



Full wwPDB NMR Structure Validation Report ⓘ

Mar 15, 2026 – 01:41 PM UTC

PDB ID : 6FZK / pdb_00006fzk
BMRB ID : 34246
Title : NMR structure of UB2H, regulatory domain of PBP1b from E. coli
Authors : Simorre, J.P.; Maya Martinez, R.C.; Bougault, C.; Egan, A.J.F.; Vollmer, W.
Deposited on : 2018-03-15

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

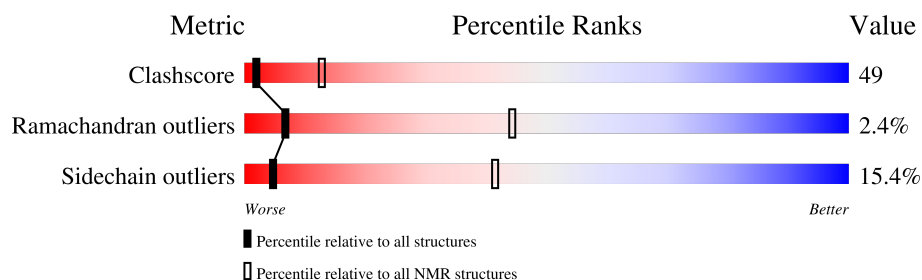
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	114	23% 41% 5% 31%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:109-A:156, A:168-A:198 (79)	0.52	4

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

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

The models can be grouped into 5 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1826 atoms, of which 904 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Penicillin-binding protein 1B.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1826	568	904	178	168	8	

There are 21 discrepancies between the modelled and reference sequences:

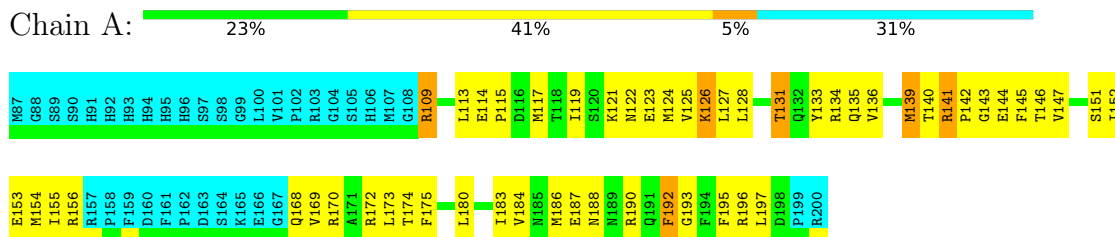
Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MET	-	initiating methionine	UNP P02919
A	88	GLY	-	expression tag	UNP P02919
A	89	SER	-	expression tag	UNP P02919
A	90	SER	-	expression tag	UNP P02919
A	91	HIS	-	expression tag	UNP P02919
A	92	HIS	-	expression tag	UNP P02919
A	93	HIS	-	expression tag	UNP P02919
A	94	HIS	-	expression tag	UNP P02919
A	95	HIS	-	expression tag	UNP P02919
A	96	HIS	-	expression tag	UNP P02919
A	97	SER	-	expression tag	UNP P02919
A	98	SER	-	expression tag	UNP P02919
A	99	GLY	-	expression tag	UNP P02919
A	100	LEU	-	expression tag	UNP P02919
A	101	VAL	-	expression tag	UNP P02919
A	102	PRO	-	expression tag	UNP P02919
A	103	ARG	-	expression tag	UNP P02919
A	104	GLY	-	expression tag	UNP P02919
A	105	SER	-	expression tag	UNP P02919
A	106	HIS	-	expression tag	UNP P02919
A	107	MET	-	expression tag	UNP P02919

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Penicillin-binding protein 1B

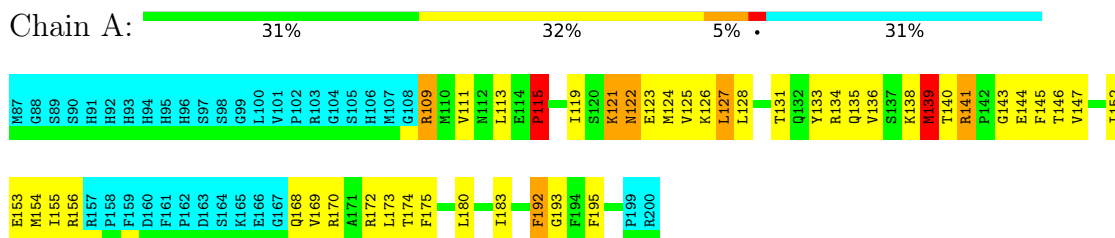


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

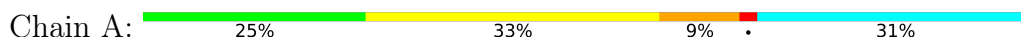
4.2.1 Score per residue for model 1

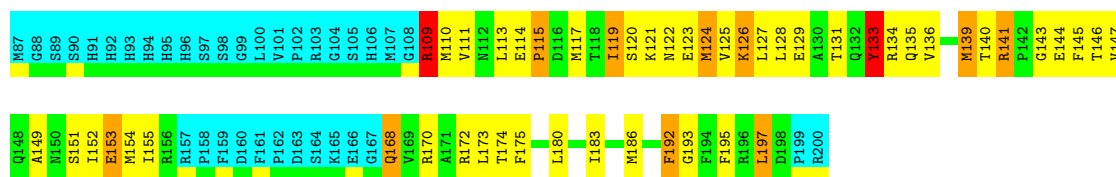
- Molecule 1: Penicillin-binding protein 1B



4.2.2 Score per residue for model 2

- Molecule 1: Penicillin-binding protein 1B

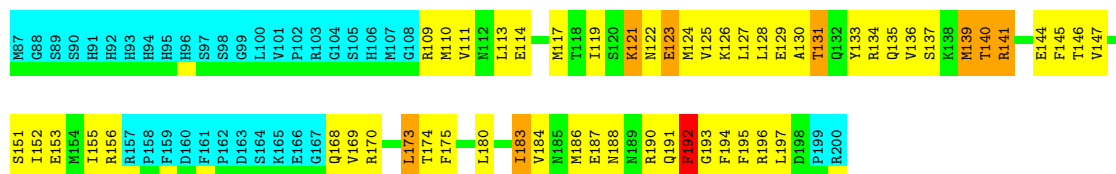




4.2.3 Score per residue for model 3

- Molecule 1: Penicillin-binding protein 1B

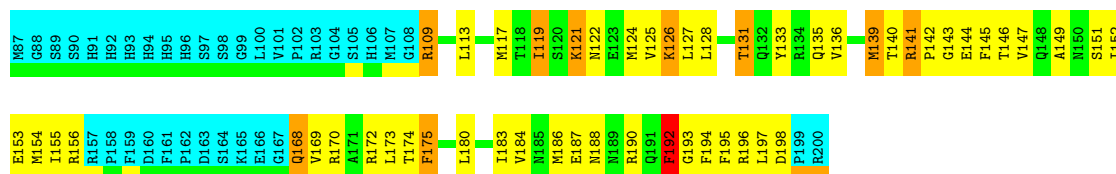
Chain A: 21% 40% 7% 31%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Penicillin-binding protein 1B

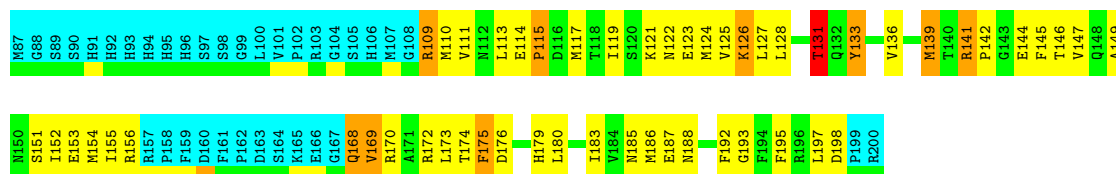
Chain A: 24% 37% 8% 31%



4.2.5 Score per residue for model 5

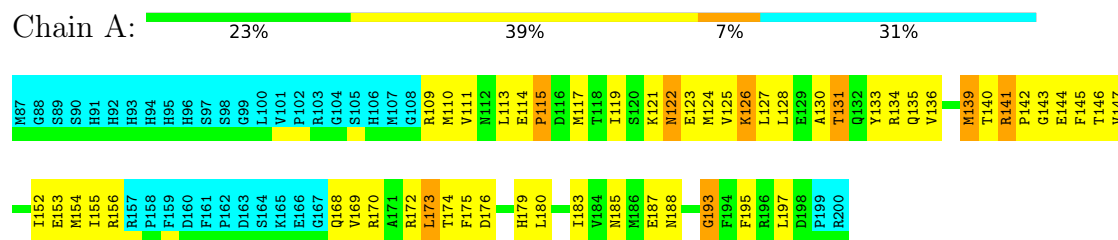
- Molecule 1: Penicillin-binding protein 1B

Chain A: 23% 38% 8% 31%



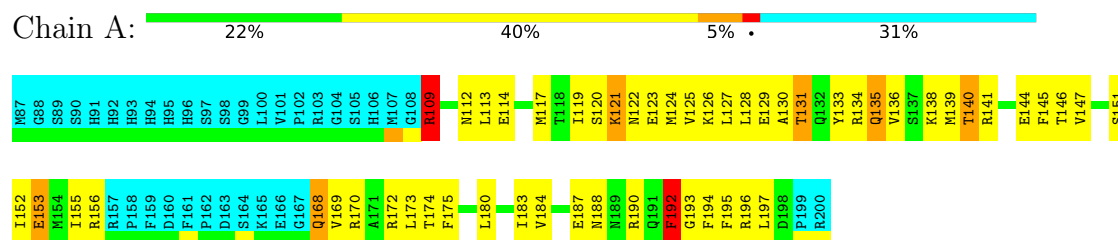
4.2.6 Score per residue for model 6

- Molecule 1: Penicillin-binding protein 1B



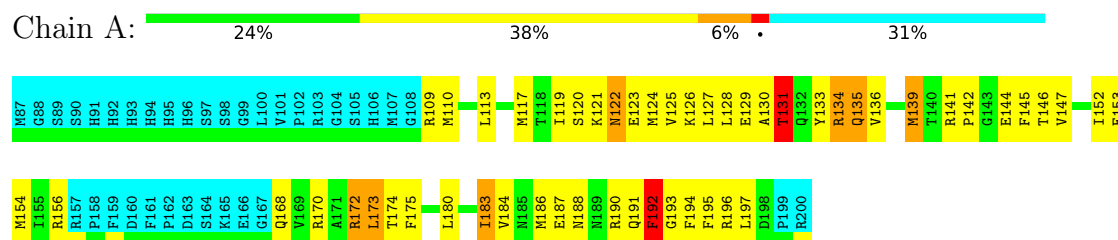
4.2.7 Score per residue for model 7

- Molecule 1: Penicillin-binding protein 1B



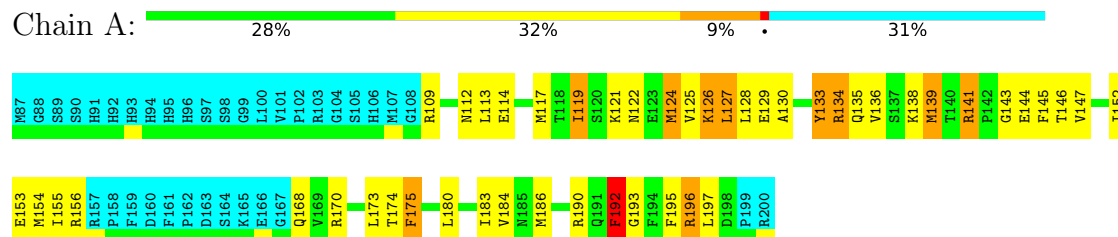
4.2.8 Score per residue for model 8

- Molecule 1: Penicillin-binding protein 1B



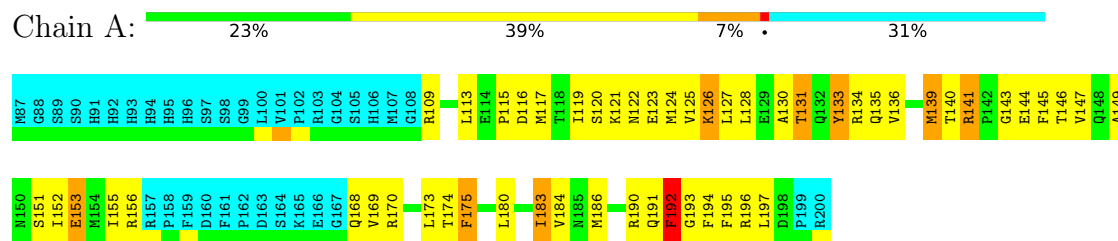
4.2.9 Score per residue for model 9

- Molecule 1: Penicillin-binding protein 1B



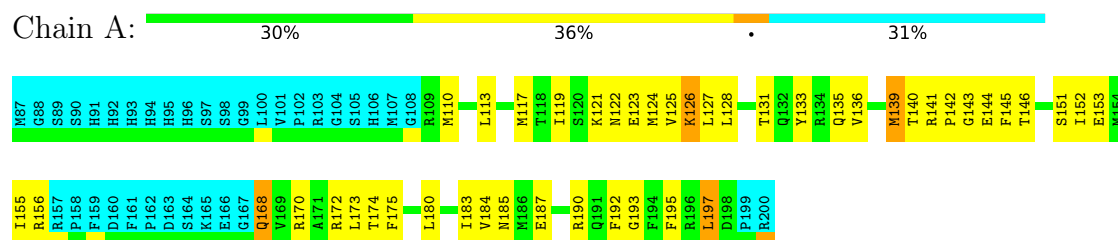
4.2.10 Score per residue for model 10

- Molecule 1: Penicillin-binding protein 1B



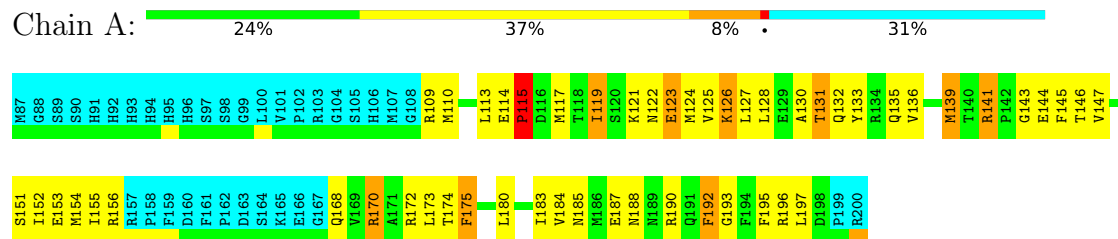
4.2.11 Score per residue for model 11

- Molecule 1: Penicillin-binding protein 1B



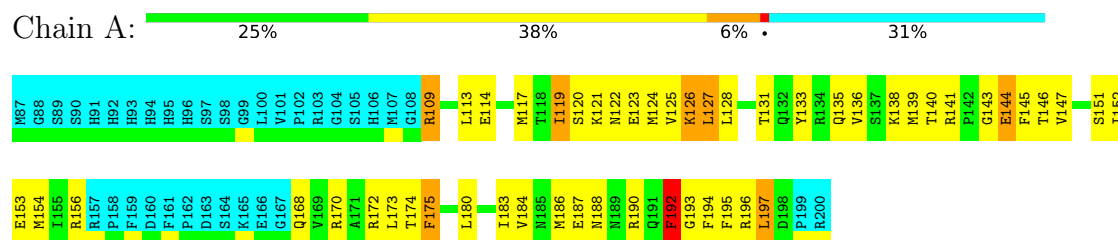
4.2.12 Score per residue for model 12

- Molecule 1: Penicillin-binding protein 1B



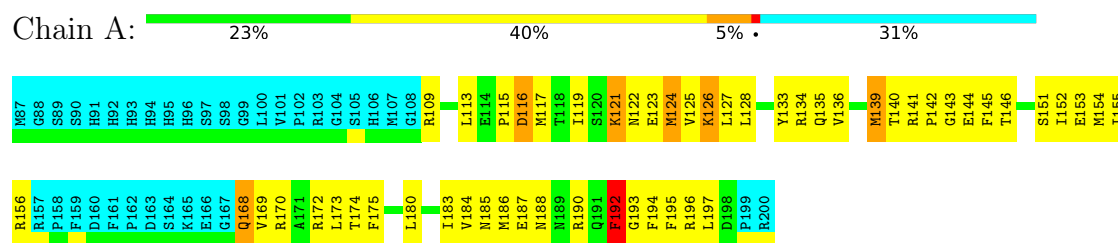
4.2.13 Score per residue for model 13

- Molecule 1: Penicillin-binding protein 1B



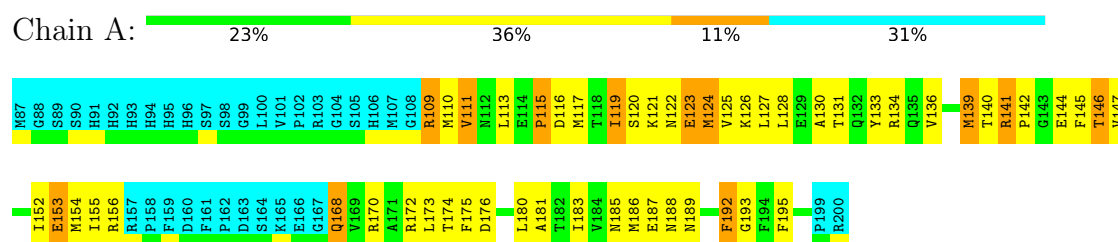
4.2.14 Score per residue for model 14

- Molecule 1: Penicillin-binding protein 1B



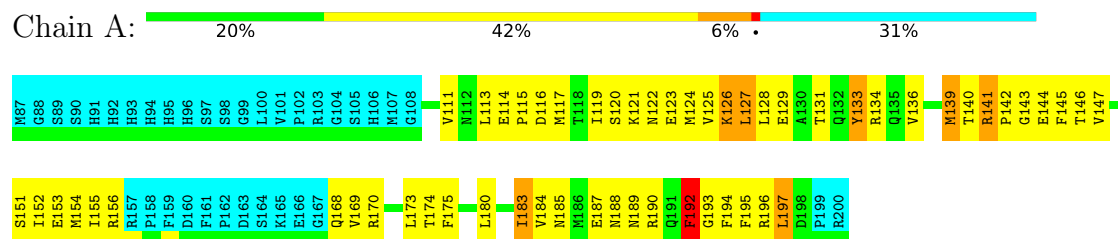
4.2.15 Score per residue for model 15

- Molecule 1: Penicillin-binding protein 1B



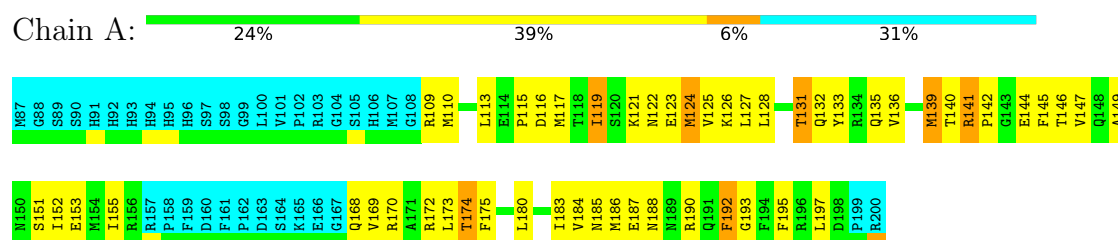
4.2.16 Score per residue for model 16

- Molecule 1: Penicillin-binding protein 1B



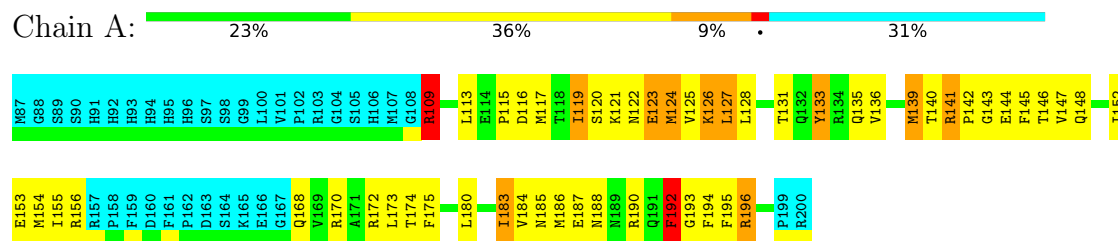
4.2.17 Score per residue for model 17

- Molecule 1: Penicillin-binding protein 1B



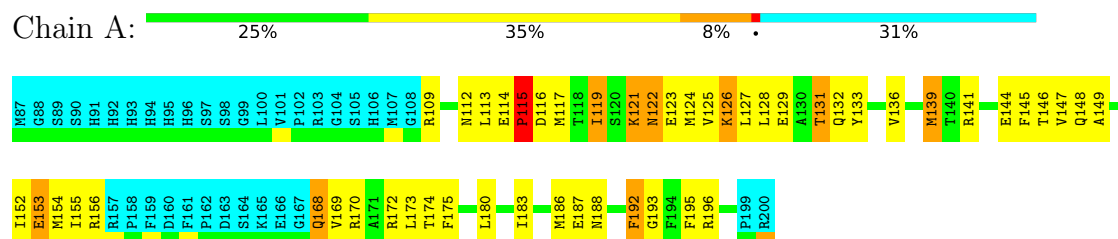
4.2.18 Score per residue for model 18

- Molecule 1: Penicillin-binding protein 1B



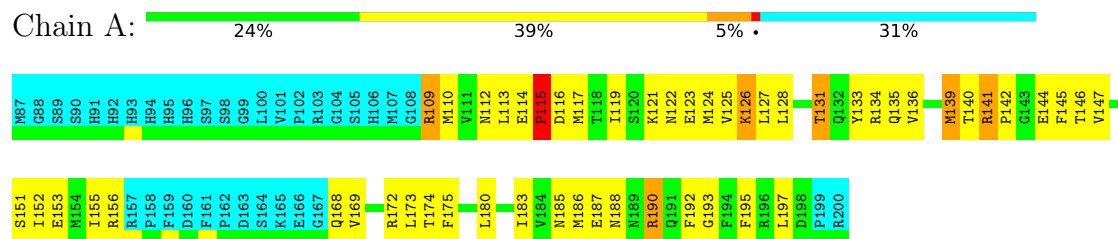
4.2.19 Score per residue for model 19

- Molecule 1: Penicillin-binding protein 1B



4.2.20 Score per residue for model 20

- Molecule 1: Penicillin-binding protein 1B



5 Refinement protocol and experimental data overview

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

Of the 750 calculated structures, 20 were deposited, based on the following criterion: *20*.

