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	15	1.26
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	20	1.26
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	18	1.26
(1,77)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	16	1.26
(1,64)	1:36:A:HIS:N	1:36:A:HIS:CA	1:36:A:HIS:C	1:37:A:LEU:N	16	1.26
(1,22)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:VAL:N	14	1.26
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	19	1.26
(1,109)	1:58:A:SER:C	1:59:A:GLU:N	1:59:A:GLU:CA	1:59:A:GLU:C	11	1.25
(1,104)	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	1:57:A:LEU:N	18	1.25
(1,91)	1:49:A:SER:C	1:50:A:GLY:N	1:50:A:GLY:CA	1:50:A:GLY:C	5	1.25
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	18	1.25
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	9	1.24
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	18	1.24
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	8	1.24
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	19	1.24
(1,125)	1:67:A:VAL:C	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	8	1.24
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	15	1.24
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	15	1.24
(1,82)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:GLU:N	20	1.24
(1,62)	1:35:A:THR:N	1:35:A:THR:CA	1:35:A:THR:C	1:36:A:HIS:N	7	1.24
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	2	1.24
(1,9)	1:5:A:LEU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	13	1.24
(1,8)	1:5:A:LEU:N	1:5:A:LEU:CA	1:5:A:LEU:C	1:6:A:LYS:N	4	1.24
(1,340)	1:192:A:ALA:N	1:192:A:ALA:CA	1:192:A:ALA:C	1:193:A:LEU:N	8	1.23
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	19	1.23
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	10	1.23
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	3	1.23
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	19	1.23
(1,60)	1:34:A:TYR:N	1:34:A:TYR:CA	1:34:A:TYR:C	1:35:A:THR:N	18	1.23
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	12	1.23
(1,5)	1:3:A:GLU:C	1:4:A:LYS:N	1:4:A:LYS:CA	1:4:A:LYS:C	15	1.23
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	3	1.22
(1,225)	1:131:A:LYS:C	1:132:A:ARG:N	1:132:A:ARG:CA	1:132:A:ARG:C	12	1.22
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	12	1.22
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	6	1.22
(1,99)	1:53:A:ARG:C	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	13	1.22
(1,64)	1:36:A:HIS:N	1:36:A:HIS:CA	1:36:A:HIS:C	1:37:A:LEU:N	12	1.22
(1,19)	1:11:A:ILE:C	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	18	1.22
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	13	1.22
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	6	1.21
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	1	1.21
(1,125)	1:67:A:VAL:C	1:68:A:PRO:N	1:68:A:PRO:CA	1:68:A:PRO:C	11	1.21
(1,100)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:LYS:N	18	1.21
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	3	1.21

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,71)	1:39:A:THR:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	5	1.21
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	3	1.2
(1,278)	1:159:A:PRO:N	1:159:A:PRO:CA	1:159:A:PRO:C	1:160:A:VAL:N	11	1.2
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	6	1.2
(1,124)	1:67:A:VAL:N	1:67:A:VAL:CA	1:67:A:VAL:C	1:68:A:PRO:N	6	1.2
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	11	1.2