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

Software name	Classification	Version
ARIA	structure calculation	2.3
CNS	refinement	1.2
UNIO	structure calculation	2.0.2

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	1098
Number of shifts mapped to atoms	1098
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.97±0.04	0±1/656 (0.1± 0.1%)	1.05±0.03	1±1/882 (0.1± 0.1%)
All	All	0.97	9/13120 (0.1%)	1.05	21/17640 (0.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.4
All	All	0	19

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	133	TYR	CE1-CZ	6.41	1.53	1.38	2	3
1	A	133	TYR	CE2-CZ	-5.74	1.24	1.38	2	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	114	GLU	CA-C-N	6.04	127.40	119.84	5	5
1	A	114	GLU	C-N-CA	6.04	127.40	119.84	5	5
1	A	131	THR	N-CA-C	-5.93	105.81	113.16	7	11

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	192	PHE	Peptide	16
1	A	139	MET	Peptide	1
1	A	133	TYR	Sidechain	1
1	A	193	GLY	Peptide	1

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	647	651	650	64±8
All	All	12940	13020	13000	1276

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 49.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:ARG:HG2	1:A:186:MET:HE3	1.05	1.26	3	5
1:A:133:TYR:CE1	1:A:144:GLU:HG2	0.89	2.02	7	4
1:A:121:LYS:HA	1:A:124:MET:SD	0.87	2.09	18	2
1:A:122:ASN:O	1:A:125:VAL:HG12	0.85	1.71	6	20
1:A:170:ARG:CG	1:A:186:MET:HE3	0.82	2.04	3	2
1:A:124:MET:HE2	1:A:124:MET:HA	0.80	1.53	4	5
1:A:119:ILE:HD11	1:A:124:MET:HE3	0.80	1.53	4	5
1:A:145:PHE:HB2	1:A:153:GLU:O	0.79	1.76	6	15
1:A:121:LYS:HG2	1:A:147:VAL:HG21	0.77	1.56	5	14
1:A:124:MET:HG3	1:A:152:ILE:HG21	0.75	1.56	15	2
1:A:115:PRO:CD	1:A:193:GLY:HA2	0.74	2.11	5	2
1:A:113:LEU:HB2	1:A:195:PHE:O	0.74	1.82	4	19
1:A:109:ARG:HA	1:A:122:ASN:O	0.74	1.83	17	4
1:A:124:MET:HE2	1:A:173:LEU:HD23	0.74	1.57	7	3
1:A:113:LEU:HD13	1:A:173:LEU:HD21	0.73	1.58	13	2
1:A:133:TYR:CE1	1:A:144:GLU:HG3	0.73	2.17	12	10
1:A:124:MET:SD	1:A:152:ILE:HD12	0.73	2.24	11	2
1:A:136:VAL:HG12	1:A:145:PHE:O	0.73	1.83	3	16
1:A:124:MET:O	1:A:128:LEU:HG	0.73	1.82	4	20
1:A:113:LEU:HD12	1:A:195:PHE:HB3	0.72	1.61	13	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:ARG:HG2	1:A:197:LEU:HD22	0.72	1.62	5	1
1:A:155:ILE:HA	1:A:169:VAL:O	0.71	1.84	19	11
1:A:156:ARG:O	1:A:168:GLN:HA	0.71	1.85	4	15
1:A:127:LEU:HD13	1:A:197:LEU:HD13	0.71	1.61	8	1
1:A:128:LEU:HB3	1:A:145:PHE:CE2	0.69	2.23	10	20
1:A:127:LEU:HG	1:A:197:LEU:HD13	0.69	1.63	7	5
1:A:125:VAL:HG13	1:A:126:LYS:HE3	0.69	1.64	6	4
1:A:124:MET:SD	1:A:128:LEU:HD21	0.68	2.28	2	1
1:A:136:VAL:HG23	1:A:146:THR:HG22	0.68	1.64	2	4
1:A:172:ARG:O	1:A:183:ILE:HA	0.68	1.87	6	15
1:A:109:ARG:HB2	1:A:126:LYS:CG	0.67	2.19	18	2
1:A:124:MET:SD	1:A:173:LEU:HD23	0.67	2.30	1	6
1:A:135:GLN:HG3	1:A:147:VAL:O	0.67	1.90	12	7
1:A:124:MET:SD	1:A:173:LEU:HD22	0.67	2.29	13	1
1:A:147:VAL:HG23	1:A:152:ILE:HG12	0.66	1.66	10	15
1:A:133:TYR:CD1	1:A:144:GLU:HG2	0.65	2.26	7	3
1:A:126:LYS:CE	1:A:126:LYS:HA	0.65	2.21	4	13
1:A:124:MET:SD	1:A:152:ILE:HD13	0.65	2.32	15	3
1:A:115:PRO:HD3	1:A:183:ILE:HD12	0.64	1.70	20	5
1:A:113:LEU:HA	1:A:117:MET:HE1	0.64	1.69	8	4
1:A:124:MET:HE3	1:A:127:LEU:HD22	0.64	1.69	10	1
1:A:127:LEU:HD23	1:A:128:LEU:HD23	0.64	1.69	11	8
1:A:128:LEU:HD22	1:A:145:PHE:CD2	0.64	2.27	17	13
1:A:113:LEU:HD21	1:A:173:LEU:HD21	0.63	1.70	7	5
1:A:184:VAL:HA	1:A:190:ARG:O	0.63	1.92	14	13
1:A:133:TYR:CG	1:A:144:GLU:HA	0.63	2.28	13	10
1:A:111:VAL:HG12	1:A:127:LEU:N	0.63	2.07	6	1
1:A:119:ILE:HG22	1:A:180:LEU:HB2	0.63	1.70	2	16
1:A:127:LEU:CG	1:A:197:LEU:HD13	0.63	2.24	7	6
1:A:124:MET:HG3	1:A:152:ILE:HD12	0.62	1.71	6	2
1:A:196:ARG:N	1:A:196:ARG:HD3	0.62	2.10	10	2
1:A:133:TYR:CZ	1:A:144:GLU:HG3	0.62	2.29	9	8
1:A:119:ILE:HG21	1:A:124:MET:HE3	0.62	1.72	11	1
1:A:172:ARG:CB	1:A:184:VAL:HB	0.62	2.24	8	1
1:A:139:MET:HB2	1:A:144:GLU:CD	0.62	2.20	13	1
1:A:140:THR:O	1:A:141:ARG:HD3	0.61	1.96	1	2
1:A:119:ILE:CG2	1:A:180:LEU:HB2	0.60	2.26	17	17
1:A:156:ARG:O	1:A:156:ARG:HD3	0.60	1.95	19	1
1:A:121:LYS:O	1:A:125:VAL:HB	0.60	1.95	15	12
1:A:113:LEU:HB2	1:A:195:PHE:HB3	0.60	1.73	2	8
1:A:128:LEU:HD22	1:A:145:PHE:CG	0.60	2.32	12	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:PRO:HD3	1:A:183:ILE:CD1	0.60	2.26	20	4
1:A:195:PHE:C	1:A:196:ARG:HD2	0.60	2.22	12	3
1:A:155:ILE:HG22	1:A:168:GLN:HG2	0.59	1.73	5	1
1:A:113:LEU:HB3	1:A:183:ILE:CD1	0.59	2.27	20	3
1:A:113:LEU:HA	1:A:117:MET:CE	0.59	2.27	8	6
1:A:151:SER:HA	1:A:173:LEU:O	0.59	1.98	20	13
1:A:183:ILE:HB	1:A:192:PHE:CB	0.59	2.27	19	13
1:A:124:MET:CE	1:A:173:LEU:HD23	0.59	2.28	7	4
1:A:109:ARG:HB3	1:A:126:LYS:CG	0.59	2.27	9	2
1:A:110:MET:H	1:A:123:GLU:HA	0.58	1.59	3	6
1:A:136:VAL:HG13	1:A:146:THR:HG22	0.58	1.74	6	11
1:A:139:MET:SD	1:A:146:THR:HG23	0.58	2.38	20	4
1:A:133:TYR:HB2	1:A:143:GLY:O	0.58	1.97	10	6
1:A:113:LEU:HD11	1:A:127:LEU:CD1	0.58	2.28	13	2
1:A:124:MET:CG	1:A:152:ILE:HD13	0.58	2.29	15	3
1:A:113:LEU:HD23	1:A:173:LEU:HD11	0.58	1.74	9	1
1:A:153:GLU:HG2	1:A:186:MET:SD	0.58	2.39	10	6
1:A:117:MET:SD	1:A:180:LEU:HB3	0.58	2.39	14	2
1:A:124:MET:O	1:A:127:LEU:HB3	0.57	1.99	16	18
1:A:124:MET:SD	1:A:128:LEU:HD11	0.57	2.39	15	3
1:A:156:ARG:HD3	1:A:156:ARG:C	0.57	2.24	19	1
1:A:195:PHE:C	1:A:196:ARG:HD3	0.57	2.23	13	2
1:A:155:ILE:HG23	1:A:168:GLN:HG3	0.57	1.74	12	2
1:A:185:ASN:OD1	1:A:187:GLU:HG2	0.57	1.99	12	7
1:A:113:LEU:HA	1:A:117:MET:HE3	0.57	1.75	10	3
1:A:124:MET:HE2	1:A:127:LEU:HG	0.57	1.76	17	1
1:A:133:TYR:CE2	1:A:144:GLU:HG3	0.57	2.34	9	2
1:A:112:ASN:O	1:A:117:MET:HE1	0.56	2.00	19	3
1:A:138:LYS:HD2	1:A:138:LYS:C	0.56	2.26	7	4
1:A:154:MET:O	1:A:170:ARG:HA	0.56	2.01	12	9
1:A:141:ARG:HG3	1:A:144:GLU:CD	0.56	2.25	12	8
1:A:136:VAL:CG1	1:A:146:THR:HG22	0.56	2.30	15	10
1:A:156:ARG:NH1	1:A:198:ASP:HB3	0.56	2.14	5	1
1:A:124:MET:SD	1:A:152:ILE:HB	0.56	2.41	13	1
1:A:140:THR:C	1:A:141:ARG:HD3	0.56	2.25	1	2
1:A:183:ILE:HB	1:A:192:PHE:HB2	0.56	1.76	12	7
1:A:124:MET:SD	1:A:152:ILE:HG21	0.56	2.41	2	1
1:A:155:ILE:HG12	1:A:170:ARG:HG3	0.56	1.78	2	7
1:A:111:VAL:HG11	1:A:127:LEU:N	0.55	2.16	15	1
1:A:124:MET:SD	1:A:154:MET:HE1	0.55	2.41	12	1
1:A:127:LEU:HA	1:A:197:LEU:CD1	0.55	2.32	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ILE:CG2	1:A:168:GLN:HG3	0.55	2.31	4	10
1:A:152:ILE:O	1:A:173:LEU:HB2	0.55	2.02	6	14
1:A:196:ARG:HD3	1:A:196:ARG:H	0.55	1.62	16	2
1:A:133:TYR:CD1	1:A:144:GLU:HA	0.55	2.36	13	16
1:A:117:MET:SD	1:A:180:LEU:HD22	0.55	2.42	17	3
1:A:156:ARG:HG2	1:A:197:LEU:CD2	0.54	2.31	5	1
1:A:141:ARG:HG2	1:A:144:GLU:CD	0.54	2.27	1	3
1:A:127:LEU:HD12	1:A:128:LEU:HD23	0.54	1.77	2	3
1:A:113:LEU:HD22	1:A:195:PHE:HB3	0.54	1.78	9	3
1:A:120:SER:H	1:A:123:GLU:HB2	0.54	1.62	15	5
1:A:175:PHE:HA	1:A:180:LEU:HA	0.54	1.79	20	19
1:A:127:LEU:CD1	1:A:128:LEU:HD23	0.54	2.32	2	4
1:A:170:ARG:HG2	1:A:186:MET:CE	0.54	2.32	13	3
1:A:124:MET:HA	1:A:124:MET:CE	0.54	2.30	4	2
1:A:124:MET:CG	1:A:152:ILE:HD12	0.54	2.32	6	2
1:A:110:MET:HB3	1:A:123:GLU:CG	0.54	2.32	2	2
1:A:121:LYS:HA	1:A:124:MET:CE	0.54	2.33	2	1
1:A:124:MET:HG2	1:A:128:LEU:HD21	0.54	1.78	15	1
1:A:115:PRO:HD3	1:A:193:GLY:CA	0.53	2.33	6	1
1:A:124:MET:CE	1:A:128:LEU:HD11	0.53	2.33	15	3
1:A:127:LEU:HA	1:A:197:LEU:HD12	0.53	1.79	16	2
1:A:139:MET:HB3	1:A:146:THR:CG2	0.53	2.33	5	9
1:A:136:VAL:CG2	1:A:146:THR:HG22	0.53	2.34	4	2
1:A:187:GLU:HG3	1:A:188:ASN:N	0.53	2.18	7	14
1:A:115:PRO:CD	1:A:193:GLY:HA3	0.53	2.34	6	1
1:A:109:ARG:O	1:A:109:ARG:HD3	0.53	2.03	18	1
1:A:196:ARG:HD3	1:A:196:ARG:N	0.53	2.19	16	2
1:A:133:TYR:HB3	1:A:145:PHE:CD2	0.53	2.38	9	14
1:A:128:LEU:HA	1:A:131:THR:HG22	0.53	1.79	1	6
1:A:119:ILE:HG21	1:A:124:MET:HE2	0.53	1.80	6	1
1:A:121:LYS:HG2	1:A:147:VAL:CG2	0.53	2.33	10	3
1:A:119:ILE:HG13	1:A:123:GLU:CB	0.53	2.34	16	8
1:A:124:MET:HE2	1:A:128:LEU:HD21	0.53	1.81	18	1
1:A:126:LYS:HA	1:A:126:LYS:HE2	0.52	1.79	4	6
1:A:124:MET:HE3	1:A:124:MET:HA	0.52	1.80	9	1
1:A:113:LEU:CD1	1:A:195:PHE:HB3	0.52	2.33	13	1
1:A:170:ARG:HB3	1:A:186:MET:HB2	0.52	1.79	9	8
1:A:122:ASN:HA	1:A:125:VAL:HB	0.52	1.81	7	11
1:A:117:MET:HE3	1:A:180:LEU:HD13	0.52	1.79	4	5
1:A:119:ILE:HG21	1:A:124:MET:HE1	0.52	1.81	3	1
1:A:114:GLU:CB	1:A:117:MET:HE3	0.52	2.34	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:LEU:CD2	1:A:197:LEU:HD13	0.52	2.35	3	1
1:A:185:ASN:CG	1:A:187:GLU:HG2	0.52	2.30	16	4
1:A:136:VAL:HG11	1:A:139:MET:HB2	0.52	1.82	15	9
1:A:127:LEU:HG	1:A:197:LEU:CD1	0.52	2.35	10	2
1:A:115:PRO:HA	1:A:180:LEU:CD2	0.51	2.35	19	5
1:A:113:LEU:CD2	1:A:195:PHE:HB3	0.51	2.35	9	5
1:A:136:VAL:HG23	1:A:146:THR:CG2	0.51	2.36	1	1
1:A:109:ARG:CB	1:A:126:LYS:HG2	0.51	2.34	18	1
1:A:114:GLU:H	1:A:117:MET:HE3	0.51	1.66	9	1
1:A:113:LEU:HG	1:A:173:LEU:HD21	0.51	1.82	10	1
1:A:119:ILE:HA	1:A:123:GLU:OE1	0.51	2.06	5	1
1:A:113:LEU:CB	1:A:195:PHE:HB3	0.51	2.35	2	4
1:A:145:PHE:HA	1:A:154:MET:HA	0.51	1.83	16	14
1:A:175:PHE:N	1:A:175:PHE:CD1	0.51	2.79	5	11
1:A:124:MET:HE3	1:A:128:LEU:HD11	0.51	1.83	2	1
1:A:117:MET:CE	1:A:180:LEU:HD13	0.50	2.36	4	5
1:A:115:PRO:CD	1:A:193:GLY:CA	0.50	2.89	6	1
1:A:145:PHE:HA	1:A:153:GLU:O	0.50	2.07	11	3
1:A:127:LEU:HA	1:A:197:LEU:HD11	0.50	1.82	2	1
1:A:139:MET:SD	1:A:145:PHE:HA	0.50	2.46	12	4
1:A:110:MET:O	1:A:123:GLU:HB3	0.50	2.06	20	1
1:A:146:THR:OG1	1:A:153:GLU:HB2	0.50	2.06	19	4
1:A:113:LEU:CG	1:A:173:LEU:HD21	0.50	2.37	10	1
1:A:127:LEU:HD11	1:A:154:MET:SD	0.50	2.46	16	3
1:A:121:LYS:HA	1:A:152:ILE:HD11	0.50	1.82	3	5
1:A:139:MET:O	1:A:139:MET:HG2	0.50	2.04	18	6
1:A:120:SER:O	1:A:124:MET:SD	0.50	2.70	7	1
1:A:125:VAL:HG13	1:A:126:LYS:CE	0.49	2.37	17	5
1:A:113:LEU:HB3	1:A:183:ILE:HD13	0.49	1.83	6	3
1:A:113:LEU:HD21	1:A:124:MET:SD	0.49	2.47	19	1
1:A:113:LEU:HB2	1:A:195:PHE:CB	0.49	2.36	6	1
1:A:140:THR:O	1:A:141:ARG:HD2	0.49	2.06	20	3
1:A:127:LEU:C	1:A:127:LEU:HD13	0.49	2.32	7	5
1:A:156:ARG:HB2	1:A:195:PHE:CZ	0.49	2.42	12	1
1:A:196:ARG:O	1:A:197:LEU:HD23	0.49	2.08	13	1
1:A:133:TYR:CE1	1:A:136:VAL:HB	0.49	2.43	20	14
1:A:133:TYR:OH	1:A:136:VAL:HG11	0.49	2.07	9	1
1:A:120:SER:O	1:A:124:MET:HG2	0.49	2.08	8	2
1:A:196:ARG:N	1:A:196:ARG:CD	0.49	2.75	9	1
1:A:115:PRO:HA	1:A:180:LEU:HD23	0.49	1.84	20	5
1:A:196:ARG:N	1:A:196:ARG:HD2	0.49	2.22	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:VAL:HG21	1:A:139:MET:CB	0.48	2.38	1	4
1:A:114:GLU:N	1:A:117:MET:HE3	0.48	2.22	7	3
1:A:122:ASN:O	1:A:125:VAL:CG1	0.48	2.61	16	16
1:A:124:MET:CG	1:A:128:LEU:HD21	0.48	2.39	15	1
1:A:115:PRO:HD2	1:A:193:GLY:HA2	0.48	1.85	15	5
1:A:133:TYR:HB3	1:A:145:PHE:CE2	0.48	2.43	12	3
1:A:170:ARG:HB3	1:A:186:MET:HE3	0.48	1.86	17	4
1:A:128:LEU:HD22	1:A:145:PHE:CD1	0.47	2.44	16	2
1:A:146:THR:O	1:A:152:ILE:HA	0.47	2.09	14	1
1:A:115:PRO:HA	1:A:180:LEU:CD1	0.47	2.40	2	1
1:A:113:LEU:HD12	1:A:113:LEU:N	0.47	2.23	10	3
1:A:196:ARG:H	1:A:196:ARG:HD2	0.47	1.68	18	1
1:A:111:VAL:HB	1:A:197:LEU:HD12	0.47	1.84	5	1
1:A:114:GLU:O	1:A:117:MET:HG2	0.47	2.10	6	4
1:A:173:LEU:N	1:A:173:LEU:HD12	0.47	2.24	6	3
1:A:124:MET:HG3	1:A:152:ILE:HD13	0.47	1.86	18	2
1:A:124:MET:SD	1:A:127:LEU:HD13	0.47	2.48	10	1
1:A:136:VAL:CG1	1:A:139:MET:HB3	0.47	2.39	14	3
1:A:141:ARG:HE	1:A:144:GLU:CD	0.47	2.17	15	1
1:A:117:MET:HE1	1:A:180:LEU:HD13	0.47	1.84	17	1
1:A:173:LEU:N	1:A:173:LEU:CD1	0.47	2.78	6	6
1:A:175:PHE:N	1:A:175:PHE:HD1	0.47	2.08	5	7
1:A:117:MET:HE2	1:A:180:LEU:HD22	0.47	1.86	8	1
1:A:109:ARG:HB2	1:A:126:LYS:HG2	0.47	1.86	18	1
1:A:113:LEU:HD13	1:A:173:LEU:HD11	0.47	1.86	18	1
1:A:172:ARG:HB2	1:A:186:MET:SD	0.47	2.50	4	1
1:A:155:ILE:HG12	1:A:170:ARG:CG	0.47	2.40	7	7
1:A:194:PHE:HB2	1:A:196:ARG:HD3	0.47	1.87	4	1
1:A:183:ILE:HD12	1:A:193:GLY:HA2	0.47	1.85	6	1
1:A:136:VAL:HG21	1:A:139:MET:HB2	0.46	1.87	4	3
1:A:127:LEU:HD23	1:A:197:LEU:HG	0.46	1.87	2	1
1:A:127:LEU:HD22	1:A:197:LEU:HD12	0.46	1.87	6	1
1:A:124:MET:HG3	1:A:127:LEU:CB	0.46	2.40	9	1
1:A:128:LEU:HD13	1:A:145:PHE:CZ	0.46	2.46	15	1
1:A:145:PHE:CD1	1:A:145:PHE:C	0.46	2.93	20	11
1:A:109:ARG:HB2	1:A:126:LYS:HG3	0.46	1.86	18	1
1:A:119:ILE:CG2	1:A:124:MET:HE3	0.46	2.41	11	1
1:A:185:ASN:HB3	1:A:190:ARG:HG2	0.46	1.86	20	1
1:A:147:VAL:CG2	1:A:152:ILE:HG12	0.46	2.41	18	2
1:A:176:ASP:HB3	1:A:179:HIS:CD2	0.46	2.46	6	2
1:A:139:MET:HA	1:A:144:GLU:OE1	0.46	2.10	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:PRO:HD3	1:A:193:GLY:HA2	0.46	1.86	5	2
1:A:119:ILE:HG23	1:A:175:PHE:CE2	0.46	2.46	8	1
1:A:147:VAL:HG22	1:A:148:GLN:N	0.46	2.26	19	1
1:A:121:LYS:HA	1:A:124:MET:HE2	0.46	1.87	2	1
1:A:124:MET:HE2	1:A:127:LEU:CG	0.46	2.40	17	1
1:A:115:PRO:CG	1:A:193:GLY:HA2	0.45	2.40	2	1
1:A:141:ARG:O	1:A:155:ILE:HD12	0.45	2.11	5	1
1:A:127:LEU:HD13	1:A:197:LEU:CD1	0.45	2.35	8	1
1:A:124:MET:O	1:A:124:MET:HG3	0.45	2.10	17	1
1:A:115:PRO:O	1:A:116:ASP:HB3	0.45	2.12	17	8
1:A:112:ASN:C	1:A:113:LEU:HD12	0.45	2.36	9	1
1:A:119:ILE:HG23	1:A:175:PHE:CZ	0.45	2.47	2	3
1:A:124:MET:HE1	1:A:147:VAL:HB	0.45	1.88	2	1
1:A:113:LEU:HD22	1:A:195:PHE:CD1	0.45	2.45	5	1
1:A:172:ARG:HB3	1:A:184:VAL:HB	0.45	1.87	11	3
1:A:133:TYR:CB	1:A:144:GLU:HA	0.45	2.41	13	1
1:A:124:MET:HG2	1:A:152:ILE:HG21	0.45	1.87	10	1
1:A:127:LEU:C	1:A:127:LEU:HD23	0.45	2.37	15	1
1:A:133:TYR:HE1	1:A:136:VAL:CB	0.45	2.25	20	3
1:A:126:LYS:CE	1:A:126:LYS:CA	0.45	2.94	16	4
1:A:134:ARG:HD2	1:A:135:GLN:N	0.45	2.27	8	1
1:A:176:ASP:HB2	1:A:181:ALA:HB2	0.45	1.87	15	1
1:A:170:ARG:HB3	1:A:186:MET:CE	0.45	2.42	17	2
1:A:110:MET:HB3	1:A:123:GLU:HG2	0.45	1.88	5	1
1:A:133:TYR:CD1	1:A:144:GLU:HG3	0.45	2.46	10	4
1:A:170:ARG:HB3	1:A:186:MET:HE2	0.45	1.89	18	1
1:A:114:GLU:HB3	1:A:117:MET:HE3	0.45	1.89	3	1
1:A:173:LEU:HB3	1:A:180:LEU:CD1	0.45	2.41	10	2
1:A:113:LEU:HD21	1:A:124:MET:HE1	0.45	1.89	17	1
1:A:133:TYR:C	1:A:145:PHE:HE2	0.44	2.19	16	4
1:A:113:LEU:HD12	1:A:195:PHE:CD1	0.44	2.47	19	2
1:A:127:LEU:HG	1:A:197:LEU:HD12	0.44	1.88	10	1
1:A:156:ARG:HB2	1:A:195:PHE:CE1	0.44	2.48	12	1
1:A:117:MET:HE2	1:A:119:ILE:HG21	0.44	1.88	14	1
1:A:134:ARG:HD3	1:A:135:GLN:N	0.44	2.27	1	1
1:A:195:PHE:CE1	1:A:197:LEU:HD21	0.44	2.47	7	1
1:A:121:LYS:H	1:A:121:LYS:HD2	0.44	1.71	8	2
1:A:127:LEU:HD23	1:A:197:LEU:CG	0.44	2.42	2	1
1:A:156:ARG:O	1:A:156:ARG:HG3	0.44	2.12	5	1
1:A:110:MET:HB3	1:A:123:GLU:HG3	0.44	1.89	20	2
1:A:133:TYR:CE1	1:A:144:GLU:CG	0.44	2.94	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:ILE:HB	1:A:192:PHE:HB3	0.44	1.89	5	2
1:A:183:ILE:O	1:A:191:GLN:HA	0.44	2.13	10	3
1:A:192:PHE:O	1:A:194:PHE:N	0.44	2.50	8	9
1:A:153:GLU:CD	1:A:172:ARG:HE	0.44	2.20	8	1
1:A:124:MET:SD	1:A:152:ILE:CG2	0.44	3.06	2	1
1:A:119:ILE:CG1	1:A:123:GLU:HB3	0.43	2.43	11	1
1:A:121:LYS:CA	1:A:124:MET:SD	0.43	2.97	18	1
1:A:133:TYR:CE1	1:A:136:VAL:HG13	0.43	2.48	4	2
1:A:109:ARG:NH1	1:A:125:VAL:HG21	0.43	2.28	2	1
1:A:113:LEU:HD11	1:A:124:MET:SD	0.43	2.53	12	1
1:A:144:GLU:HG3	1:A:145:PHE:N	0.43	2.27	13	1
1:A:151:SER:HB2	1:A:153:GLU:OE2	0.43	2.14	13	1
1:A:119:ILE:HG12	1:A:124:MET:SD	0.43	2.53	20	1
1:A:124:MET:HG2	1:A:127:LEU:CB	0.43	2.43	13	1
1:A:128:LEU:HD22	1:A:145:PHE:CE1	0.43	2.49	16	1
1:A:124:MET:HE3	1:A:173:LEU:HD23	0.43	1.89	6	1
1:A:117:MET:CE	1:A:119:ILE:HD13	0.43	2.44	12	1
1:A:141:ARG:HG2	1:A:144:GLU:OE1	0.43	2.13	1	1
1:A:113:LEU:N	1:A:113:LEU:CD1	0.43	2.81	10	4
1:A:133:TYR:CG	1:A:134:ARG:N	0.43	2.87	2	9
1:A:119:ILE:CD1	1:A:124:MET:HE3	0.43	2.40	5	1
1:A:187:GLU:CG	1:A:188:ASN:N	0.43	2.82	15	5
1:A:117:MET:HG3	1:A:180:LEU:HB3	0.43	1.91	5	2
1:A:139:MET:HG3	1:A:144:GLU:HB3	0.43	1.90	2	2
1:A:113:LEU:CD2	1:A:173:LEU:HD21	0.43	2.44	4	1
1:A:144:GLU:CG	1:A:145:PHE:N	0.43	2.82	13	1
1:A:180:LEU:C	1:A:180:LEU:HD13	0.43	2.39	2	1
1:A:124:MET:CE	1:A:173:LEU:HD22	0.42	2.44	10	1
1:A:120:SER:C	1:A:122:ASN:N	0.42	2.75	7	1
1:A:175:PHE:CE1	1:A:180:LEU:HD12	0.42	2.49	10	1
1:A:141:ARG:HG3	1:A:144:GLU:OE1	0.42	2.14	12	1
1:A:124:MET:CE	1:A:127:LEU:HD22	0.42	2.41	10	1
1:A:133:TYR:HE1	1:A:136:VAL:HB	0.42	1.73	3	3
1:A:119:ILE:HG13	1:A:123:GLU:HB2	0.42	1.90	5	3
1:A:139:MET:HB3	1:A:146:THR:HG23	0.42	1.91	10	3
1:A:183:ILE:CD1	1:A:193:GLY:HA2	0.42	2.45	6	1
1:A:139:MET:HG3	1:A:144:GLU:C	0.42	2.39	3	1
1:A:125:VAL:HG13	1:A:126:LYS:N	0.42	2.29	7	8
1:A:172:ARG:HB2	1:A:184:VAL:HB	0.42	1.88	8	1
1:A:185:ASN:HB3	1:A:190:ARG:CG	0.42	2.45	20	1
1:A:111:VAL:O	1:A:111:VAL:HG23	0.42	2.14	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:LEU:O	1:A:130:ALA:HB3	0.42	2.14	6	1
1:A:140:THR:N	1:A:144:GLU:OE1	0.42	2.52	7	1
1:A:114:GLU:H	1:A:117:MET:CE	0.42	2.27	9	1
1:A:133:TYR:CE1	1:A:144:GLU:HB2	0.42	2.49	13	1
1:A:196:ARG:H	1:A:196:ARG:CD	0.42	2.28	7	1
1:A:124:MET:HE1	1:A:180:LEU:HD12	0.42	1.91	11	1
1:A:109:ARG:CB	1:A:126:LYS:CG	0.42	2.95	18	1
1:A:124:MET:HE2	1:A:124:MET:CA	0.42	2.37	4	1
1:A:156:ARG:NH1	1:A:197:LEU:HA	0.42	2.30	8	1
1:A:136:VAL:HG11	1:A:139:MET:CB	0.42	2.45	14	1
1:A:196:ARG:O	1:A:196:ARG:HD2	0.42	2.14	14	1
1:A:113:LEU:HD22	1:A:117:MET:HE1	0.42	1.92	2	1
1:A:168:GLN:HG2	1:A:169:VAL:N	0.41	2.30	7	1
1:A:133:TYR:C	1:A:145:PHE:CE2	0.41	2.99	1	2
1:A:113:LEU:HD11	1:A:124:MET:HE1	0.41	1.92	4	1
1:A:119:ILE:HG13	1:A:123:GLU:HB3	0.41	1.92	11	2
1:A:155:ILE:CG1	1:A:170:ARG:HG3	0.41	2.45	4	1
1:A:142:PRO:HB3	1:A:168:GLN:NE2	0.41	2.30	5	1
1:A:141:ARG:CG	1:A:144:GLU:HG2	0.41	2.45	10	1
1:A:139:MET:SD	1:A:153:GLU:HB3	0.41	2.55	3	1
1:A:127:LEU:O	1:A:131:THR:HB	0.41	2.15	5	1
1:A:115:PRO:HA	1:A:180:LEU:HD12	0.41	1.91	2	1
1:A:140:THR:HA	1:A:155:ILE:CD1	0.41	2.46	3	1
1:A:125:VAL:CG1	1:A:126:LYS:N	0.41	2.83	5	2
1:A:110:MET:O	1:A:126:LYS:HB2	0.41	2.15	6	1
1:A:127:LEU:O	1:A:131:THR:N	0.41	2.51	8	1
1:A:113:LEU:N	1:A:113:LEU:HD12	0.41	2.30	14	1
1:A:148:GLN:OE1	1:A:148:GLN:HA	0.41	2.15	18	1
1:A:115:PRO:HG2	1:A:193:GLY:N	0.41	2.31	1	1
1:A:141:ARG:HD3	1:A:144:GLU:CD	0.41	2.41	3	1
1:A:127:LEU:HD13	1:A:127:LEU:C	0.41	2.41	17	2
1:A:113:LEU:HD11	1:A:127:LEU:HD11	0.41	1.93	13	1
1:A:139:MET:HG3	1:A:144:GLU:CB	0.40	2.46	4	1
1:A:139:MET:HB2	1:A:144:GLU:HB3	0.40	1.91	11	1
1:A:185:ASN:O	1:A:189:ASN:N	0.40	2.48	16	2
1:A:185:ASN:HB3	1:A:187:GLU:HG2	0.40	1.92	11	1
1:A:128:LEU:HD13	1:A:145:PHE:CE1	0.40	2.51	6	1
1:A:109:ARG:CB	1:A:126:LYS:HG3	0.40	2.46	10	1
1:A:113:LEU:HB2	1:A:195:PHE:C	0.40	2.42	16	1
1:A:117:MET:HE3	1:A:119:ILE:HG21	0.40	1.93	8	1
1:A:196:ARG:HD2	1:A:196:ARG:N	0.40	2.31	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:ASN:OD1	1:A:122:ASN:N	0.40	2.55	1	1
1:A:126:LYS:HE3	1:A:126:LYS:HA	0.40	1.92	12	1
1:A:172:ARG:HE	1:A:174:THR:HG23	0.40	1.77	17	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	79/114 (69%)	67±2 (85±3%)	10±2 (13±2%)	2±1 (2±1%)	7	44
All	All	1580/2280 (69%)	1337 (85%)	205 (13%)	38 (2%)	7	44