(1,77)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	8	1.2
(1,77)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	17	1.2
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	18	1.19
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	14	1.19
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	17	1.19
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	15	1.19
(1,103)	1:55:A:LYS:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	5	1.19
(1,54)	1:31:A:LYS:N	1:31:A:LYS:CA	1:31:A:LYS:C	1:32:A:TYR:N	1	1.19
(1,197)	1:115:A:LEU:C	1:116:A:LEU:N	1:116:A:LEU:CA	1:116:A:LEU:C	8	1.18
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	20	1.18
(1,340)	1:192:A:ALA:N	1:192:A:ALA:CA	1:192:A:ALA:C	1:193:A:LEU:N	17	1.17
(1,310)	1:176:A:GLU:N	1:176:A:GLU:CA	1:176:A:GLU:C	1:177:A:GLY:N	19	1.17
(1,291)	1:165:A:GLU:C	1:166:A:LYS:N	1:166:A:LYS:CA	1:166:A:LYS:C	17	1.17
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	12	1.17
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	8	1.17
(1,197)	1:115:A:LEU:C	1:116:A:LEU:N	1:116:A:LEU:CA	1:116:A:LEU:C	16	1.17
(1,195)	1:114:A:LEU:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	13	1.17
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	5	1.17
(1,103)	1:55:A:LYS:C	1:56:A:LYS:N	1:56:A:LYS:CA	1:56:A:LYS:C	19	1.17
(1,249)	1:144:A:GLU:C	1:145:A:THR:N	1:145:A:THR:CA	1:145:A:THR:C	2	1.16
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	6	1.16
(1,83)	1:45:A:SER:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	16	1.16
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	6	1.16
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	9	1.15
(1,222)	1:130:A:LEU:N	1:130:A:LEU:CA	1:130:A:LEU:C	1:131:A:LYS:N	4	1.15
(1,165)	1:89:A:GLY:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	7	1.15
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	14	1.15
(1,64)	1:36:A:HIS:N	1:36:A:HIS:CA	1:36:A:HIS:C	1:37:A:LEU:N	2	1.15
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	5	1.15
(1,30)	1:19:A:SER:N	1:19:A:SER:CA	1:19:A:SER:C	1:20:A:GLY:N	6	1.15
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	5	1.14
(1,242)	1:141:A:ASP:N	1:141:A:ASP:CA	1:141:A:ASP:C	1:142:A:ASN:N	7	1.14
(1,199)	1:116:A:LEU:C	1:117:A:TYR:N	1:117:A:TYR:CA	1:117:A:TYR:C	10	1.14
(1,83)	1:45:A:SER:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	10	1.14
(1,64)	1:36:A:HIS:N	1:36:A:HIS:CA	1:36:A:HIS:C	1:37:A:LEU:N	15	1.14
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	15	1.14
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	7	1.14
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	13	1.13
(1,195)	1:114:A:LEU:C	1:115:A:LEU:N	1:115:A:LEU:CA	1:115:A:LEU:C	20	1.13
(1,149)	1:79:A:ALA:C	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	14	1.13
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	8	1.13
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	2	1.13
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	10	1.13
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	18	1.12
(1,273)	1:156:A:ALA:C	1:157:A:THR:N	1:157:A:THR:CA	1:157:A:THR:C	3	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,151)	1:80:A:MET:C	1:81:A:VAL:N	1:81:A:VAL:CA	1:81:A:VAL:C	19	1.12
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	12	1.12
(1,133)	1:71:A:THR:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	12	1.12
(1,129)	1:69:A:LEU:C	1:70:A:GLU:N	1:70:A:GLU:CA	1:70:A:GLU:C	1	1.12
(1,67)	1:37:A:LEU:C	1:38:A:SER:N	1:38:A:SER:CA	1:38:A:SER:C	2	1.12
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	2	1.12
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	1	1.11
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	8	1.11
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	9	1.11
(1,82)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:GLU:N	17	1.11
(1,22)	1:13:A:VAL:N	1:13:A:VAL:CA	1:13:A:VAL:C	1:14:A:VAL:N	9	1.11
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	16	1.11
(1,9)	1:5:A:LEU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	3	1.11
(1,333)	1:188:A:THR:C	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	20	1.1
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	4	1.1
(1,176)	1:105:A:PHE:N	1:105:A:PHE:CA	1:105:A:PHE:C	1:106:A:GLU:N	17	1.1
(1,26)	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	1:18:A:GLY:N	6	1.1
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	6	1.09
(1,190)	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	1:113:A:THR:N	4	1.09
(1,181)	1:107:A:ARG:C	1:108:A:ARG:N	1:108:A:ARG:CA	1:108:A:ARG:C	6	1.09
(1,169)	1:91:A:LEU:C	1:92:A:ILE:N	1:92:A:ILE:CA	1:92:A:ILE:C	18	1.09
(1,161)	1:87:A:SER:C	1:88:A:LYS:N	1:88:A:LYS:CA	1:88:A:LYS:C	3	1.09
(1,157)	1:84:A:VAL:C	1:85:A:ASN:N	1:85:A:ASN:CA	1:85:A:ASN:C	11	1.09
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	13	1.09
(1,133)	1:71:A:THR:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	16	1.09
(1,77)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	4	1.09
(1,13)	1:7:A:LYS:C	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	16	1.09
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	10	1.09
(1,8)	1:5:A:LEU:N	1:5:A:LEU:CA	1:5:A:LEU:C	1:6:A:LYS:N	20	1.09
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	14	1.09
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	15	1.09
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	10	1.08
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	2	1.08
(1,184)	1:109:A:ILE:N	1:109:A:ILE:CA	1:109:A:ILE:C	1:110:A:GLY:N	18	1.08
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	20	1.08
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	2	1.07
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	13	1.07
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	1	1.07
(1,268)	1:154:A:TYR:N	1:154:A:TYR:CA	1:154:A:TYR:C	1:155:A:LYS:N	11	1.07
(1,217)	1:127:A:GLN:C	1:128:A:ARG:N	1:128:A:ARG:CA	1:128:A:ARG:C	5	1.07
(1,177)	1:105:A:PHE:C	1:106:A:GLU:N	1:106:A:GLU:CA	1:106:A:GLU:C	12	1.07
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	7	1.07
(1,334)	1:189:A:HIS:N	1:189:A:HIS:CA	1:189:A:HIS:C	1:190:A:LEU:N	12	1.06
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	2	1.06
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	15	1.06
(1,247)	1:143:A:GLU:C	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	2	1.06
(1,191)	1:112:A:PRO:C	1:113:A:THR:N	1:113:A:THR:CA	1:113:A:THR:C	9	1.06
(1,88)	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	1:49:A:SER:N	6	1.06
(1,82)	1:45:A:SER:N	1:45:A:SER:CA	1:45:A:SER:C	1:46:A:GLU:N	11	1.06
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	12	1.06
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	3	1.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:6:A:LYS:C	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	16	1.06