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

Mol	Chain	Res	Type	Models (Total)
1	A	193	GLY	12
1	A	109	ARG	10
1	A	115	PRO	8
1	A	149	ALA	6
1	A	116	ASP	1
1	A	168	GLN	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	72/102 (71%)	61±2 (85±3%)	11±2 (15±3%)	5	41
All	All	1440/2040 (71%)	1218 (85%)	222 (15%)	5	41

All 34 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	141	ARG	20
1	A	174	THR	20
1	A	139	MET	18
1	A	126	LYS	15
1	A	131	THR	12
1	A	192	PHE	12
1	A	135	GLN	10
1	A	140	THR	10
1	A	119	ILE	9
1	A	109	ARG	7
1	A	129	GLU	7
1	A	168	GLN	7
1	A	121	LYS	6
1	A	124	MET	6
1	A	197	LEU	6
1	A	175	PHE	6
1	A	111	VAL	5
1	A	127	LEU	5
1	A	153	GLU	5
1	A	123	GLU	5
1	A	183	ILE	5
1	A	115	PRO	4
1	A	122	ASN	4
1	A	173	LEU	3
1	A	134	ARG	3
1	A	132	GLN	3
1	A	196	ARG	2
1	A	137	SER	1
1	A	169	VAL	1
1	A	172	ARG	1
1	A	170	ARG	1
1	A	144	GLU	1
1	A	146	THR	1
1	A	190	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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 82% for the well-defined parts and 69% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *UB2H_dep_2018.str*

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	1098
Number of shifts mapped to atoms	1098
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	95	-0.02 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	89	-0.23 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	85	-0.13 ± 0.18	None needed (< 0.5 ppm)
^{15}N	85	-1.23 ± 0.33	Should be applied

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 82%, i.e. 939 atoms were assigned a chemical shift out of a possible 1144. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	373/394 (95%)	150/159 (94%)	152/158 (96%)	71/77 (92%)
Sidechain	510/683 (75%)	344/440 (78%)	166/205 (81%)	0/38 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	56/67 (84%)	28/33 (85%)	28/32 (88%)	0/2 (0%)
Overall	939/1144 (82%)	522/632 (83%)	346/395 (88%)	71/117 (61%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 1098 atoms were assigned a chemical shift out of a possible 1598. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	443/566 (78%)	178/230 (77%)	180/228 (79%)	85/108 (79%)
Sidechain	585/889 (66%)	392/573 (68%)	193/268 (72%)	0/48 (0%)
Aromatic	70/143 (49%)	35/71 (49%)	35/56 (62%)	0/16 (0%)
Overall	1098/1598 (69%)	605/874 (69%)	408/552 (74%)	85/172 (49%)

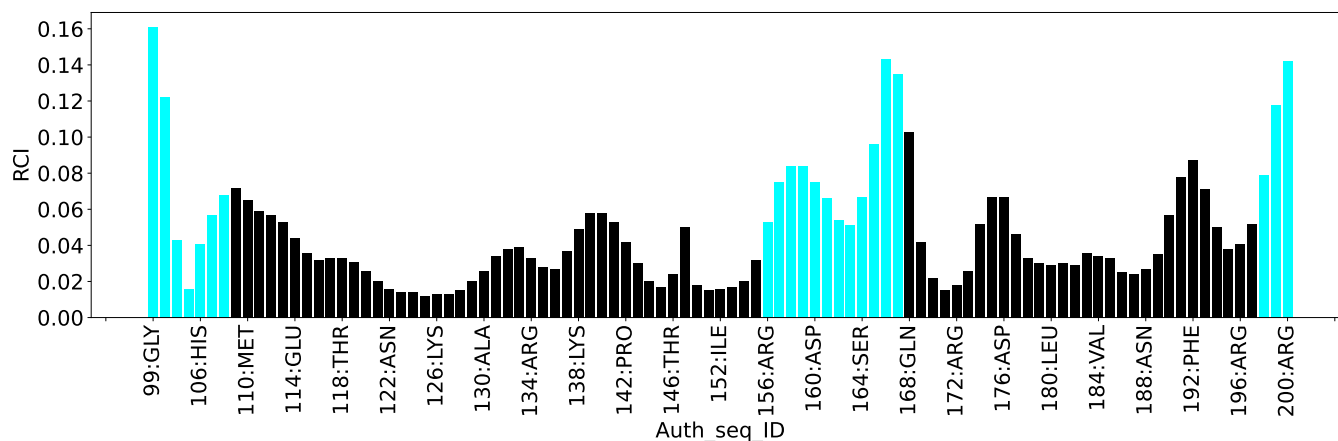
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1974
Intra-residue ($ i-j =0$)	693
Sequential ($ i-j =1$)	457
Medium range ($ i-j >1$ and $ i-j <5$)	258
Long range ($ i-j \geq 5$)	566
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	170
Number of unmapped restraints	0
Number of restraints per residue	18.8
Number of long range restraints per residue ¹	5.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	111.1	0.2
0.2-0.5 (Medium)	198.0	0.5
>0.5 (Large)	179.8	4.94

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)	29.4	9.91
10.0-20.0 (Medium)	2.5	19.94
>20.0 (Large)	3.0	28.77

9 Distance violation analysis ⓘ

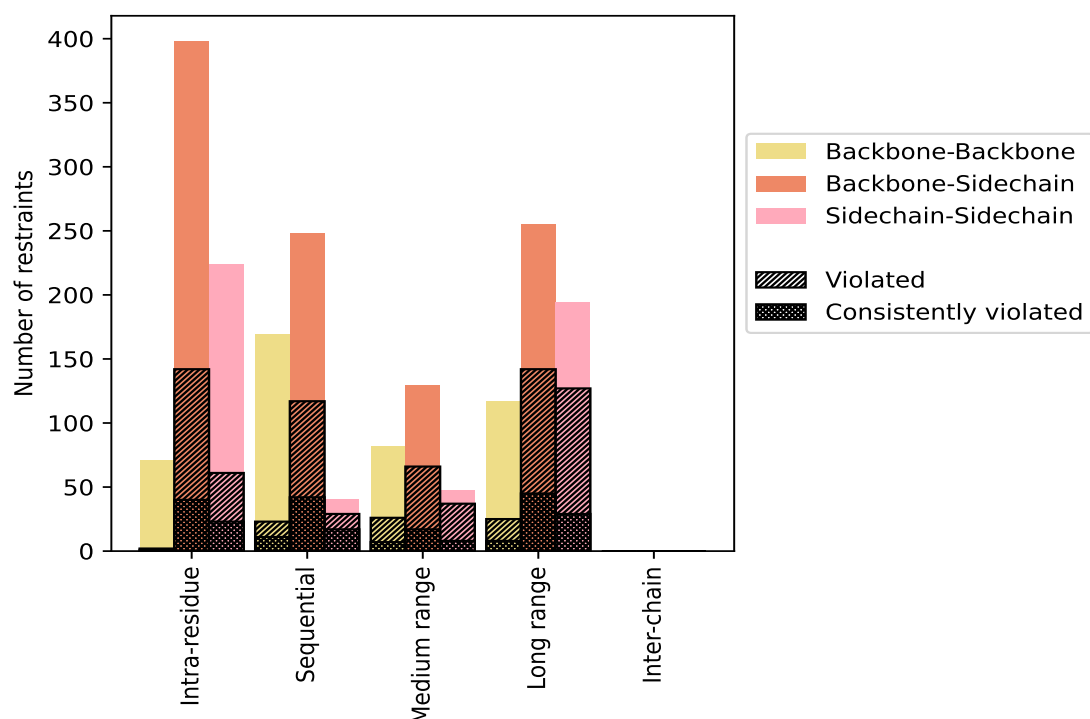
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	693	35.1	205	29.6	10.4	64	9.2	3.2
Backbone-Backbone	71	3.6	2	2.8	0.1	1	1.4	0.1
Backbone-Sidechain	398	20.2	142	35.7	7.2	40	10.1	2.0
Sidechain-Sidechain	224	11.3	61	27.2	3.1	23	10.3	1.2
Sequential ($i-j =1$)	457	23.2	169	37.0	8.6	70	15.3	3.5
Backbone-Backbone	169	8.6	23	13.6	1.2	11	6.5	0.6
Backbone-Sidechain	248	12.6	117	47.2	5.9	42	16.9	2.1
Sidechain-Sidechain	40	2.0	29	72.5	1.5	17	42.5	0.9
Medium range ($i-j >1$ & $i-j <5$)	258	13.1	129	50.0	6.5	32	12.4	1.6
Backbone-Backbone	82	4.2	26	31.7	1.3	7	8.5	0.4
Backbone-Sidechain	129	6.5	66	51.2	3.3	17	13.2	0.9
Sidechain-Sidechain	47	2.4	37	78.7	1.9	8	17.0	0.4
Long range ($i-j \geq 5$)	566	28.7	294	51.9	14.9	82	14.5	4.2
Backbone-Backbone	117	5.9	25	21.4	1.3	8	6.8	0.4
Backbone-Sidechain	255	12.9	142	55.7	7.2	45	17.6	2.3
Sidechain-Sidechain	194	9.8	127	65.5	6.4	29	14.9	1.5
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1974	100.0	797	40.4	40.4	248	12.6	12.6
Backbone-Backbone	439	22.2	76	17.3	3.9	27	6.2	1.4
Backbone-Sidechain	1030	52.2	467	45.3	23.7	144	14.0	7.3
Sidechain-Sidechain	505	25.6	254	50.3	12.9	77	15.2	3.9