(1,312)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	9	1.05
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	17	1.05
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	3	1.05
(1,220)	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	1:130:A:LEU:N	18	1.05
(1,180)	1:107:A:ARG:N	1:107:A:ARG:CA	1:107:A:ARG:C	1:108:A:ARG:N	5	1.05
(1,100)	1:54:A:GLY:N	1:54:A:GLY:CA	1:54:A:GLY:C	1:55:A:LYS:N	16	1.05
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	18	1.05
(1,14)	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	1:9:A:LYS:N	19	1.05
(1,338)	1:191:A:ASP:N	1:191:A:ASP:CA	1:191:A:ASP:C	1:192:A:ALA:N	7	1.04
(1,189)	1:111:A:GLN:C	1:112:A:PRO:N	1:112:A:PRO:CA	1:112:A:PRO:C	19	1.04
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	1	1.04
(1,154)	1:82:A:ALA:N	1:82:A:ALA:CA	1:82:A:ALA:C	1:83:A:LYS:N	12	1.04
(1,149)	1:79:A:ALA:C	1:80:A:MET:N	1:80:A:MET:CA	1:80:A:MET:C	7	1.04
(1,98)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:GLY:N	11	1.04
(1,74)	1:41:A:ASP:N	1:41:A:ASP:CA	1:41:A:ASP:C	1:42:A:LEU:N	2	1.04
(1,71)	1:39:A:THR:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	12	1.04
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	5	1.04
(1,280)	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	1:161:A:ILE:N	20	1.03
(1,145)	1:77:A:ARG:C	1:78:A:ASP:N	1:78:A:ASP:CA	1:78:A:ASP:C	10	1.03
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	4	1.03
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	15	1.03
(1,87)	1:47:A:VAL:C	1:48:A:SER:N	1:48:A:SER:CA	1:48:A:SER:C	13	1.03
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	18	1.03
(1,13)	1:7:A:LYS:C	1:8:A:THR:N	1:8:A:THR:CA	1:8:A:THR:C	5	1.03
(1,225)	1:131:A:LYS:C	1:132:A:ARG:N	1:132:A:ARG:CA	1:132:A:ARG:C	1	1.02
(1,144)	1:77:A:ARG:N	1:77:A:ARG:CA	1:77:A:ARG:C	1:78:A:ASP:N	5	1.02
(1,101)	1:54:A:GLY:C	1:55:A:LYS:N	1:55:A:LYS:CA	1:55:A:LYS:C	9	1.02
(1,97)	1:52:A:ALA:C	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	16	1.02
(1,20)	1:12:A:PHE:N	1:12:A:PHE:CA	1:12:A:PHE:C	1:13:A:VAL:N	4	1.02
(1,288)	1:164:A:TYR:N	1:164:A:TYR:CA	1:164:A:TYR:C	1:165:A:GLU:N	14	1.01
(1,269)	1:154:A:TYR:C	1:155:A:LYS:N	1:155:A:LYS:CA	1:155:A:LYS:C	6	1.01
(1,259)	1:149:A:ARG:C	1:150:A:LEU:N	1:150:A:LEU:CA	1:150:A:LEU:C	18	1.01
(1,236)	1:137:A:GLY:N	1:137:A:GLY:CA	1:137:A:GLY:C	1:138:A:ARG:N	4	1.01
(1,219)	1:128:A:ARG:C	1:129:A:LEU:N	1:129:A:LEU:CA	1:129:A:LEU:C	5	1.01
(1,133)	1:71:A:THR:C	1:72:A:VAL:N	1:72:A:VAL:CA	1:72:A:VAL:C	18	1.01
(1,122)	1:66:A:LEU:N	1:66:A:LEU:CA	1:66:A:LEU:C	1:67:A:VAL:N	19	1.01
(1,77)	1:42:A:LEU:C	1:43:A:LEU:N	1:43:A:LEU:CA	1:43:A:LEU:C	20	1.01
(1,41)	1:24:A:GLN:C	1:25:A:CYS:N	1:25:A:CYS:CA	1:25:A:CYS:C	16	1.01
(1,39)	1:23:A:THR:C	1:24:A:GLN:N	1:24:A:GLN:CA	1:24:A:GLN:C	8	1.01
(1,9)	1:5:A:LEU:C	1:6:A:LYS:N	1:6:A:LYS:CA	1:6:A:LYS:C	9	1.01
(1,3)	1:2:A:GLU:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	9	1.01
(1,312)	1:178:A:SER:N	1:178:A:SER:CA	1:178:A:SER:C	1:179:A:VAL:N	16	1.0
(1,279)	1:159:A:PRO:C	1:160:A:VAL:N	1:160:A:VAL:CA	1:160:A:VAL:C	3	1.0
(1,217)	1:127:A:GLN:C	1:128:A:ARG:N	1:128:A:ARG:CA	1:128:A:ARG:C	20	1.0
(1,98)	1:53:A:ARG:N	1:53:A:ARG:CA	1:53:A:ARG:C	1:54:A:GLY:N	3	1.0
(1,71)	1:39:A:THR:C	1:40:A:GLY:N	1:40:A:GLY:CA	1:40:A:GLY:C	1	1.0
(1,70)	1:39:A:THR:N	1:39:A:THR:CA	1:39:A:THR:C	1:40:A:GLY:N	9	1.0
(1,12)	1:7:A:LYS:N	1:7:A:LYS:CA	1:7:A:LYS:C	1:8:A:THR:N	7	1.0