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	117	119	81	176	0	493	0.56	4.94	0.55	0.37
2	125	121	83	187	0	516	0.61	3.47	0.59	0.4
3	132	119	78	160	0	489	0.5	3.7	0.41	0.38
4	128	116	80	168	0	492	0.51	2.77	0.44	0.36
5	135	118	83	170	0	506	0.51	3.67	0.47	0.36
6	124	120	74	161	0	479	0.53	3.46	0.5	0.37
7	127	127	70	170	0	494	0.51	2.84	0.42	0.36
8	131	124	74	165	0	494	0.48	2.64	0.39	0.35
9	125	120	83	166	0	494	0.53	2.95	0.47	0.36
10	129	116	80	180	0	505	0.49	2.73	0.39	0.36

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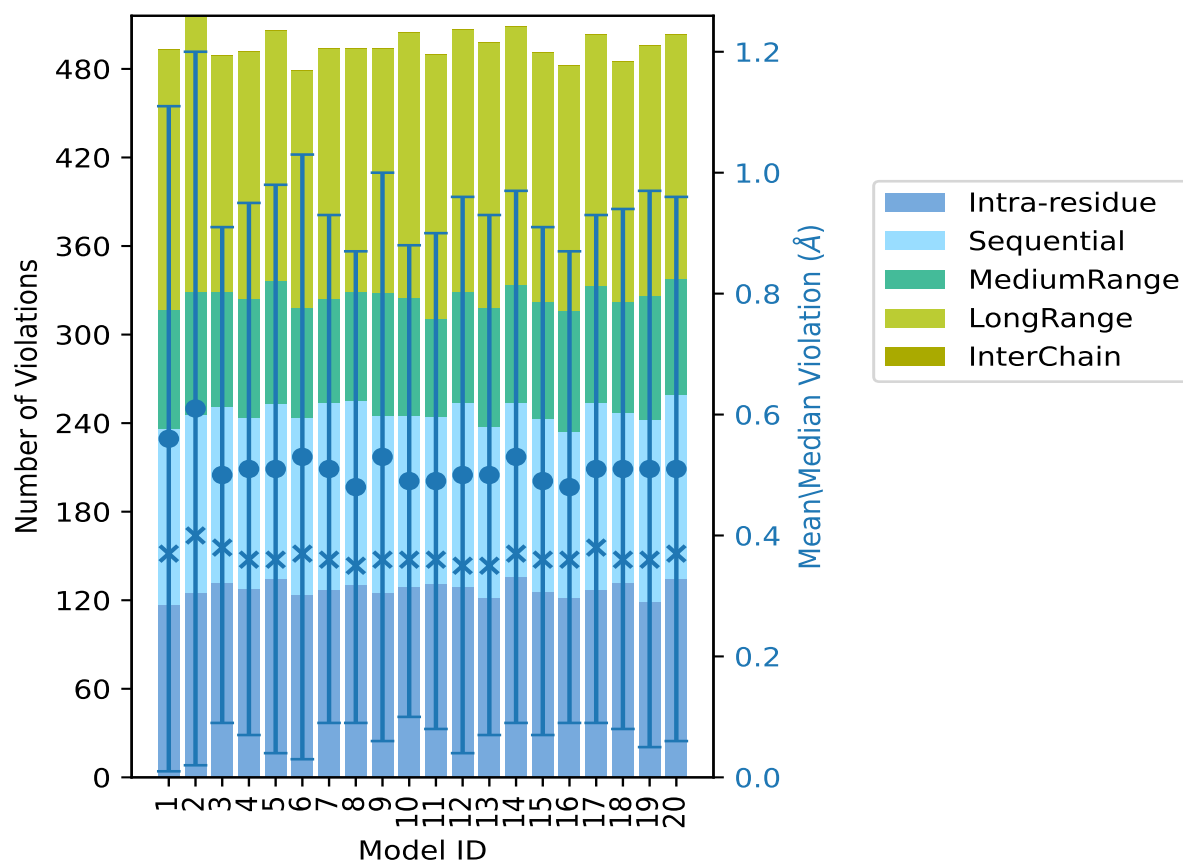
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	131	113	67	179	0	490	0.49	2.71	0.41	0.36
12	129	125	75	178	0	507	0.5	3.72	0.46	0.35
13	122	116	80	180	0	498	0.5	2.94	0.43	0.35
14	136	118	80	175	0	509	0.53	2.88	0.44	0.37
15	126	117	79	169	0	491	0.49	2.92	0.42	0.36
16	122	112	82	166	0	482	0.48	2.93	0.39	0.36
17	127	127	79	170	0	503	0.51	2.73	0.42	0.38
18	132	115	75	163	0	485	0.51	2.92	0.43	0.36
19	119	123	84	170	0	496	0.51	3.66	0.46	0.36
20	135	124	79	165	0	503	0.51	3.69	0.45	0.37

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble ⓘ

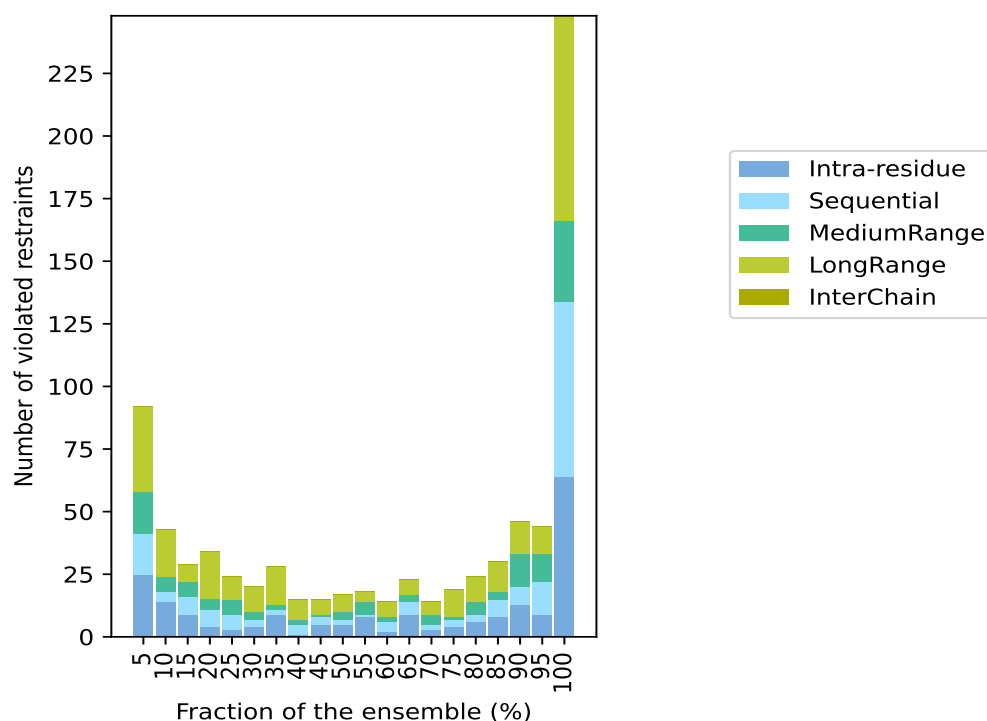
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1177(IR:488, SQ:288, MR:129, LR:272, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
25	16	17	34	0	92	1	5.0
14	4	6	19	0	43	2	10.0
9	7	6	7	0	29	3	15.0
4	7	4	19	0	34	4	20.0
3	6	6	9	0	24	5	25.0
4	3	3	10	0	20	6	30.0
9	2	2	15	0	28	7	35.0
1	4	2	8	0	15	8	40.0
5	3	1	6	0	15	9	45.0
5	2	3	7	0	17	10	50.0
8	1	5	4	0	18	11	55.0
2	4	2	6	0	14	12	60.0
9	5	3	6	0	23	13	65.0
3	2	4	5	0	14	14	70.0
4	3	1	11	0	19	15	75.0
6	3	5	10	0	24	16	80.0
8	7	3	12	0	30	17	85.0
13	7	13	13	0	46	18	90.0
9	13	11	11	0	44	19	95.0
64	70	32	82	0	248	20	100.0

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

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

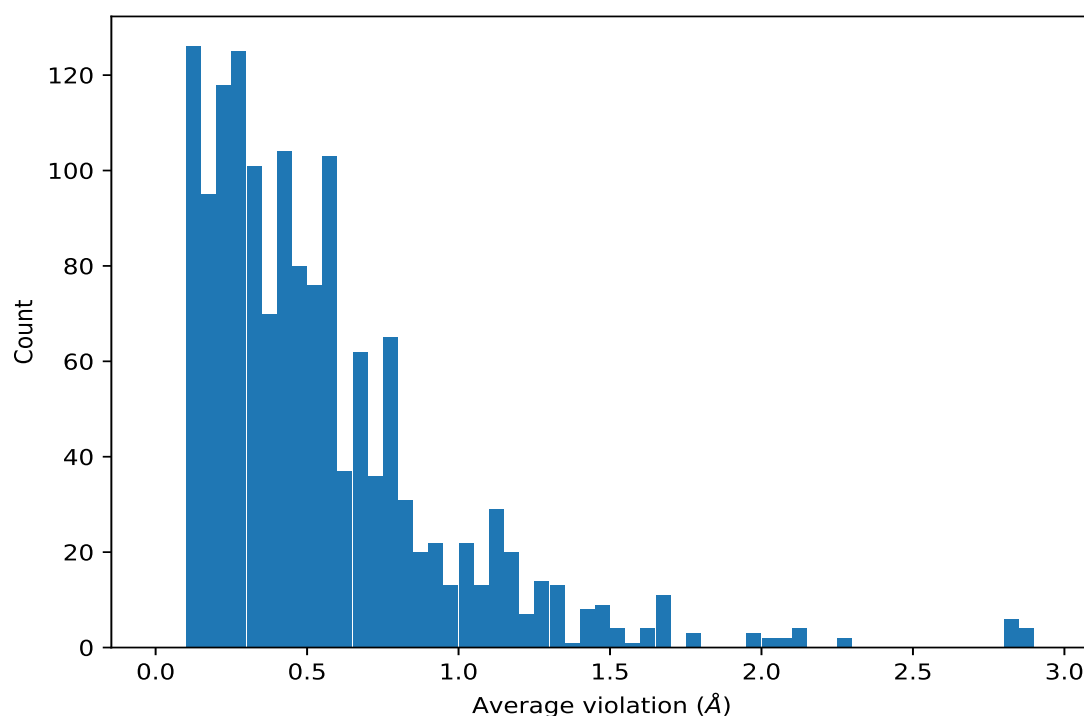
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	20	2.83	0.13	2.82
(2,99)	1:182:A:THR:H	1:152:A:ILE:HD13	20	2.83	0.13	2.82
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD13	20	2.83	0.13	2.82
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD12	20	2.83	0.13	2.82
(2,99)	1:182:A:THR:H	1:184:A:VAL:HG13	20	2.83	0.13	2.82
(2,99)	1:182:A:THR:H	1:184:A:VAL:HG11	20	2.83	0.13	2.82
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG13	20	2.1	0.32	2.18
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	20	2.1	0.32	2.18
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG12	20	2.1	0.32	2.18
(2,151)	1:112:A:ASN:HB3	1:111:A:VAL:HG13	20	2.1	0.32	2.18
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	20	1.97	0.19	1.98
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	20	1.97	0.19	1.98
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG21	20	1.97	0.19	1.98
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	20	1.75	0.25	1.7
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	20	1.75	0.25	1.7
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB2	20	1.75	0.25	1.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	20	1.69	0.14	1.63
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	20	1.64	0.05	1.65
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	20	1.55	0.09	1.57
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	20	1.52	0.14	1.54
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	20	1.49	0.33	1.59
(1,1436)	1:136:A:VAL:HG21	1:144:A:GLU:HB2	20	1.49	0.33	1.59
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	20	1.49	0.33	1.59
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG13	20	1.47	0.45	1.32
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	20	1.47	0.45	1.32
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	20	1.47	0.45	1.32
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG21	20	1.46	0.49	1.47
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	20	1.46	0.49	1.47
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG22	20	1.46	0.49	1.47
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	20	1.45	0.23	1.48
(2,69)	1:159:A:PHE:H	1:156:A:ARG:HB2	20	1.45	0.23	1.48
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	20	1.44	0.68	1.42
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	20	1.35	0.42	1.5
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD11	20	1.32	0.62	1.52
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB3	20	1.32	0.62	1.52
(2,5)	1:196:A:ARG:H	1:111:A:VAL:HG11	20	1.32	0.62	1.52
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD13	20	1.32	0.62	1.52
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB2	20	1.32	0.62	1.52
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB1	20	1.32	0.62	1.52
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD12	20	1.32	0.62	1.52
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	20	1.31	0.43	1.24
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD22	20	1.3	0.03	1.29
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	20	1.3	0.03	1.29
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	20	1.3	0.03	1.29
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	20	1.29	0.51	1.25
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	20	1.28	0.22	1.37
(2,198)	1:169:A:VAL:HG11	1:170:A:ARG:HB3	20	1.28	0.22	1.37
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	20	1.28	0.22	1.37
(2,198)	1:141:A:ARG:HB3	1:140:A:THR:HG23	20	1.28	0.22	1.37
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	20	1.27	0.22	1.23
(1,1373)	1:128:A:LEU:HD23	1:154:A:MET:HB2	20	1.27	0.22	1.23
(1,1373)	1:128:A:LEU:HD21	1:154:A:MET:HB2	20	1.27	0.22	1.23
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	20	1.27	0.2	1.3
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	20	1.27	0.2	1.3
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG22	20	1.27	0.2	1.3
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	20	1.24	0.52	1.21
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	20	1.22	0.93	0.54
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	20	1.22	0.93	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG22	20	1.22	0.93	0.54
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	20	1.21	0.15	1.29
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	20	1.21	0.15	1.29
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	20	1.2	0.48	1.05
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	20	1.2	0.48	1.05
(2,186)	1:173:A:LEU:HD13	1:195:A:PHE:HB2	20	1.2	0.48	1.05
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	20	1.19	0.37	1.08
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD11	20	1.19	0.37	1.08
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD13	20	1.19	0.37	1.08
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	20	1.18	0.2	1.23
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	20	1.18	0.61	1.04
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG23	20	1.18	0.61	1.04
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG21	20	1.18	0.61	1.04
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	20	1.18	0.15	1.26
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	20	1.18	0.15	1.26
(2,53)	1:134:A:ARG:H	1:141:A:ARG:HG3	20	1.18	0.15	1.26
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	20	1.15	0.12	1.17
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	20	1.15	0.03	1.13
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	20	1.15	0.02	1.14
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	20	1.14	0.54	0.86
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD11	20	1.14	0.54	0.86
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD12	20	1.14	0.54	0.86
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD21	20	1.11	0.18	1.14
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	20	1.11	0.18	1.14
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD22	20	1.11	0.18	1.14
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD12	20	1.11	0.18	1.14
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	20	1.08	0.03	1.1
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD21	20	1.08	0.82	0.57
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD21	20	1.08	0.82	0.57
(1,1409)	1:131:A:THR:HG21	1:127:A:LEU:HD22	20	1.08	0.82	0.57
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD22	20	1.08	0.82	0.57
(1,1409)	1:131:A:THR:HG21	1:127:A:LEU:HD21	20	1.08	0.82	0.57
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD22	20	1.08	0.82	0.57
(1,1409)	1:131:A:THR:HG21	1:127:A:LEU:HD23	20	1.08	0.82	0.57
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD23	20	1.08	0.82	0.57
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	20	1.04	0.54	1.14
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG21	20	1.04	0.05	1.02
(1,1579)	1:184:A:VAL:HG11	1:183:A:ILE:HG22	20	1.04	0.05	1.02
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG22	20	1.04	0.05	1.02
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG21	20	1.04	0.05	1.02
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG22	20	1.04	0.05	1.02
(1,1579)	1:184:A:VAL:HG11	1:183:A:ILE:HG23	20	1.04	0.05	1.02

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG23	20	1.04	0.05	1.02
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	20	1.02	0.46	0.82
(1,1456)	1:130:A:ALA:HB3	1:132:A:GLN:HG3	20	1.02	0.46	0.82
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	20	1.02	0.46	0.82
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	20	0.98	0.01	0.98
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	20	0.96	0.89	0.4
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	20	0.96	0.15	0.95
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG23	20	0.96	0.21	1.04
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	20	0.96	0.21	1.04
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG22	20	0.96	0.21	1.04
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	20	0.92	0.07	0.93
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	20	0.92	0.05	0.92
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	20	0.91	0.26	1.0
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	20	0.91	0.26	1.0
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG22	20	0.91	0.26	1.0
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD22	20	0.91	0.6	0.64
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	20	0.91	0.6	0.64
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	20	0.91	0.6	0.64
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	20	0.9	0.59	0.67
(2,173)	1:124:A:MET:HB3	1:123:A:GLU:HB3	20	0.9	0.59	0.67
(2,173)	1:125:A:VAL:HB	1:124:A:MET:HB3	20	0.9	0.59	0.67
(2,173)	1:124:A:MET:HB3	1:121:A:LYS:HB3	20	0.9	0.59	0.67
(2,173)	1:124:A:MET:HB3	1:121:A:LYS:HB2	20	0.9	0.59	0.67
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	20	0.89	0.03	0.9
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	20	0.89	0.23	0.9
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG13	20	0.89	0.23	0.9
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG12	20	0.89	0.23	0.9
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	20	0.88	0.02	0.88
(1,1468)	1:152:A:ILE:HG23	1:145:A:PHE:HB3	20	0.88	0.18	0.9
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	20	0.88	0.18	0.9
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	20	0.88	0.18	0.9
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD13	20	0.86	0.61	0.48
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD11	20	0.86	0.61	0.48
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	20	0.86	0.61	0.48
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD13	20	0.86	0.08	0.87
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD11	20	0.86	0.08	0.87
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD11	20	0.86	0.08	0.87
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD13	20	0.86	0.08	0.87
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD12	20	0.86	0.08	0.87
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD12	20	0.86	0.08	0.87
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	20	0.84	0.75	0.32
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	20	0.84	0.02	0.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	20	0.84	0.64	0.54
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	20	0.84	0.64	0.54
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG11	20	0.84	0.64	0.54
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	20	0.82	0.05	0.82
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB1	20	0.82	0.05	0.82
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	20	0.82	0.05	0.82
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	20	0.81	0.61	0.38
(2,166)	1:122:A:ASN:HB3	1:125:A:VAL:HB	20	0.81	0.12	0.83
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	20	0.81	0.12	0.83
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	20	0.8	0.07	0.8
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	20	0.79	0.1	0.72
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	20	0.79	0.48	0.76
(2,117)	1:124:A:MET:HA	1:111:A:VAL:HG23	20	0.79	0.48	0.76
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD11	20	0.79	0.48	0.76
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD12	20	0.79	0.48	0.76
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	20	0.78	0.13	0.78
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG11	20	0.78	0.13	0.78
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	20	0.78	0.13	0.78
(1,1416)	1:147:A:VAL:HG11	1:147:A:VAL:HA	20	0.78	0.02	0.78
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	20	0.78	0.02	0.78
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	20	0.78	0.02	0.78
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD11	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD23	1:119:A:ILE:HD11	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD13	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD12	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD13	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD11	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD11	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD12	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD13	20	0.77	0.37	0.7
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD12	20	0.77	0.37	0.7
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	20	0.75	0.29	0.81
(2,1)	1:170:A:ARG:H	1:154:A:MET:HG2	20	0.75	0.29	0.81
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	20	0.75	0.05	0.76
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD11	20	0.75	0.05	0.76
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD12	20	0.75	0.05	0.76
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	20	0.74	0.07	0.76
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	20	0.74	0.07	0.76
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB1	20	0.74	0.07	0.76
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG11	20	0.74	0.06	0.74
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG12	20	0.74	0.06	0.74
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	20	0.74	0.06	0.74

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	20	0.73	0.07	0.72
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	20	0.73	0.07	0.72
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD12	20	0.73	0.07	0.72
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	20	0.73	0.2	0.68
(2,93)	1:188:A:ASN:H	1:186:A:MET:HB3	20	0.73	0.2	0.68
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	20	0.73	0.07	0.75
(2,214)	1:112:A:ASN:HB3	1:111:A:VAL:HA	20	0.73	0.07	0.75
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	20	0.72	0.22	0.73
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB3	20	0.72	0.22	0.73
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD21	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD21	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD23	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD23	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD22	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB1	1:180:A:LEU:HD22	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD22	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB1	1:180:A:LEU:HD23	20	0.71	0.06	0.7
(1,1452)	1:181:A:ALA:HB1	1:180:A:LEU:HD21	20	0.71	0.06	0.7
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	20	0.7	0.12	0.75
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE3	20	0.7	0.12	0.75
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE1	20	0.7	0.12	0.75
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	20	0.69	0.21	0.7
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD23	20	0.69	0.21	0.7
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	20	0.69	0.21	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	20	0.69	0.02	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	20	0.69	0.02	0.7
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	20	0.68	0.07	0.68
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG13	20	0.68	0.07	0.68
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG11	20	0.68	0.07	0.68
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	20	0.68	0.55	0.38
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD2	20	0.68	0.55	0.38
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	20	0.67	0.03	0.68
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	20	0.67	0.03	0.68
(1,1475)	1:119:A:ILE:HG23	1:119:A:ILE:HA	20	0.67	0.03	0.68
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	20	0.67	0.9	0.23
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	20	0.67	0.09	0.7
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	20	0.67	0.09	0.7
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD12	20	0.67	0.09	0.7
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	20	0.67	0.33	0.53
(1,1490)	1:119:A:ILE:HD11	1:119:A:ILE:HA	20	0.67	0.33	0.53
(1,1490)	1:119:A:ILE:HD13	1:119:A:ILE:HA	20	0.67	0.33	0.53
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	20	0.67	0.1	0.7

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE2	20	0.67	0.1	0.7
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	20	0.66	0.39	0.44
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG23	20	0.66	0.02	0.66
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	20	0.66	0.02	0.66
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	20	0.66	0.02	0.66
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	20	0.66	0.16	0.64
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	20	0.66	0.16	0.64
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD13	20	0.66	0.16	0.64
(2,81)	1:140:A:THR:H	1:136:A:VAL:HG11	20	0.66	0.16	0.64
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	20	0.66	0.03	0.67
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD3	20	0.66	0.03	0.67
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	20	0.65	0.07	0.64
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	20	0.65	0.07	0.64
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB2	20	0.65	0.07	0.64
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	20	0.63	0.11	0.64
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD11	20	0.63	0.11	0.64
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD13	20	0.63	0.11	0.64
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD21	20	0.63	0.09	0.65
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	20	0.63	0.09	0.65
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD22	20	0.63	0.09	0.65
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	20	0.63	0.13	0.64
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD23	20	0.63	0.18	0.64
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	20	0.63	0.18	0.64
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	20	0.63	0.18	0.64
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	20	0.61	0.04	0.61
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	20	0.61	0.04	0.61
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD13	20	0.61	0.04	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	20	0.61	0.01	0.61
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	20	0.6	0.09	0.62
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG22	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG22	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG23	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG21	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG23	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG22	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG21	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG23	20	0.6	0.25	0.58
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG21	20	0.6	0.25	0.58
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	20	0.6	0.11	0.58
(2,192)	1:125:A:VAL:HG12	1:109:A:ARG:H	20	0.59	0.1	0.59
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	20	0.59	0.1	0.59
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG11	20	0.59	0.1	0.59

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG12	20	0.59	0.1	0.59
(2,192)	1:125:A:VAL:HG11	1:109:A:ARG:H	20	0.59	0.1	0.59
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	20	0.58	0.32	0.46
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	20	0.58	0.32	0.46
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG23	20	0.58	0.32	0.46
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	20	0.58	0.13	0.59
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	20	0.58	0.13	0.59
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD22	20	0.58	0.13	0.59
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	20	0.58	0.09	0.52
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	20	0.58	0.06	0.58
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	20	0.58	1.01	0.33
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	20	0.58	1.01	0.33
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	20	0.57	0.07	0.59
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	20	0.56	0.06	0.57
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD12	20	0.56	0.06	0.57
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD11	20	0.56	0.06	0.57
(1,1701)	1:133:A:TYR:HE1	1:134:A:ARG:H	20	0.56	0.07	0.54
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	20	0.56	0.07	0.54
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG22	20	0.56	0.49	0.35
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	20	0.56	0.49	0.35
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	20	0.56	0.49	0.35
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD12	20	0.56	0.21	0.56
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	20	0.56	0.21	0.56
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD13	20	0.56	0.21	0.56
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	20	0.56	0.08	0.57
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG13	20	0.56	0.08	0.57
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	20	0.56	0.08	0.57
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	20	0.55	0.03	0.55
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	20	0.55	0.04	0.55
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG11	20	0.55	0.04	0.55
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	20	0.55	0.04	0.55
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	20	0.55	0.04	0.55
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG21	20	0.55	0.04	0.55
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	20	0.55	0.04	0.55
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	20	0.54	0.11	0.54
(1,1424)	1:128:A:LEU:HD21	1:127:A:LEU:HB2	20	0.54	0.11	0.54
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	20	0.54	0.11	0.54
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	20	0.54	0.17	0.55
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	20	0.54	0.17	0.55
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG21	20	0.54	0.17	0.55
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG23	20	0.54	0.08	0.54
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	20	0.54	0.08	0.54

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG22	20	0.54	0.08	0.54
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG23	20	0.53	0.05	0.54
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	20	0.53	0.05	0.54
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	20	0.53	0.05	0.54
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG23	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG23	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG21	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG22	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG21	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG22	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG23	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG22	20	0.53	0.06	0.53
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG21	20	0.53	0.06	0.53
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	20	0.52	0.03	0.52
(1,1454)	1:130:A:ALA:HB1	1:128:A:LEU:H	20	0.52	0.03	0.52
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	20	0.52	0.03	0.52
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	20	0.51	0.07	0.51
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	20	0.51	0.07	0.51
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD11	20	0.51	0.07	0.51
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	20	0.51	0.1	0.48
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD12	20	0.51	0.1	0.48
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD11	20	0.51	0.1	0.48
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	20	0.51	0.06	0.5
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	20	0.5	0.3	0.44
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	20	0.5	0.08	0.52
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	20	0.5	0.08	0.52
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD12	20	0.5	0.08	0.52
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	20	0.5	0.19	0.53
(2,197)	1:184:A:VAL:HG22	1:172:A:ARG:HG2	20	0.5	0.19	0.53
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	20	0.5	0.19	0.53
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG3	20	0.5	0.19	0.53
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	20	0.5	0.27	0.35
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	20	0.49	0.07	0.5
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG23	20	0.49	0.07	0.5
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG21	20	0.49	0.07	0.5
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG21	20	0.49	0.06	0.5
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	20	0.49	0.06	0.5
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG23	20	0.49	0.06	0.5
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	20	0.48	0.18	0.43
(1,450)	1:174:A:THR:H	1:174:A:THR:HG21	20	0.48	0.07	0.48
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	20	0.48	0.07	0.48
(1,450)	1:174:A:THR:H	1:174:A:THR:HG23	20	0.48	0.07	0.48

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG21	20	0.48	0.13	0.44
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	20	0.48	0.13	0.44
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	20	0.48	0.13	0.44
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	20	0.46	0.17	0.44
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG21	20	0.46	0.09	0.48
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG23	20	0.46	0.09	0.48
(1,1590)	1:171:A:ALA:HB2	1:183:A:ILE:HG22	20	0.46	0.09	0.48
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG22	20	0.46	0.09	0.48
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG23	20	0.46	0.09	0.48
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG21	20	0.46	0.09	0.48
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG22	20	0.46	0.09	0.48
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG22	20	0.46	0.17	0.53
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	20	0.46	0.17	0.53
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG21	20	0.46	0.17	0.53
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB2	20	0.46	0.33	0.42
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	20	0.46	0.33	0.42
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	20	0.46	0.33	0.42
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	20	0.46	0.1	0.48
(1,1634)	1:195:A:PHE:HE1	1:195:A:PHE:HB2	20	0.46	0.1	0.48
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	20	0.45	0.1	0.49
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	20	0.45	0.57	0.33
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD11	20	0.45	0.57	0.33
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD12	20	0.45	0.57	0.33
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	20	0.44	0.4	0.26
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG22	20	0.44	0.37	0.27
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	20	0.44	0.37	0.27
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	20	0.44	0.37	0.27
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	20	0.43	0.01	0.43
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	20	0.42	0.14	0.46
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	20	0.42	0.09	0.4
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG23	20	0.42	0.09	0.4
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	20	0.42	0.09	0.4
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	20	0.42	0.22	0.56
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	20	0.42	0.07	0.44
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB1	20	0.42	0.07	0.44
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB2	20	0.42	0.07	0.44
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	20	0.42	0.4	0.2
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	20	0.42	0.0	0.42
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	20	0.42	0.08	0.42
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB3	20	0.42	0.08	0.42
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	20	0.41	0.14	0.36
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG13	20	0.41	0.14	0.36

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG12	20	0.41	0.14	0.36
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG12	20	0.41	0.14	0.36
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG11	20	0.41	0.14	0.36
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG11	20	0.41	0.14	0.36
(1,1585)	1:136:A:VAL:HG21	1:136:A:VAL:HG11	20	0.41	0.14	0.36
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	20	0.4	0.32	0.3
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG12	20	0.4	0.32	0.3
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG11	20	0.4	0.32	0.3
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	20	0.4	0.15	0.44
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	20	0.4	0.29	0.32
(1,678)	1:124:A:MET:H	1:120:A:SER:H	20	0.4	0.27	0.32
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG22	20	0.4	0.02	0.4
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	20	0.4	0.02	0.4
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	20	0.4	0.02	0.4
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	20	0.39	0.12	0.4
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	20	0.39	0.12	0.4
(1,1562)	1:173:A:LEU:HD12	1:174:A:THR:H	20	0.39	0.12	0.4
(1,1485)	1:183:A:ILE:HD13	1:115:A:PRO:HA	20	0.39	0.08	0.4
(1,1485)	1:183:A:ILE:HD12	1:115:A:PRO:HA	20	0.39	0.08	0.4
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	20	0.39	0.08	0.4
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	20	0.38	0.1	0.4
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	20	0.37	0.21	0.29
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	20	0.37	0.05	0.39
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	20	0.37	0.03	0.37
(2,167)	1:109:A:ARG:HB3	1:126:A:LYS:H	20	0.37	0.03	0.37
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	20	0.37	0.03	0.37
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	20	0.37	0.17	0.31
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	20	0.37	0.01	0.37
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	20	0.36	0.02	0.36
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	20	0.36	0.07	0.38
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG11	20	0.36	0.07	0.38
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG13	20	0.36	0.07	0.38
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	20	0.36	0.12	0.38
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	20	0.36	0.12	0.38
(1,1459)	1:183:A:ILE:HG23	1:172:A:ARG:HB3	20	0.36	0.12	0.38
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	20	0.36	0.01	0.36
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	20	0.36	0.12	0.37
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	20	0.36	0.12	0.37
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD12	20	0.36	0.12	0.37
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD13	20	0.35	0.11	0.33
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	20	0.35	0.11	0.33
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD11	20	0.35	0.11	0.33

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	20	0.35	0.02	0.35
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG22	20	0.35	0.05	0.36
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	20	0.35	0.05	0.36
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG21	20	0.35	0.05	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	20	0.35	0.02	0.36
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	20	0.34	0.05	0.35
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	20	0.34	0.09	0.34
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	20	0.34	0.06	0.34
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	20	0.33	0.16	0.3
(2,55)	1:123:A:GLU:H	1:109:A:ARG:HA	20	0.33	0.16	0.3
(2,55)	1:123:A:GLU:H	1:124:A:MET:HA	20	0.33	0.16	0.3
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG23	20	0.33	0.04	0.34
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	20	0.33	0.04	0.34
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	20	0.33	0.04	0.34
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	20	0.33	0.16	0.27
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	20	0.33	0.08	0.34
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	20	0.33	0.04	0.34
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG21	20	0.32	0.03	0.32
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	20	0.32	0.03	0.32
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	20	0.32	0.03	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	20	0.32	0.02	0.32
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	20	0.32	0.06	0.31
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG21	20	0.31	0.05	0.3
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	20	0.31	0.05	0.3
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	20	0.31	0.05	0.3
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	20	0.31	0.06	0.3
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	20	0.31	0.06	0.32
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG21	20	0.31	0.06	0.32
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	20	0.31	0.06	0.32
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	20	0.3	0.05	0.3
(1,1414)	1:147:A:VAL:HG11	1:145:A:PHE:HZ	20	0.3	0.08	0.32
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	20	0.3	0.08	0.32
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	20	0.3	0.08	0.32
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	20	0.3	0.03	0.29
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	20	0.29	0.09	0.26
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	20	0.29	0.09	0.26
(1,1413)	1:171:A:ALA:HB1	1:195:A:PHE:HZ	20	0.29	0.09	0.26
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	20	0.29	0.07	0.29
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD3	20	0.29	0.07	0.29
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	20	0.29	0.03	0.3
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	20	0.29	0.04	0.29
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG22	20	0.29	0.04	0.29

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG23	20	0.29	0.04	0.29
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	20	0.28	0.02	0.29
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	20	0.28	0.02	0.29
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	20	0.28	0.04	0.28
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	20	0.28	0.03	0.27
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	20	0.27	0.1	0.25
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	20	0.27	0.1	0.25
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG23	20	0.27	0.1	0.25
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	20	0.27	0.06	0.3
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	20	0.27	0.02	0.27
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	20	0.27	0.05	0.27
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	20	0.26	0.01	0.26
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	20	0.26	0.01	0.26
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG22	20	0.26	0.01	0.26
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	20	0.26	0.05	0.26
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	20	0.26	0.02	0.26
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	20	0.26	0.05	0.26
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	20	0.26	0.05	0.26
(1,1494)	1:155:A:ILE:HD13	1:155:A:ILE:HB	20	0.26	0.05	0.26
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	20	0.26	0.06	0.27
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB1	20	0.26	0.06	0.27
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	20	0.26	0.06	0.27
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	20	0.25	0.02	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	20	0.25	0.01	0.25
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	20	0.25	0.05	0.24
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	20	0.25	0.06	0.24
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG23	20	0.25	0.01	0.25
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	20	0.25	0.01	0.25
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	20	0.25	0.01	0.25
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	20	0.25	0.08	0.22
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	20	0.25	0.02	0.24
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	20	0.24	0.06	0.22
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	20	0.24	0.06	0.22
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG23	20	0.24	0.06	0.22
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	20	0.23	0.06	0.24
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	20	0.23	0.04	0.23
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	20	0.23	0.03	0.22
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	20	0.23	0.03	0.23
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG22	20	0.23	0.06	0.22
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	20	0.23	0.06	0.22
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG21	20	0.23	0.06	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	20	0.23	0.01	0.22

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	20	0.22	0.01	0.22
(1,1369)	1:197:A:LEU:HD11	1:197:A:LEU:HG	20	0.22	0.04	0.22
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	20	0.22	0.04	0.22
(1,1369)	1:197:A:LEU:HD12	1:197:A:LEU:HG	20	0.22	0.04	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	20	0.22	0.01	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG23	20	0.22	0.01	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG21	20	0.22	0.01	0.22
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	20	0.21	0.03	0.22
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	20	0.21	0.03	0.22
(1,1571)	1:197:A:LEU:HD22	1:197:A:LEU:HG	20	0.21	0.03	0.22
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	20	0.21	0.01	0.21
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	20	0.2	0.0	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	20	0.2	0.0	0.2
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	20	0.2	0.02	0.2
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	20	0.2	0.04	0.2
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	20	0.2	0.01	0.19
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	20	0.19	0.02	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	20	0.19	0.01	0.19
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	20	0.19	0.05	0.21
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	20	0.18	0.04	0.18
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	20	0.18	0.03	0.18
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	20	0.18	0.04	0.18
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	20	0.18	0.06	0.16
(2,146)	1:163:A:ASP:HB2	1:161:A:PHE:HB3	20	0.18	0.06	0.16
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	20	0.18	0.04	0.16
(1,661)	1:182:A:THR:H	1:182:A:THR:HG21	20	0.18	0.04	0.16
(1,661)	1:182:A:THR:H	1:182:A:THR:HG22	20	0.18	0.04	0.16
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	20	0.18	0.01	0.18
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	20	0.18	0.04	0.18
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	20	0.16	0.03	0.15
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	20	0.16	0.01	0.16
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	20	0.16	0.02	0.16
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	20	0.15	0.02	0.16
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG21	20	0.15	0.01	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	20	0.15	0.01	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	20	0.15	0.01	0.15
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	20	0.15	0.01	0.14
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	20	0.14	0.02	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	20	0.14	0.01	0.15
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	19	0.83	0.12	0.83
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	19	0.69	0.14	0.75
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD23	19	0.69	0.14	0.75

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD22	19	0.69	0.14	0.75
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD13	19	0.68	0.3	0.57
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	19	0.68	0.3	0.57
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD12	19	0.68	0.3	0.57
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	19	0.68	0.45	0.52
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	19	0.68	0.45	0.52
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	19	0.68	0.1	0.66
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	19	0.68	0.1	0.66
(1,1397)	1:125:A:VAL:HG12	1:122:A:ASN:HB3	19	0.68	0.1	0.66
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	19	0.59	0.14	0.65
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	19	0.59	0.19	0.55
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	19	0.59	0.19	0.55
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG13	19	0.59	0.19	0.55
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	19	0.56	0.17	0.61
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD11	19	0.56	0.17	0.61
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD13	19	0.56	0.17	0.61
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	19	0.56	0.1	0.56
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	19	0.56	0.1	0.56
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE2	19	0.56	0.1	0.56
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	19	0.55	0.1	0.58
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	19	0.55	0.1	0.58
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB2	19	0.55	0.1	0.58
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	19	0.54	0.16	0.62
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD12	19	0.54	0.16	0.62
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD11	19	0.54	0.16	0.62
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	19	0.51	0.1	0.5
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD13	19	0.51	0.1	0.5
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD11	19	0.51	0.1	0.5
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD23	19	0.48	0.08	0.51
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	19	0.48	0.08	0.51
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD21	19	0.48	0.08	0.51
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	19	0.48	0.16	0.45
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	19	0.45	0.18	0.4
(2,56)	1:110:A:MET:H	1:109:A:ARG:HB3	19	0.45	0.18	0.4
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	19	0.43	0.1	0.41
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG13	19	0.43	0.1	0.41
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	19	0.43	0.1	0.41
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	19	0.39	0.05	0.39
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	19	0.39	0.24	0.34
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	19	0.39	0.18	0.39
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD13	19	0.39	0.18	0.39
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD11	19	0.39	0.18	0.39

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	19	0.38	0.07	0.4
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	19	0.38	0.06	0.41
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	19	0.32	0.04	0.3
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	19	0.3	0.1	0.31
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	19	0.3	0.05	0.31
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	19	0.29	0.07	0.28
(2,147)	1:112:A:ASN:HB2	1:114:A:GLU:HB2	19	0.29	0.07	0.28
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG23	19	0.28	0.08	0.27
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	19	0.28	0.08	0.27
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	19	0.28	0.08	0.27
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	19	0.28	0.05	0.29
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	19	0.26	0.03	0.26
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	19	0.26	0.07	0.24
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	19	0.26	0.07	0.24
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD13	19	0.26	0.07	0.24
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	19	0.25	0.04	0.25
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	19	0.23	0.07	0.22
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD21	19	0.23	0.04	0.23
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	19	0.23	0.04	0.23
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD22	19	0.23	0.04	0.23
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	19	0.22	0.2	0.19
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	19	0.22	0.12	0.18
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	19	0.22	0.06	0.2
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	19	0.22	0.23	0.17
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	19	0.22	0.06	0.23
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	19	0.21	0.05	0.21
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	19	0.21	0.07	0.2
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG23	19	0.21	0.07	0.2
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG22	19	0.21	0.07	0.2
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	19	0.19	0.03	0.19
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	19	0.18	0.02	0.19
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	19	0.16	0.03	0.16
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	19	0.16	0.02	0.16
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	19	0.15	0.03	0.15
(1,1382)	1:127:A:LEU:HD22	1:124:A:MET:HB2	18	1.63	1.49	0.84
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	18	1.63	1.49	0.84
(1,1382)	1:127:A:LEU:HD21	1:124:A:MET:HB2	18	1.63	1.49	0.84
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	18	1.2	0.15	1.18
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG23	18	1.2	0.15	1.18
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG21	18	1.2	0.15	1.18
(1,1370)	1:197:A:LEU:HD13	1:127:A:LEU:HD13	18	1.1	0.95	0.64
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD11	18	1.1	0.95	0.64

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD13	18	1.1	0.95	0.64
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD13	18	1.1	0.95	0.64
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD12	18	1.1	0.95	0.64
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD12	18	1.1	0.95	0.64
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD11	18	1.1	0.95	0.64
(1,1370)	1:197:A:LEU:HD13	1:127:A:LEU:HD11	18	1.1	0.95	0.64
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	18	1.03	0.56	1.28
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG23	18	1.03	0.56	1.28
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG11	18	1.03	0.56	1.28
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG22	18	1.03	0.56	1.28
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG13	18	1.03	0.56	1.28
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD13	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD12	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD13	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD11	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD13	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD11	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD11	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD12	18	0.77	0.59	0.74
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD12	18	0.77	0.59	0.74
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG22	18	0.77	0.15	0.78
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG21	18	0.77	0.15	0.78
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG23	18	0.77	0.15	0.78
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	18	0.73	0.02	0.73
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	18	0.72	0.04	0.71
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG22	18	0.67	0.29	0.7
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	18	0.67	0.29	0.7
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG21	18	0.67	0.29	0.7
(1,1648)	1:195:A:PHE:HE1	1:183:A:ILE:HG23	18	0.67	0.29	0.7
(1,1648)	1:195:A:PHE:HE1	1:183:A:ILE:HG22	18	0.67	0.29	0.7
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HD3	18	0.64	0.37	0.52
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HG2	18	0.64	0.37	0.52
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HG2	18	0.64	0.37	0.52
(2,199)	1:140:A:THR:HG22	1:138:A:LYS:HG2	18	0.64	0.37	0.52
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HD3	18	0.64	0.37	0.52
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	18	0.64	0.27	0.52
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE1	18	0.64	0.27	0.52
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE3	18	0.64	0.27	0.52
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	18	0.59	0.11	0.6
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG23	18	0.59	0.11	0.6
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG21	18	0.59	0.11	0.6
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	18	0.58	0.1	0.62

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,183)	1:158:A:PRO:HG2	1:158:A:PRO:HA	18	0.58	0.1	0.62
(1,1483)	1:183:A:ILE:HD11	1:195:A:PHE:HD1	18	0.56	0.25	0.51
(1,1483)	1:183:A:ILE:HD11	1:195:A:PHE:HD2	18	0.56	0.25	0.51
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD1	18	0.56	0.25	0.51
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD2	18	0.56	0.25	0.51
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD1	18	0.56	0.25	0.51
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD2	18	0.56	0.25	0.51
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	18	0.54	0.23	0.54
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD13	18	0.54	0.23	0.54
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD11	18	0.54	0.23	0.54
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	18	0.49	0.12	0.52
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD22	18	0.49	0.12	0.52
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD23	18	0.49	0.12	0.52
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG23	18	0.49	0.19	0.55
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	18	0.49	0.19	0.55
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG21	18	0.49	0.19	0.55
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	18	0.48	0.11	0.49
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	18	0.48	0.11	0.49
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG22	18	0.48	0.11	0.49
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	18	0.47	0.18	0.45
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD2	18	0.47	0.18	0.45
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	18	0.44	0.31	0.34
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	18	0.44	0.31	0.34
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG11	18	0.44	0.31	0.34
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	18	0.44	0.15	0.41
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	18	0.44	0.15	0.41
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD11	18	0.44	0.15	0.41
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD21	18	0.43	0.29	0.34
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD22	18	0.43	0.29	0.34
(1,1481)	1:152:A:ILE:HD11	1:128:A:LEU:HD23	18	0.43	0.29	0.34
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD23	18	0.43	0.29	0.34
(1,1481)	1:152:A:ILE:HD13	1:128:A:LEU:HD21	18	0.43	0.29	0.34
(1,1481)	1:152:A:ILE:HD11	1:128:A:LEU:HD21	18	0.43	0.29	0.34
(1,1481)	1:152:A:ILE:HD13	1:128:A:LEU:HD22	18	0.43	0.29	0.34
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB1	18	0.43	0.17	0.4
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB2	18	0.43	0.17	0.4
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB3	18	0.43	0.17	0.4
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB3	18	0.43	0.17	0.4
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB1	18	0.43	0.17	0.4
(1,1366)	1:173:A:LEU:HD13	1:171:A:ALA:HB1	18	0.43	0.17	0.4
(1,1366)	1:173:A:LEU:HD13	1:171:A:ALA:HB2	18	0.43	0.17	0.4
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB2	18	0.43	0.17	0.4

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	18	0.41	0.52	0.2
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	18	0.41	0.12	0.44
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	18	0.38	0.13	0.43
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD2	18	0.38	0.13	0.43
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	18	0.38	0.74	0.21
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	18	0.36	0.11	0.38
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	18	0.36	0.14	0.38
(1,1734)	1:195:A:PHE:HD1	1:195:A:PHE:HB2	18	0.36	0.14	0.38
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	18	0.35	0.11	0.34
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG21	18	0.35	0.11	0.34
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG22	18	0.35	0.11	0.34
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	18	0.34	0.1	0.34
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD13	18	0.34	0.1	0.34
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD11	18	0.34	0.1	0.34
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD11	18	0.32	0.13	0.35
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	18	0.32	0.13	0.35
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD13	18	0.32	0.13	0.35
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG22	18	0.31	0.08	0.32
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	18	0.31	0.08	0.32
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG21	18	0.31	0.08	0.32
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	18	0.29	0.04	0.3
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	18	0.28	0.09	0.28
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG22	18	0.26	0.07	0.28
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	18	0.26	0.07	0.28
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	18	0.26	0.07	0.28
(1,1591)	1:183:A:ILE:HG23	1:173:A:LEU:HD13	18	0.22	0.09	0.2
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD11	18	0.22	0.09	0.2
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD13	18	0.22	0.09	0.2
(1,1591)	1:183:A:ILE:HG23	1:173:A:LEU:HD11	18	0.22	0.09	0.2
(1,1591)	1:183:A:ILE:HG22	1:173:A:LEU:HD13	18	0.22	0.09	0.2
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD12	18	0.22	0.09	0.2
(1,1591)	1:183:A:ILE:HG22	1:173:A:LEU:HD12	18	0.22	0.09	0.2
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	18	0.18	0.02	0.18
(2,178)	1:165:A:LYS:HD2	1:165:A:LYS:HG3	18	0.18	0.02	0.18
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	18	0.17	0.06	0.16
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	18	0.17	0.02	0.17
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	18	0.17	0.04	0.17
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	18	0.16	0.03	0.16
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	18	0.15	0.03	0.16
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB3	18	0.14	0.02	0.14
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	18	0.14	0.02	0.14
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB1	18	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG23	18	0.13	0.02	0.12
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG22	18	0.13	0.02	0.12
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG21	18	0.13	0.02	0.12
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	18	0.12	0.01	0.12
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	17	1.45	1.04	0.77
(1,1420)	1:113:A:LEU:HD23	1:154:A:MET:HG2	17	1.45	1.04	0.77
(1,1420)	1:113:A:LEU:HD22	1:154:A:MET:HG2	17	1.45	1.04	0.77
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	17	0.83	0.27	0.89
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG13	17	0.83	0.27	0.89
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG12	17	0.83	0.27	0.89
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG23	17	0.83	0.27	0.89
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	17	0.79	0.39	0.79
(2,132)	1:167:A:GLY:HA3	1:168:A:GLN:HG2	17	0.79	0.39	0.79
(2,132)	1:167:A:GLY:HA3	1:158:A:PRO:HB2	17	0.79	0.39	0.79
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG3	17	0.79	0.39	0.79
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	17	0.78	0.94	0.29
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG12	17	0.78	0.94	0.29
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG11	17	0.78	0.94	0.29
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	17	0.64	0.23	0.57
(2,133)	1:167:A:GLY:HA2	1:166:A:GLU:HG3	17	0.64	0.23	0.57
(2,133)	1:167:A:GLY:HA2	1:168:A:GLN:HG2	17	0.64	0.23	0.57
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	17	0.54	0.29	0.47
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG13	17	0.54	0.29	0.47
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG12	17	0.54	0.29	0.47
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	17	0.5	0.14	0.47
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	17	0.44	0.05	0.43
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD2	17	0.44	0.05	0.43
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	17	0.41	0.16	0.47
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	17	0.41	0.16	0.47
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD11	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD11	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD13	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD11	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD12	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD12	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD12	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD13	17	0.4	0.17	0.36
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD13	17	0.4	0.17	0.36
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	17	0.36	0.19	0.27
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	17	0.36	0.12	0.38
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD12	17	0.36	0.12	0.38
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD13	17	0.36	0.12	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	17	0.34	0.26	0.3
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD12	17	0.34	0.26	0.3
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD13	17	0.34	0.26	0.3
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	17	0.32	0.11	0.34
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB1	17	0.32	0.11	0.34
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB3	17	0.32	0.11	0.34
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	17	0.32	0.09	0.32
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD13	17	0.31	0.16	0.26
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	17	0.31	0.16	0.26
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD12	17	0.31	0.16	0.26
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	17	0.3	0.06	0.3
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD13	17	0.28	0.12	0.28
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD12	17	0.28	0.12	0.28
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	17	0.28	0.12	0.28
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG11	17	0.25	0.09	0.23
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	17	0.25	0.09	0.23
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG12	17	0.25	0.09	0.23
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG21	17	0.21	0.07	0.18
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG23	17	0.21	0.07	0.18
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	17	0.21	0.07	0.18
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	17	0.2	0.03	0.2
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	17	0.19	0.08	0.16
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	17	0.19	0.06	0.18
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	17	0.18	0.05	0.17
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	17	0.15	0.1	0.14
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	17	0.15	0.04	0.14
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB3	17	0.15	0.04	0.14
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	17	0.14	0.03	0.14
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	17	0.14	0.02	0.13
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	17	0.14	0.02	0.13
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB3	17	0.14	0.02	0.13
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	17	0.13	0.02	0.13
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	17	0.13	0.01	0.13
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD21	16	1.67	1.35	2.68
(1,1746)	1:128:A:LEU:HD23	1:127:A:LEU:HD21	16	1.67	1.35	2.68
(1,1746)	1:128:A:LEU:HD21	1:127:A:LEU:HD21	16	1.67	1.35	2.68
(1,1746)	1:128:A:LEU:HD21	1:127:A:LEU:HD22	16	1.67	1.35	2.68
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD23	16	1.67	1.35	2.68
(1,1746)	1:128:A:LEU:HD23	1:127:A:LEU:HD22	16	1.67	1.35	2.68
(1,1746)	1:128:A:LEU:HD23	1:127:A:LEU:HD23	16	1.67	1.35	2.68
(1,1746)	1:128:A:LEU:HD21	1:127:A:LEU:HD23	16	1.67	1.35	2.68
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG23	16	0.99	0.05	0.99

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG21	16	0.99	0.05	0.99
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG22	16	0.99	0.05	0.99
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	16	0.96	0.42	1.17
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG23	16	0.79	0.03	0.78
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	16	0.79	0.03	0.78
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	16	0.79	0.03	0.78
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG21	16	0.66	0.05	0.68
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	16	0.66	0.05	0.68
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	16	0.66	0.05	0.68
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG11	16	0.62	0.08	0.62
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG13	16	0.62	0.08	0.62
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG12	16	0.62	0.08	0.62
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	16	0.58	0.08	0.61
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG22	16	0.58	0.08	0.61
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG23	16	0.58	0.08	0.61
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	16	0.58	0.32	0.49
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD12	16	0.58	0.32	0.49
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD11	16	0.58	0.32	0.49
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD22	16	0.58	0.32	0.49
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD13	16	0.51	0.24	0.53
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD12	16	0.51	0.24	0.53
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD11	16	0.51	0.24	0.53
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	16	0.44	0.33	0.31
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG13	16	0.44	0.33	0.31
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG11	16	0.44	0.33	0.31
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG12	16	0.43	0.11	0.42
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG11	16	0.43	0.11	0.42
(2,52)	1:134:A:ARG:H	1:128:A:LEU:HB3	16	0.43	0.11	0.42
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG13	16	0.43	0.11	0.42
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	16	0.43	0.3	0.26
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	16	0.43	0.14	0.42
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG13	16	0.43	0.14	0.42
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG12	16	0.43	0.14	0.42
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	16	0.41	0.19	0.36
(1,1479)	1:152:A:ILE:HD13	1:175:A:PHE:HE1	16	0.39	0.17	0.3
(1,1479)	1:152:A:ILE:HD12	1:175:A:PHE:HE1	16	0.39	0.17	0.3
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE2	16	0.39	0.17	0.3
(1,1479)	1:152:A:ILE:HD12	1:175:A:PHE:HE2	16	0.39	0.17	0.3
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE1	16	0.39	0.17	0.3
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	16	0.36	0.14	0.38
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	16	0.36	0.13	0.34
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG13	16	0.36	0.13	0.34

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG12	16	0.36	0.13	0.34
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	16	0.35	0.08	0.38
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG23	16	0.35	0.08	0.38
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	16	0.35	0.08	0.38
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	16	0.26	0.1	0.28
(1,1435)	1:136:A:VAL:HG21	1:139:A:MET:HB2	16	0.24	0.07	0.23
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	16	0.24	0.07	0.23
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	16	0.24	0.07	0.23
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	16	0.23	0.08	0.24
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	16	0.19	0.06	0.18
(1,333)	1:124:A:MET:H	1:110:A:MET:H	16	0.19	0.04	0.2
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	16	0.16	0.04	0.16
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	15	0.73	0.27	0.81
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HG3	15	0.73	0.27	0.81
(2,126)	1:112:A:ASN:HA	1:197:A:LEU:HG	15	0.73	0.27	0.81
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB2	15	0.73	0.27	0.81
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	15	0.56	0.7	0.15
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD12	15	0.46	0.14	0.47
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD13	15	0.46	0.14	0.47
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD11	15	0.46	0.14	0.47
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	15	0.44	0.09	0.45
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG22	15	0.41	0.15	0.41
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG23	15	0.41	0.15	0.41
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG21	15	0.41	0.15	0.41
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	15	0.36	0.07	0.38
(2,7)	1:135:A:GLN:H	1:136:A:VAL:HG11	15	0.34	0.14	0.26
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	15	0.34	0.14	0.26
(2,7)	1:135:A:GLN:H	1:136:A:VAL:HG13	15	0.34	0.14	0.26
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB1	15	0.32	0.05	0.31
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	15	0.32	0.05	0.31
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB3	15	0.32	0.05	0.31
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	15	0.26	0.18	0.25
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	15	0.25	0.09	0.22
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD22	15	0.25	0.09	0.22
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD21	15	0.25	0.09	0.22
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	15	0.24	0.08	0.23
(2,66)	1:168:A:GLN:H	1:142:A:PRO:HA	15	0.24	0.08	0.23
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	15	0.23	0.31	0.14
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	15	0.23	0.09	0.22
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	15	0.23	0.09	0.22
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	15	0.2	0.05	0.21
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE2	15	0.2	0.05	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	15	0.18	0.03	0.19
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	15	0.14	0.03	0.13
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	15	0.13	0.03	0.11
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	15	0.12	0.01	0.12
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	15	0.11	0.01	0.11
(1,1421)	1:113:A:LEU:HD11	1:113:A:LEU:HB3	14	1.16	0.02	1.15
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	14	1.16	0.02	1.15
(1,1421)	1:113:A:LEU:HD13	1:113:A:LEU:HB3	14	1.16	0.02	1.15
(2,201)	1:111:A:VAL:HG11	1:130:A:ALA:HB3	14	1.11	0.36	1.25
(2,201)	1:111:A:VAL:HG12	1:130:A:ALA:HB3	14	1.11	0.36	1.25
(2,201)	1:111:A:VAL:HG21	1:127:A:LEU:HB3	14	1.11	0.36	1.25
(2,201)	1:111:A:VAL:HG11	1:130:A:ALA:HB2	14	1.11	0.36	1.25
(2,201)	1:111:A:VAL:HG12	1:130:A:ALA:HB2	14	1.11	0.36	1.25
(2,201)	1:111:A:VAL:HG22	1:130:A:ALA:HB2	14	1.11	0.36	1.25
(2,201)	1:111:A:VAL:HG13	1:130:A:ALA:HB2	14	1.11	0.36	1.25
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD23	14	0.9	0.49	0.76
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD21	14	0.9	0.49	0.76
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD22	14	0.9	0.49	0.76
(2,54)	1:129:A:GLU:H	1:129:A:GLU:HG2	14	0.57	0.14	0.55
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	14	0.57	0.14	0.55
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	14	0.54	0.27	0.55
(1,1476)	1:119:A:ILE:HG22	1:117:A:MET:HG3	14	0.54	0.45	0.36
(1,1476)	1:119:A:ILE:HG21	1:117:A:MET:HG3	14	0.54	0.45	0.36
(1,1476)	1:119:A:ILE:HG23	1:117:A:MET:HG3	14	0.54	0.45	0.36
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	14	0.46	0.16	0.47
(2,170)	1:110:A:MET:H	1:109:A:ARG:HB3	14	0.46	0.16	0.47
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE1	14	0.38	0.12	0.4
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE2	14	0.38	0.12	0.4
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE3	14	0.38	0.12	0.4
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	14	0.28	0.11	0.29
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	14	0.23	0.13	0.18
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	14	0.2	0.06	0.19
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	14	0.2	0.05	0.22
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	14	0.18	0.07	0.15
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG3	14	0.18	0.07	0.15
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	14	0.16	0.03	0.16
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG22	14	0.16	0.03	0.16
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG23	14	0.16	0.03	0.16
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	13	1.25	0.6	1.38
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD2	13	1.25	0.6	1.38
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	13	0.98	0.06	0.94
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	13	0.96	0.95	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG11	13	0.83	0.07	0.81
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG12	13	0.83	0.07	0.81
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG13	13	0.83	0.07	0.81
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD13	13	0.64	0.15	0.66
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD12	13	0.64	0.15	0.66
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD11	13	0.64	0.15	0.66
(1,1403)	1:180:A:LEU:HD12	1:183:A:ILE:HD11	13	0.64	0.15	0.66
(1,1403)	1:180:A:LEU:HD13	1:183:A:ILE:HD12	13	0.64	0.15	0.66
(1,1403)	1:180:A:LEU:HD13	1:183:A:ILE:HD11	13	0.64	0.15	0.66
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG23	13	0.59	0.46	0.4
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG21	13	0.59	0.46	0.4
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG22	13	0.59	0.46	0.4
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	13	0.55	0.03	0.57
(2,143)	1:138:A:LYS:HE3	1:138:A:LYS:HG3	13	0.55	0.03	0.57
(1,1461)	1:183:A:ILE:HG23	1:183:A:ILE:HG13	13	0.52	0.15	0.54
(1,1461)	1:183:A:ILE:HG21	1:183:A:ILE:HG13	13	0.52	0.15	0.54
(1,1461)	1:183:A:ILE:HG22	1:183:A:ILE:HG13	13	0.52	0.15	0.54
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	13	0.36	0.05	0.34
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG23	13	0.31	0.13	0.28
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG22	13	0.31	0.13	0.28
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG21	13	0.31	0.13	0.28
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB1	13	0.29	0.38	0.13
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB3	13	0.29	0.38	0.13
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB2	13	0.29	0.38	0.13
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	13	0.28	0.16	0.27
(2,105)	1:115:A:PRO:HA	1:181:A:ALA:HA	13	0.28	0.16	0.27
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	13	0.24	0.01	0.24
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB3	13	0.24	0.09	0.25
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB2	13	0.24	0.09	0.25
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB1	13	0.24	0.09	0.25
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	13	0.19	0.07	0.14
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	13	0.18	0.07	0.15
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	13	0.17	0.05	0.15
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	13	0.17	0.05	0.17
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	13	0.16	0.04	0.15
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	13	0.15	0.04	0.14
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	13	0.15	0.04	0.15
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB2	13	0.13	0.02	0.14
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB3	13	0.13	0.02	0.14
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB1	13	0.13	0.02	0.14
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	13	0.11	0.01	0.11
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	12	0.8	0.09	0.84

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	12	0.6	0.05	0.61
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD13	12	0.57	0.71	0.37
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD11	12	0.57	0.71	0.37
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD12	12	0.57	0.71	0.37
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	12	0.53	0.56	0.15
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG13	12	0.53	0.56	0.15
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG12	12	0.53	0.56	0.15
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG21	12	0.46	0.14	0.51
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG22	12	0.46	0.14	0.51
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG23	12	0.46	0.14	0.51
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG22	12	0.44	0.17	0.5
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG23	12	0.44	0.17	0.5
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG21	12	0.44	0.17	0.5
(1,1462)	1:195:A:PHE:HD1	1:183:A:ILE:HG23	12	0.44	0.17	0.5
(2,161)	1:186:A:MET:HG3	1:170:A:ARG:HD3	12	0.42	0.19	0.41
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	12	0.42	0.19	0.41
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD2	12	0.42	0.19	0.41
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD2	12	0.31	0.12	0.34
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD1	12	0.31	0.12	0.34
(1,1474)	1:119:A:ILE:HG22	1:175:A:PHE:HD2	12	0.31	0.12	0.34
(1,1474)	1:119:A:ILE:HG22	1:175:A:PHE:HD1	12	0.31	0.12	0.34
(1,1474)	1:119:A:ILE:HG21	1:175:A:PHE:HD1	12	0.31	0.12	0.34
(1,1474)	1:119:A:ILE:HG21	1:175:A:PHE:HD2	12	0.31	0.12	0.34
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	12	0.31	0.01	0.3
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	12	0.3	0.21	0.2
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	12	0.24	0.08	0.23
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG23	12	0.24	0.08	0.23
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG21	12	0.24	0.08	0.23
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB3	12	0.13	0.03	0.12
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB2	12	0.13	0.03	0.12
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB1	12	0.13	0.03	0.12
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	12	0.13	0.02	0.12
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	12	0.1	0.0	0.1
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	11	1.09	0.07	1.11
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	11	0.93	0.6	1.36
(1,1384)	1:127:A:LEU:HD21	1:127:A:LEU:HA	11	0.9	0.23	0.94
(1,1384)	1:127:A:LEU:HD22	1:127:A:LEU:HA	11	0.9	0.23	0.94
(1,1384)	1:127:A:LEU:HD23	1:127:A:LEU:HA	11	0.9	0.23	0.94
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	11	0.7	0.29	0.72
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD13	11	0.58	0.11	0.63
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD12	11	0.58	0.11	0.63
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD11	11	0.58	0.11	0.63

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD12	11	0.5	0.07	0.49
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD11	11	0.5	0.07	0.49
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD13	11	0.5	0.07	0.49
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	11	0.42	0.39	0.14
(2,202)	1:184:A:VAL:HG11	1:172:A:ARG:HG2	11	0.34	0.17	0.28
(2,202)	1:184:A:VAL:HG12	1:172:A:ARG:HG2	11	0.34	0.17	0.28
(2,202)	1:184:A:VAL:HG13	1:172:A:ARG:HG2	11	0.34	0.17	0.28
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD23	11	0.32	0.11	0.35
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD21	11	0.32	0.11	0.35
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD22	11	0.32	0.11	0.35
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	11	0.26	0.12	0.23
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB2	11	0.26	0.12	0.23
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	11	0.24	0.07	0.26
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD23	11	0.24	0.11	0.21
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD22	11	0.24	0.11	0.21
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD21	11	0.24	0.11	0.21
(2,42)	1:128:A:LEU:H	1:129:A:GLU:HG2	11	0.2	0.08	0.17
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	11	0.2	0.08	0.17
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE2	11	0.2	0.08	0.17
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG23	11	0.2	0.08	0.2
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG21	11	0.2	0.08	0.2
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG22	11	0.2	0.08	0.2
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	11	0.16	0.08	0.13
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	11	0.13	0.02	0.14
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	11	0.13	0.03	0.12
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB1	11	0.11	0.01	0.11
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB2	11	0.11	0.01	0.11
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB3	11	0.11	0.01	0.11
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD13	10	1.02	0.11	0.98
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD11	10	1.02	0.11	0.98
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD12	10	1.02	0.11	0.98
(1,1477)	1:186:A:MET:HE1	1:170:A:ARG:HD2	10	0.82	0.66	0.85
(1,1477)	1:186:A:MET:HE2	1:170:A:ARG:HD2	10	0.82	0.66	0.85
(1,1477)	1:186:A:MET:HE3	1:170:A:ARG:HD2	10	0.82	0.66	0.85
(1,1578)	1:140:A:THR:HG21	1:138:A:LYS:HE3	10	0.6	0.45	0.33
(1,1578)	1:140:A:THR:HG23	1:138:A:LYS:HE3	10	0.6	0.45	0.33
(1,1578)	1:140:A:THR:HG22	1:138:A:LYS:HE3	10	0.6	0.45	0.33
(1,1406)	1:180:A:LEU:HD13	1:175:A:PHE:HD1	10	0.48	0.75	0.18
(1,1406)	1:180:A:LEU:HD11	1:175:A:PHE:HD1	10	0.48	0.75	0.18
(1,1406)	1:180:A:LEU:HD12	1:175:A:PHE:HD1	10	0.48	0.75	0.18
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG13	10	0.36	0.18	0.38
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG11	10	0.36	0.18	0.38

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG12	10	0.36	0.18	0.38
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD13	10	0.31	0.09	0.29
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD12	10	0.31	0.09	0.29
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD11	10	0.31	0.09	0.29
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	10	0.28	0.28	0.17
(2,136)	1:172:A:ARG:HD2	1:172:A:ARG:HB2	10	0.28	0.28	0.17
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	10	0.26	0.1	0.26
(2,62)	1:120:A:SER:H	1:123:A:GLU:HA	10	0.26	0.1	0.26
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	10	0.2	0.06	0.2
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG21	10	0.2	0.02	0.2
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG22	10	0.2	0.02	0.2
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG23	10	0.2	0.02	0.2
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	10	0.19	0.04	0.18
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	10	0.18	0.04	0.2
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	10	0.16	0.02	0.15
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	10	0.13	0.02	0.12
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	10	0.12	0.01	0.13
(2,209)	1:194:A:PHE:HD1	1:194:A:PHE:HB3	10	0.12	0.02	0.12
(2,209)	1:194:A:PHE:HD2	1:194:A:PHE:HB2	10	0.12	0.02	0.12
(2,209)	1:194:A:PHE:HD1	1:194:A:PHE:HB2	10	0.12	0.02	0.12
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	10	0.11	0.01	0.11
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	9	1.06	0.03	1.05
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD23	9	1.06	0.03	1.05
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	9	0.98	0.52	1.3
(1,1570)	1:127:A:LEU:HD12	1:127:A:LEU:HB2	9	0.83	0.06	0.82
(1,1570)	1:127:A:LEU:HD13	1:127:A:LEU:HB2	9	0.83	0.06	0.82
(1,1570)	1:127:A:LEU:HD11	1:127:A:LEU:HB2	9	0.83	0.06	0.82
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG22	9	0.75	0.39	0.62
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG23	9	0.75	0.39	0.62
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG21	9	0.75	0.39	0.62
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	9	0.73	0.39	0.58
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD23	9	0.73	0.39	0.58
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD12	9	0.47	0.12	0.47
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD13	9	0.47	0.12	0.47
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD11	9	0.47	0.12	0.47
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD23	9	0.38	0.18	0.38
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD21	9	0.38	0.18	0.38
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD22	9	0.38	0.18	0.38
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD23	9	0.31	0.12	0.27
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD22	9	0.31	0.12	0.27
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD21	9	0.31	0.12	0.27
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	9	0.25	0.11	0.19

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD3	9	0.25	0.11	0.19
(1,81)	1:186:A:MET:H	1:186:A:MET:HE3	9	0.21	0.14	0.14
(1,81)	1:186:A:MET:H	1:186:A:MET:HE2	9	0.21	0.14	0.14
(1,81)	1:186:A:MET:H	1:186:A:MET:HE1	9	0.21	0.14	0.14
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	9	0.21	0.05	0.21
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	9	0.19	0.06	0.18
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG21	9	0.18	0.05	0.17
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG22	9	0.18	0.05	0.17
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG23	9	0.18	0.05	0.17
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	9	0.15	0.03	0.16
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD2	9	0.14	0.03	0.13
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD3	9	0.14	0.03	0.13
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD12	8	0.82	0.23	0.94
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD21	8	0.82	0.23	0.94
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD22	8	0.82	0.23	0.94
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG21	8	0.51	0.21	0.58
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG23	8	0.51	0.21	0.58
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG22	8	0.51	0.21	0.58
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	8	0.36	0.14	0.34
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB2	8	0.35	0.07	0.38
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB3	8	0.35	0.07	0.38
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	8	0.28	0.06	0.26
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	8	0.25	0.23	0.17
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	8	0.19	0.06	0.18
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	8	0.17	0.05	0.16
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	8	0.16	0.03	0.15
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	8	0.15	0.05	0.15
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	8	0.15	0.02	0.15
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	8	0.15	0.03	0.14
(1,1471)	1:119:A:ILE:HG23	1:175:A:PHE:HE2	8	0.14	0.04	0.13
(1,1471)	1:119:A:ILE:HG23	1:175:A:PHE:HE1	8	0.14	0.04	0.13
(1,1471)	1:119:A:ILE:HG22	1:175:A:PHE:HE2	8	0.14	0.04	0.13
(1,1471)	1:119:A:ILE:HG22	1:175:A:PHE:HE1	8	0.14	0.04	0.13
(1,1471)	1:119:A:ILE:HG21	1:175:A:PHE:HE1	8	0.14	0.04	0.13
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	8	0.14	0.01	0.14
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	8	0.13	0.02	0.14
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	7	1.24	0.46	1.4
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	7	0.89	0.24	0.99
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD12	7	0.77	0.07	0.75
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD11	7	0.77	0.07	0.75
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD13	7	0.77	0.07	0.75
(1,1395)	1:197:A:LEU:HD22	1:156:A:ARG:HG3	7	0.75	0.29	0.87

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1395)	1:197:A:LEU:HD21	1:156:A:ARG:HG3	7	0.75	0.29	0.87
(1,1395)	1:197:A:LEU:HD23	1:156:A:ARG:HG3	7	0.75	0.29	0.87
(1,1487)	1:183:A:ILE:HD11	1:183:A:ILE:HB	7	0.46	0.02	0.46
(1,1487)	1:183:A:ILE:HD13	1:183:A:ILE:HB	7	0.46	0.02	0.46
(1,1487)	1:183:A:ILE:HD12	1:183:A:ILE:HB	7	0.46	0.02	0.46
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG23	7	0.41	0.34	0.29
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG21	7	0.41	0.34	0.29
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG22	7	0.41	0.34	0.29
(2,38)	1:113:A:LEU:H	1:196:A:ARG:HD2	7	0.35	0.13	0.4
(2,38)	1:176:A:ASP:H	1:179:A:HIS:HB3	7	0.35	0.13	0.4
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG21	7	0.34	0.01	0.34
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG23	7	0.34	0.01	0.34
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG22	7	0.34	0.01	0.34
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD21	7	0.31	0.14	0.33
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD23	7	0.31	0.14	0.33
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD22	7	0.31	0.14	0.33
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG13	7	0.28	0.13	0.22
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG12	7	0.28	0.13	0.22
(2,12)	1:195:A:PHE:H	1:197:A:LEU:HD22	7	0.28	0.13	0.22
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	7	0.25	0.05	0.27
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG23	7	0.22	0.12	0.19
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG22	7	0.22	0.12	0.19
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	7	0.22	0.01	0.22
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD22	7	0.21	0.05	0.2
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD21	7	0.21	0.05	0.2
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD23	7	0.21	0.05	0.2
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	7	0.2	0.09	0.17
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	7	0.19	0.04	0.2
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD1	7	0.17	0.04	0.16
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD2	7	0.17	0.04	0.16
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB3	7	0.16	0.05	0.15
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB2	7	0.16	0.05	0.15
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB1	7	0.16	0.05	0.15
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE3	7	0.16	0.03	0.15
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE1	7	0.16	0.03	0.15
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE2	7	0.16	0.03	0.15
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	7	0.15	0.03	0.15
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	7	0.15	0.03	0.13
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	7	0.14	0.04	0.12
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	7	0.14	0.02	0.14
(1,1491)	1:119:A:ILE:HD11	1:119:A:ILE:HB	7	0.13	0.02	0.13
(1,1491)	1:119:A:ILE:HD12	1:119:A:ILE:HB	7	0.13	0.02	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1491)	1:119:A:ILE:HD13	1:119:A:ILE:HB	7	0.13	0.02	0.13
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG22	7	0.13	0.02	0.13
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG21	7	0.13	0.02	0.13
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG21	7	0.13	0.02	0.13
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG22	7	0.13	0.02	0.13
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG23	7	0.13	0.02	0.13
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	7	0.12	0.01	0.12
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	7	0.12	0.01	0.12
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD21	6	2.07	0.28	2.08
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD23	6	2.07	0.28	2.08
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD13	6	1.51	0.18	1.54
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD11	6	1.51	0.18	1.54
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD12	6	1.51	0.18	1.54
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD12	6	1.12	0.2	1.08
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD13	6	1.12	0.2	1.08
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD11	6	1.12	0.2	1.08
(1,1510)	1:129:A:GLU:HG2	1:126:A:LYS:HD3	6	1.09	0.25	1.01
(1,1049)	1:156:A:ARG:HD3	1:197:A:LEU:HA	6	0.93	0.3	0.94
(1,719)	1:138:A:LYS:H	1:137:A:SER:HB2	6	0.88	0.04	0.87
(1,1735)	1:190:A:ARG:HD2	1:185:A:ASN:HB2	6	0.74	0.44	0.6
(1,761)	1:129:A:GLU:HA	1:129:A:GLU:HG3	6	0.66	0.13	0.71
(1,72)	1:139:A:MET:H	1:139:A:MET:HE3	6	0.63	0.15	0.7
(1,72)	1:139:A:MET:H	1:139:A:MET:HE1	6	0.63	0.15	0.7
(1,72)	1:139:A:MET:H	1:139:A:MET:HE2	6	0.63	0.15	0.7
(1,1607)	1:155:A:ILE:HD13	1:170:A:ARG:HG2	6	0.49	0.22	0.37
(1,1607)	1:155:A:ILE:HD12	1:170:A:ARG:HG2	6	0.49	0.22	0.37
(1,1607)	1:155:A:ILE:HD11	1:170:A:ARG:HG2	6	0.49	0.22	0.37
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD13	6	0.48	0.6	0.18
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD12	6	0.48	0.6	0.18
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD11	6	0.48	0.6	0.18
(1,1312)	1:126:A:LYS:HD3	1:109:A:ARG:HB3	6	0.28	0.28	0.17
(2,175)	1:119:A:ILE:HA	1:123:A:GLU:HB3	6	0.27	0.14	0.26
(2,175)	1:123:A:GLU:HB3	1:124:A:MET:HA	6	0.27	0.14	0.26
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG21	6	0.19	0.1	0.16
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG23	6	0.19	0.1	0.16
(2,141)	1:126:A:LYS:HE3	1:109:A:ARG:HA	6	0.19	0.09	0.16
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB1	6	0.18	0.04	0.2
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB3	6	0.18	0.04	0.2
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB2	6	0.18	0.04	0.2
(1,1166)	1:153:A:GLU:HG3	1:172:A:ARG:HB2	6	0.18	0.09	0.14
(1,1389)	1:138:A:LYS:HG3	1:139:A:MET:H	6	0.17	0.03	0.16
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD12	6	0.16	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD13	6	0.16	0.04	0.15
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD11	6	0.16	0.04	0.15
(2,61)	1:133:A:TYR:H	1:129:A:GLU:HB3	6	0.16	0.06	0.14
(1,1718)	1:138:A:LYS:HA	1:136:A:VAL:HG13	5	1.67	0.75	1.99
(1,1718)	1:138:A:LYS:HA	1:136:A:VAL:HG12	5	1.67	0.75	1.99
(1,1431)	1:146:A:THR:HG22	1:139:A:MET:HE3	5	0.76	0.12	0.78
(1,1431)	1:146:A:THR:HG23	1:139:A:MET:HE2	5	0.76	0.12	0.78
(1,1431)	1:146:A:THR:HG21	1:139:A:MET:HE1	5	0.76	0.12	0.78
(1,1431)	1:146:A:THR:HG21	1:139:A:MET:HE3	5	0.76	0.12	0.78
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD12	5	0.74	0.16	0.72
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD11	5	0.74	0.16	0.72
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD13	5	0.74	0.16	0.72
(1,1029)	1:190:A:ARG:HD2	1:188:A:ASN:HB2	5	0.66	0.15	0.64
(1,1655)	1:195:A:PHE:HZ	1:156:A:ARG:HD2	5	0.58	0.44	0.51
(1,1531)	1:126:A:LYS:HB2	1:126:A:LYS:HE3	5	0.56	0.03	0.56
(1,1503)	1:122:A:ASN:HB3	1:123:A:GLU:HB2	5	0.39	0.54	0.11
(2,34)	1:166:A:GLU:H	1:159:A:PHE:HB2	5	0.36	0.2	0.23
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD12	5	0.3	0.1	0.31
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD13	5	0.3	0.1	0.31
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD11	5	0.3	0.1	0.31
(1,229)	1:200:A:ARG:H	1:200:A:ARG:HG2	5	0.28	0.12	0.23
(2,32)	1:166:A:GLU:H	1:164:A:SER:HB3	5	0.25	0.1	0.2
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG12	5	0.22	0.08	0.19
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG13	5	0.22	0.08	0.19
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG11	5	0.22	0.08	0.19
(2,33)	1:166:A:GLU:H	1:165:A:LYS:HE2	5	0.2	0.09	0.17
(2,33)	1:166:A:GLU:H	1:165:A:LYS:HE3	5	0.2	0.09	0.17
(1,1195)	1:118:A:THR:H	1:117:A:MET:HB3	5	0.16	0.04	0.18
(1,11)	1:119:A:ILE:H	1:179:A:HIS:HB3	5	0.15	0.03	0.16
(1,956)	1:112:A:ASN:HA	1:196:A:ARG:HA	5	0.14	0.01	0.14
(2,139)	1:172:A:ARG:HD2	1:174:A:THR:HG21	5	0.14	0.01	0.13
(2,139)	1:172:A:ARG:HD2	1:174:A:THR:HG22	5	0.14	0.01	0.13
(1,770)	1:146:A:THR:HA	1:135:A:GLN:HG3	5	0.13	0.02	0.12
(1,1254)	1:196:A:ARG:HB3	1:196:A:ARG:HD3	5	0.13	0.02	0.12
(1,675)	1:120:A:SER:H	1:119:A:ILE:HG13	5	0.12	0.02	0.11
(1,1178)	1:184:A:VAL:HB	1:172:A:ARG:HB3	5	0.12	0.03	0.11
(1,630)	1:167:A:GLY:H	1:168:A:GLN:HA	5	0.12	0.01	0.12
(1,164)	1:130:A:ALA:H	1:126:A:LYS:HA	5	0.11	0.01	0.11
(1,682)	1:141:A:ARG:H	1:140:A:THR:HA	5	0.11	0.01	0.1
(1,1584)	1:146:A:THR:HG23	1:136:A:VAL:HG11	4	2.86	0.09	2.86
(1,1584)	1:146:A:THR:HG23	1:136:A:VAL:HG13	4	2.86	0.09	2.86
(1,1584)	1:146:A:THR:HG21	1:136:A:VAL:HG12	4	2.86	0.09	2.86

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1584)	1:146:A:THR:HG21	1:136:A:VAL:HG13	4	2.86	0.09	2.86
(1,702)	1:146:A:THR:HB	1:136:A:VAL:HG11	4	2.3	0.34	2.33
(1,702)	1:146:A:THR:HB	1:136:A:VAL:HG13	4	2.3	0.34	2.33
(1,620)	1:146:A:THR:H	1:136:A:VAL:HG11	4	2.04	0.06	2.06
(1,620)	1:146:A:THR:H	1:136:A:VAL:HG13	4	2.04	0.06	2.06
(1,76)	1:139:A:MET:H	1:136:A:VAL:HG13	4	1.43	0.12	1.42
(1,76)	1:139:A:MET:H	1:136:A:VAL:HG12	4	1.43	0.12	1.42
(1,529)	1:145:A:PHE:H	1:136:A:VAL:HG13	4	1.32	0.03	1.32
(1,529)	1:145:A:PHE:H	1:136:A:VAL:HG12	4	1.32	0.03	1.32
(1,1233)	1:186:A:MET:HG2	1:185:A:ASN:HA	4	1.25	0.05	1.26
(1,340)	1:172:A:ARG:H	1:186:A:MET:HG2	4	1.15	0.17	1.15
(1,316)	1:147:A:VAL:H	1:136:A:VAL:HG11	4	1.04	0.08	1.08
(1,316)	1:147:A:VAL:H	1:136:A:VAL:HG13	4	1.04	0.08	1.08
(1,614)	1:132:A:GLN:H	1:132:A:GLN:HG3	4	0.84	0.23	0.88
(1,80)	1:186:A:MET:H	1:186:A:MET:HG2	4	0.7	0.02	0.71
(1,407)	1:168:A:GLN:H	1:158:A:PRO:HD2	4	0.68	0.56	0.44
(1,1623)	1:133:A:TYR:HD1	1:136:A:VAL:HG11	4	0.58	0.06	0.57
(1,1623)	1:133:A:TYR:HD1	1:136:A:VAL:HG13	4	0.58	0.06	0.57
(1,583)	1:131:A:THR:H	1:132:A:GLN:HG3	4	0.48	0.27	0.52
(1,890)	1:135:A:GLN:HA	1:136:A:VAL:HG11	4	0.42	0.06	0.4
(1,890)	1:135:A:GLN:HA	1:136:A:VAL:HG13	4	0.42	0.06	0.4
(1,1463)	1:183:A:ILE:HG22	1:195:A:PHE:HB3	4	0.35	0.14	0.4
(1,1463)	1:183:A:ILE:HG23	1:195:A:PHE:HB3	4	0.35	0.14	0.4
(1,875)	1:154:A:MET:HA	1:131:A:THR:HG22	4	0.3	0.1	0.32
(1,875)	1:154:A:MET:HA	1:131:A:THR:HG23	4	0.3	0.1	0.32
(2,145)	1:194:A:PHE:HB3	1:114:A:GLU:HG3	4	0.3	0.12	0.3
(1,475)	1:116:A:ASP:H	1:182:A:THR:HG23	4	0.29	0.19	0.2
(1,475)	1:116:A:ASP:H	1:182:A:THR:HG21	4	0.29	0.19	0.2
(1,1220)	1:186:A:MET:HG2	1:172:A:ARG:HB3	4	0.28	0.1	0.29
(1,1007)	1:167:A:GLY:HA2	1:168:A:GLN:HB2	4	0.26	0.17	0.2
(1,1010)	1:168:A:GLN:H	1:167:A:GLY:HA3	4	0.24	0.08	0.24
(1,1527)	1:117:A:MET:HG3	1:180:A:LEU:HD21	4	0.23	0.13	0.17
(1,1527)	1:117:A:MET:HG3	1:180:A:LEU:HD23	4	0.23	0.13	0.17
(1,1527)	1:117:A:MET:HG3	1:180:A:LEU:HD22	4	0.23	0.13	0.17
(2,157)	1:122:A:ASN:HB2	1:121:A:LYS:HB2	4	0.22	0.12	0.16
(2,157)	1:122:A:ASN:HB3	1:125:A:VAL:HB	4	0.22	0.12	0.16
(2,179)	1:165:A:LYS:HD2	1:160:A:ASP:HB3	4	0.19	0.06	0.18
(2,179)	1:165:A:LYS:HD3	1:160:A:ASP:HB3	4	0.19	0.06	0.18
(1,99)	1:165:A:LYS:H	1:163:A:ASP:HA	4	0.17	0.04	0.18
(1,1315)	1:173:A:LEU:HG	1:183:A:ILE:HA	4	0.17	0.03	0.18
(1,113)	1:185:A:ASN:H	1:190:A:ARG:HB3	4	0.16	0.04	0.16
(1,963)	1:192:A:PHE:HE1	1:192:A:PHE:HA	4	0.14	0.04	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,751)	1:184:A:VAL:HA	1:192:A:PHE:HD2	4	0.14	0.04	0.12
(1,1056)	1:126:A:LYS:HE3	1:109:A:ARG:HB3	4	0.13	0.02	0.12
(1,307)	1:129:A:GLU:H	1:128:A:LEU:HD11	4	0.12	0.02	0.12
(1,307)	1:129:A:GLU:H	1:128:A:LEU:HD12	4	0.12	0.02	0.12
(1,307)	1:129:A:GLU:H	1:128:A:LEU:HD13	4	0.12	0.02	0.12
(1,580)	1:131:A:THR:H	1:129:A:GLU:HA	4	0.12	0.02	0.13
(1,1)	1:170:A:ARG:H	1:156:A:ARG:H	4	0.12	0.01	0.12
(1,1602)	1:182:A:THR:HB	1:182:A:THR:HA	4	0.11	0.01	0.11
(1,1740)	1:138:A:LYS:HB3	1:138:A:LYS:HE2	3	1.02	0.16	0.98
(1,1231)	1:186:A:MET:HB3	1:170:A:ARG:HD2	3	0.86	0.28	0.86
(1,1270)	1:139:A:MET:HG2	1:155:A:ILE:HD12	3	0.75	0.76	0.31
(1,1270)	1:139:A:MET:HG2	1:155:A:ILE:HD13	3	0.75	0.76	0.31
(1,1270)	1:139:A:MET:HG2	1:155:A:ILE:HD11	3	0.75	0.76	0.31
(1,1241)	1:117:A:MET:H	1:117:A:MET:HG3	3	0.55	0.04	0.57
(1,1045)	1:180:A:LEU:HB2	1:117:A:MET:HG3	3	0.53	0.06	0.53
(1,745)	1:131:A:THR:HA	1:132:A:GLN:HG3	3	0.52	0.21	0.62
(1,698)	1:161:A:PHE:H	1:165:A:LYS:HB2	3	0.47	0.51	0.11
(1,1158)	1:144:A:GLU:HG2	1:141:A:ARG:HG3	3	0.45	0.31	0.38
(1,1242)	1:117:A:MET:HG3	1:118:A:THR:H	3	0.38	0.02	0.38
(1,1392)	1:197:A:LEU:HD22	1:195:A:PHE:HE1	3	0.35	0.14	0.35
(1,1392)	1:197:A:LEU:HD23	1:195:A:PHE:HE1	3	0.35	0.14	0.35
(1,797)	1:175:A:PHE:HA	1:175:A:PHE:HD2	3	0.29	0.14	0.29
(1,797)	1:175:A:PHE:HA	1:175:A:PHE:HD1	3	0.29	0.14	0.29
(1,404)	1:168:A:GLN:H	1:169:A:VAL:HG22	3	0.27	0.09	0.31
(1,404)	1:168:A:GLN:H	1:169:A:VAL:HG21	3	0.27	0.09	0.31
(1,636)	1:143:A:GLY:H	1:155:A:ILE:HD12	3	0.23	0.03	0.22
(1,636)	1:143:A:GLY:H	1:155:A:ILE:HD13	3	0.23	0.03	0.22
(1,708)	1:131:A:THR:HB	1:127:A:LEU:HD11	3	0.21	0.07	0.17
(1,708)	1:131:A:THR:HB	1:127:A:LEU:HD12	3	0.21	0.07	0.17
(1,708)	1:131:A:THR:HB	1:127:A:LEU:HD13	3	0.21	0.07	0.17
(1,120)	1:175:A:PHE:H	1:174:A:THR:HG21	3	0.18	0.04	0.17
(1,120)	1:175:A:PHE:H	1:174:A:THR:HG23	3	0.18	0.04	0.17
(1,626)	1:151:A:SER:H	1:150:A:ASN:HB3	3	0.16	0.03	0.18
(1,1647)	1:195:A:PHE:HE2	1:171:A:ALA:HB1	3	0.16	0.06	0.12
(1,1647)	1:195:A:PHE:HE2	1:171:A:ALA:HB2	3	0.16	0.06	0.12
(1,1588)	1:142:A:PRO:HA	1:155:A:ILE:HG21	3	0.15	0.02	0.15
(1,1588)	1:142:A:PRO:HA	1:155:A:ILE:HG23	3	0.15	0.02	0.15
(1,415)	1:159:A:PHE:H	1:159:A:PHE:HE1	3	0.15	0.05	0.11
(1,415)	1:159:A:PHE:H	1:159:A:PHE:HE2	3	0.15	0.05	0.11
(1,142)	1:157:A:ARG:H	1:156:A:ARG:HG2	3	0.14	0.02	0.14
(1,725)	1:158:A:PRO:HA	1:158:A:PRO:HB2	3	0.14	0.02	0.12
(1,395)	1:117:A:MET:H	1:115:A:PRO:HA	3	0.13	0.01	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1722)	1:170:A:ARG:HA	1:155:A:ILE:HG13	3	0.13	0.02	0.12
(1,1328)	1:115:A:PRO:HG3	1:114:A:GLU:HA	3	0.13	0.02	0.12
(1,1390)	1:138:A:LYS:HG3	1:138:A:LYS:HA	3	0.13	0.01	0.13
(1,674)	1:114:A:GLU:H	1:117:A:MET:HE1	3	0.12	0.0	0.12
(1,674)	1:114:A:GLU:H	1:117:A:MET:HE2	3	0.12	0.0	0.12
(1,907)	1:180:A:LEU:HA	1:180:A:LEU:HD22	3	0.12	0.01	0.11
(1,763)	1:129:A:GLU:HA	1:129:A:GLU:HB3	3	0.11	0.01	0.11
(1,774)	1:136:A:VAL:HA	1:136:A:VAL:HB	3	0.11	0.01	0.1
(1,1144)	1:185:A:ASN:HB3	1:190:A:ARG:HB3	2	1.2	0.0	1.2
(1,974)	1:158:A:PRO:HD3	1:158:A:PRO:HA	2	0.94	0.06	0.94
(1,1061)	1:176:A:ASP:HB3	1:181:A:ALA:H	2	0.78	0.03	0.78
(1,1277)	1:190:A:ARG:HB3	1:190:A:ARG:HD2	2	0.57	0.29	0.57
(1,628)	1:167:A:GLY:H	1:169:A:VAL:HG22	2	0.53	0.21	0.53
(1,628)	1:167:A:GLY:H	1:169:A:VAL:HG21	2	0.53	0.21	0.53
(1,1150)	1:192:A:PHE:HE2	1:185:A:ASN:HB2	2	0.46	0.07	0.46
(1,1469)	1:128:A:LEU:HD22	1:152:A:ILE:HG21	2	0.46	0.09	0.46
(1,1469)	1:128:A:LEU:HD22	1:152:A:ILE:HG23	2	0.46	0.09	0.46
(1,424)	1:190:A:ARG:H	1:185:A:ASN:HB3	2	0.45	0.02	0.45
(1,225)	1:128:A:LEU:H	1:127:A:LEU:HD21	2	0.42	0.28	0.42
(1,199)	1:191:A:GLN:H	1:190:A:ARG:HG2	2	0.4	0.28	0.4
(1,746)	1:119:A:ILE:HA	1:117:A:MET:HG3	2	0.4	0.22	0.4
(1,160)	1:141:A:ARG:H	1:141:A:ARG:HD2	2	0.38	0.02	0.38
(1,1368)	1:141:A:ARG:HD3	1:141:A:ARG:HG3	2	0.38	0.01	0.38
(1,1489)	1:183:A:ILE:HD13	1:183:A:ILE:HG22	2	0.36	0.05	0.36
(1,1489)	1:183:A:ILE:HD12	1:183:A:ILE:HG23	2	0.36	0.05	0.36
(1,1358)	1:197:A:LEU:HG	1:197:A:LEU:H	2	0.32	0.08	0.32
(1,227)	1:200:A:ARG:H	1:199:A:PRO:HB2	2	0.3	0.05	0.3
(2,31)	1:166:A:GLU:H	1:167:A:GLY:H	2	0.29	0.09	0.29
(2,31)	1:166:A:GLU:H	1:159:A:PHE:H	2	0.29	0.09	0.29
(1,1535)	1:154:A:MET:HG3	1:173:A:LEU:HD12	2	0.28	0.09	0.28
(1,1535)	1:154:A:MET:HG3	1:173:A:LEU:HD13	2	0.28	0.09	0.28
(1,49)	1:195:A:PHE:H	1:183:A:ILE:HG22	2	0.28	0.12	0.28
(1,49)	1:195:A:PHE:H	1:183:A:ILE:HG23	2	0.28	0.12	0.28
(1,473)	1:116:A:ASP:H	1:181:A:ALA:HB3	2	0.26	0.03	0.26
(1,473)	1:116:A:ASP:H	1:181:A:ALA:HB1	2	0.26	0.03	0.26
(2,180)	1:172:A:ARG:HG2	1:151:A:SER:HB2	2	0.26	0.05	0.26
(2,180)	1:172:A:ARG:HG3	1:151:A:SER:HB2	2	0.26	0.05	0.26
(2,172)	1:170:A:ARG:HB3	1:155:A:ILE:HG12	2	0.22	0.12	0.22
(1,1626)	1:159:A:PHE:HD2	1:161:A:PHE:HD2	2	0.22	0.02	0.22
(1,202)	1:113:A:LEU:H	1:113:A:LEU:HD12	2	0.22	0.06	0.22
(1,1041)	1:180:A:LEU:HB3	1:117:A:MET:HG3	2	0.2	0.03	0.2
(1,1593)	1:119:A:ILE:H	1:119:A:ILE:HG23	2	0.2	0.04	0.2

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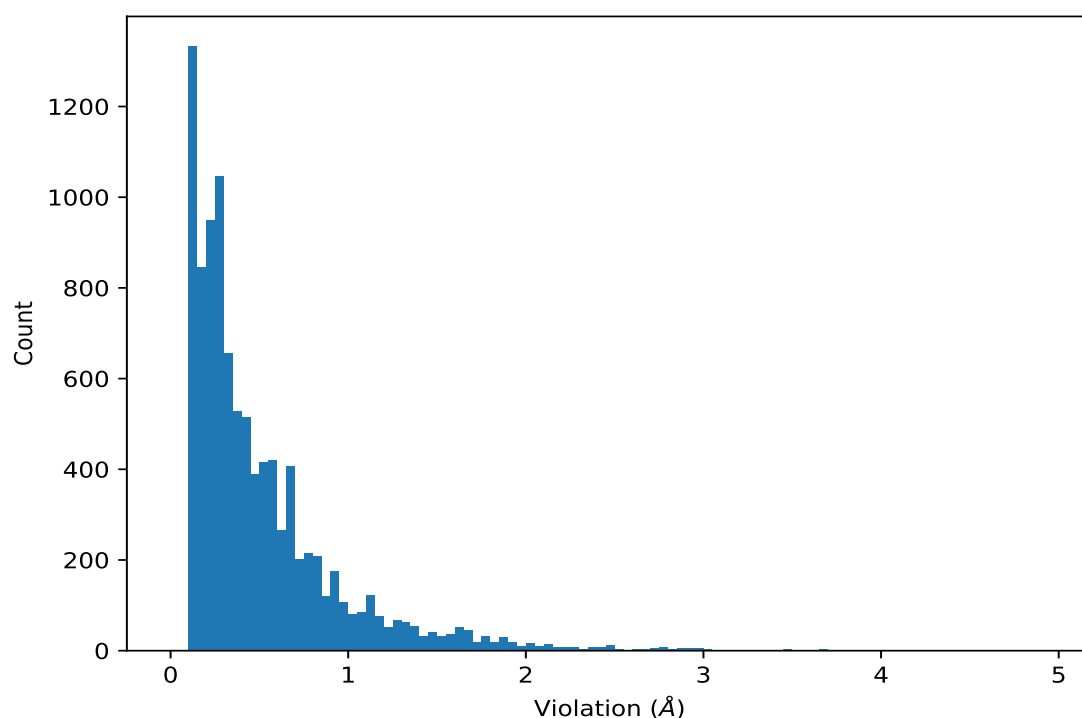
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,168)	1:130:A:ALA:H	1:129:A:GLU:HB2	2	0.18	0.01	0.18
(1,1480)	1:152:A:ILE:HD12	1:152:A:ILE:HA	2	0.18	0.02	0.18
(1,1480)	1:152:A:ILE:HD13	1:152:A:ILE:HA	2	0.18	0.02	0.18
(1,1084)	1:150:A:ASN:HB3	1:174:A:THR:HG23	2	0.18	0.02	0.18
(1,1084)	1:150:A:ASN:HB3	1:174:A:THR:HG22	2	0.18	0.02	0.18
(1,671)	1:156:A:ARG:H	1:156:A:ARG:HG2	2	0.17	0.04	0.17
(1,1646)	1:195:A:PHE:HE2	1:169:A:VAL:HG11	2	0.16	0.06	0.16
(1,1646)	1:195:A:PHE:HE1	1:169:A:VAL:HG11	2	0.16	0.06	0.16
(2,29)	1:124:A:MET:H	1:173:A:LEU:HD22	2	0.16	0.02	0.16
(1,289)	1:134:A:ARG:H	1:144:A:GLU:HA	2	0.15	0.0	0.15
(1,1573)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	2	0.15	0.0	0.15
(1,1573)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	2	0.15	0.0	0.15
(1,50)	1:195:A:PHE:H	1:195:A:PHE:HD2	2	0.14	0.02	0.14
(1,258)	1:192:A:PHE:H	1:183:A:ILE:HG22	2	0.14	0.04	0.14
(1,1408)	1:131:A:THR:HG22	1:145:A:PHE:HB2	2	0.13	0.01	0.13
(1,1460)	1:173:A:LEU:HG	1:183:A:ILE:HG21	2	0.13	0.01	0.13
(1,1460)	1:173:A:LEU:HG	1:183:A:ILE:HG23	2	0.13	0.01	0.13
(1,1551)	1:126:A:LYS:H	1:126:A:LYS:HD3	2	0.12	0.02	0.12
(1,747)	1:119:A:ILE:HA	1:123:A:GLU:HB3	2	0.12	0.01	0.12
(1,78)	1:186:A:MET:H	1:192:A:PHE:HE2	2	0.11	0.01	0.11
(1,1600)	1:184:A:VAL:H	1:182:A:THR:HB	2	0.11	0.0	0.11
(1,1628)	1:146:A:THR:H	1:146:A:THR:HB	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	1	4.94
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	12	3.72
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	3	3.7
(1,1382)	1:127:A:LEU:HD22	1:124:A:MET:HB2	20	3.69
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	5	3.67
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	19	3.66
(1,1645)	1:175:A:PHE:HE1	1:180:A:LEU:HD11	2	3.47
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD21	6	3.46
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	1	3.45
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	12	3.42
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	1	3.09
(1,1420)	1:113:A:LEU:HD23	1:154:A:MET:HG2	2	3.07
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	12	3.04
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	5	3.03
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	2	3.03
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD21	6	3.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	19	2.97
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD13	2	2.97
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	6	2.96
(1,1584)	1:146:A:THR:HG23	1:136:A:VAL:HG11	1	2.95
(1,1584)	1:146:A:THR:HG21	1:136:A:VAL:HG13	9	2.95
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD13	13	2.94
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	13	2.94
(2,99)	1:182:A:THR:H	1:184:A:VAL:HG11	16	2.93
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	2	2.93
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD13	15	2.92
(1,1420)	1:113:A:LEU:HD23	1:154:A:MET:HG2	18	2.92
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD13	14	2.88
(1,1746)	1:128:A:LEU:HD23	1:127:A:LEU:HD21	2	2.88
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	1	2.88
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	15	2.87
(1,1746)	1:128:A:LEU:HD21	1:127:A:LEU:HD23	20	2.85
(2,99)	1:182:A:THR:H	1:184:A:VAL:HG13	9	2.84
(1,1746)	1:128:A:LEU:HD21	1:127:A:LEU:HD21	7	2.84
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	20	2.83
(2,99)	1:182:A:THR:H	1:152:A:ILE:HD13	2	2.82
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD21	5	2.8
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	19	2.79
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD13	7	2.78
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG22	6	2.78
(1,1584)	1:146:A:THR:HG23	1:136:A:VAL:HG13	2	2.77
(1,1584)	1:146:A:THR:HG21	1:136:A:VAL:HG12	4	2.77
(1,1746)	1:128:A:LEU:HD23	1:127:A:LEU:HD21	12	2.76
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD12	4	2.75
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD21	19	2.74
(2,99)	1:182:A:THR:H	1:184:A:VAL:HG13	10	2.73
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD13	17	2.73
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD13	3	2.72
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD21	17	2.72
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD12	11	2.71
(1,1406)	1:180:A:LEU:HD11	1:175:A:PHE:HD1	2	2.69
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG22	13	2.68
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	6	2.67
(1,702)	1:146:A:THR:HB	1:136:A:VAL:HG11	1	2.67
(2,99)	1:182:A:THR:H	1:119:A:ILE:HD11	8	2.64
(2,99)	1:182:A:THR:H	1:184:A:VAL:HG13	18	2.64
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD11	6	2.63
(1,1746)	1:128:A:LEU:HD21	1:127:A:LEU:HD21	3	2.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,702)	1:146:A:THR:HB	1:136:A:VAL:HG11	9	2.59
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	11	2.58
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD11	2	2.55
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	2	2.51
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG12	4	2.5
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	2	2.5
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	1	2.49
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	5	2.48
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	5	2.48
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	1	2.48
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	4	2.48
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	6	2.47
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	2	2.47
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	20	2.47
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD23	18	2.46
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	9	2.46
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD21	15	2.46
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	18	2.45
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	16	2.44
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	1	2.44
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	9	2.43
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	2	2.42
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	6	2.42
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	17	2.41
(1,704)	1:174:A:THR:HB	1:180:A:LEU:HG	2	2.41
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	9	2.39
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG12	12	2.36
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD13	5	2.36
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	1	2.36
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	6	2.35
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD21	6	2.35
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	15	2.35
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	5	2.33
(2,194)	1:180:A:LEU:HD23	1:119:A:ILE:HD11	2	2.31
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG12	18	2.31
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	19	2.31
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	6	2.3
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG12	9	2.29
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	12	2.28
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	5	2.28
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD11	19	2.28
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG12	19	2.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	1	2.27
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD12	14	2.26
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	13	2.24
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG13	13	2.23
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG13	7	2.21
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	2	2.2
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	10	2.2
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG13	9	2.2
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	14	2.2
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	11	2.19
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	9	2.19
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	14	2.19
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	8	2.18
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG13	10	2.18
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG12	14	2.17
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	5	2.15
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	7	2.15
(1,1370)	1:197:A:LEU:HD13	1:127:A:LEU:HD13	20	2.14
(1,1718)	1:138:A:LYS:HA	1:136:A:VAL:HG13	1	2.13
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD21	13	2.13
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD12	12	2.13
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG13	4	2.12
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG21	14	2.12
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	7	2.12
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	2	2.11
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD11	17	2.11
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG12	17	2.1
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	6	2.1
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	11	2.1
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB2	5	2.1
(1,620)	1:146:A:THR:H	1:136:A:VAL:HG11	1	2.1
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG13	2	2.09
(2,173)	1:125:A:VAL:HB	1:124:A:MET:HB3	6	2.08
(1,1718)	1:138:A:LYS:HA	1:136:A:VAL:HG13	9	2.08
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG13	1	2.08
(1,620)	1:146:A:THR:H	1:136:A:VAL:HG11	9	2.08
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD11	7	2.07
(1,365)	1:152:A:ILE:H	1:180:A:LEU:HD13	2	2.07
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD21	5	2.06
(1,702)	1:146:A:THR:HB	1:136:A:VAL:HG13	4	2.06
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	16	2.05
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	17	2.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	4	2.05
(1,620)	1:146:A:THR:H	1:136:A:VAL:HG13	4	2.05
(2,173)	1:124:A:MET:HB3	1:121:A:LYS:HB3	8	2.04
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG13	6	2.04
(2,151)	1:112:A:ASN:HB3	1:111:A:VAL:HG13	20	2.04
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	18	2.04
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD21	1	2.03
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	20	2.03
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	16	2.02
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	17	2.02
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	4	2.01
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG21	12	2.01
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	15	2.0
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD21	7	2.0
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	5	1.99
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	20	1.99
(1,1718)	1:138:A:LYS:HA	1:136:A:VAL:HG13	2	1.99
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	8	1.99
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	2	1.98
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	9	1.98
(1,1718)	1:138:A:LYS:HA	1:136:A:VAL:HG12	4	1.97
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	6	1.97
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	12	1.97
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	13	1.96
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG13	1	1.96
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD21	3	1.95
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	7	1.95
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	16	1.95
(1,620)	1:146:A:THR:H	1:136:A:VAL:HG13	2	1.95
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	9	1.94
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG21	19	1.94
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG22	10	1.94
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	1	1.94
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG21	4	1.93
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	18	1.93
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD13	18	1.92
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	3	1.92
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	20	1.92
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	14	1.92
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	13	1.92
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	11	1.91
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	1	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	11	1.91
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	11	1.91
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	9	1.9
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	11	1.89
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	14	1.89
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	5	1.89
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	2	1.89
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	5	1.88
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB2	4	1.88
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	14	1.88
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	4	1.88
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	1	1.88
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG23	15	1.88
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	12	1.87
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	20	1.87
(1,702)	1:146:A:THR:HB	1:136:A:VAL:HG11	2	1.87
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	3	1.86
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	15	1.86
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	8	1.86
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	8	1.86
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD11	11	1.86
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	2	1.86
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	13	1.86
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG23	13	1.86
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	12	1.86
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	11	1.86
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	15	1.86
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	1	1.85
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	10	1.85
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	17	1.85
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	2	1.85
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG21	20	1.84
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	13	1.84
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	12	1.84
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	19	1.83
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	18	1.83
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB3	2	1.82
(1,1270)	1:139:A:MET:HG2	1:155:A:ILE:HD13	13	1.82
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD13	15	1.82
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	6	1.82
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	20	1.82
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG22	19	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	19	1.81
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	14	1.81
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD23	19	1.81
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	5	1.81
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	1	1.81
(1,441)	1:114:A:GLU:H	1:180:A:LEU:HD22	2	1.81
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	13	1.8
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	14	1.79
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG21	15	1.79
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	16	1.79
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	14	1.79
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD13	1	1.79
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD11	19	1.79
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	11	1.78
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	18	1.78
(1,1409)	1:131:A:THR:HG21	1:127:A:LEU:HD21	19	1.78
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD23	20	1.78
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG13	5	1.78
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	5	1.78
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	4	1.77
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	1	1.77
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	17	1.77
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD22	14	1.77
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	12	1.77
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	15	1.77
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	1	1.77
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	15	1.77
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	17	1.76
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB2	17	1.76
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	2	1.76
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	6	1.76
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	12	1.76
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	6	1.75
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	20	1.75
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG21	19	1.75
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB2	20	1.75
(1,1373)	1:128:A:LEU:HD21	1:154:A:MET:HB2	16	1.75
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	18	1.75
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	10	1.75
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG21	13	1.75
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	9	1.74
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	18	1.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	4	1.74
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	14	1.73
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	14	1.73
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB2	3	1.72
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD21	17	1.72
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	13	1.72
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	13	1.72
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	14	1.71
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	2	1.71
(2,69)	1:159:A:PHE:H	1:156:A:ARG:HB2	18	1.71
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG22	6	1.71
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD12	14	1.71
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	10	1.71
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD12	13	1.71
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD11	19	1.71
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG22	11	1.71
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	20	1.7
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	15	1.7
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	20	1.7
(1,1456)	1:130:A:ALA:HB3	1:132:A:GLN:HG3	9	1.7
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	10	1.7
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	18	1.7
(1,398)	1:117:A:MET:H	1:180:A:LEU:HD21	2	1.7
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	13	1.69
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	14	1.69
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	16	1.69
(1,1735)	1:190:A:ARG:HD2	1:185:A:ASN:HB2	14	1.69
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	12	1.69
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	10	1.69
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	1	1.69
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	12	1.69
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	3	1.69
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	16	1.69
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	14	1.69
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD11	2	1.69
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	18	1.69
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG23	8	1.68
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB2	8	1.68
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB2	7	1.68
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	5	1.68
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD21	2	1.68
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	19	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	20	1.68
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG21	19	1.68
(2,201)	1:111:A:VAL:HG11	1:130:A:ALA:HB2	20	1.67
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	20	1.67
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD2	3	1.67
(2,69)	1:159:A:PHE:H	1:156:A:ARG:HB2	3	1.67
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	2	1.67
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	12	1.67
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	16	1.67
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	17	1.67
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	1	1.67
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	6	1.67
(1,644)	1:173:A:LEU:H	1:180:A:LEU:HD13	2	1.67
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB3	7	1.66
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	2	1.66
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	5	1.66
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	7	1.66
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	8	1.66
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	14	1.66
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	20	1.66
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	2	1.65
(2,186)	1:173:A:LEU:HD13	1:195:A:PHE:HB2	19	1.65
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD11	1	1.65
(1,1639)	1:195:A:PHE:HD1	1:113:A:LEU:HD23	2	1.65
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	6	1.65
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	2	1.65
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	13	1.65
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	16	1.65
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG21	6	1.65
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	8	1.65
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	19	1.65
(1,407)	1:168:A:GLN:H	1:158:A:PRO:HD2	19	1.65
(2,173)	1:124:A:MET:HB3	1:121:A:LYS:HB2	14	1.64
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	10	1.64
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD13	4	1.64
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	2	1.64
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	15	1.64
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	16	1.64
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	10	1.64
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	15	1.64
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG22	5	1.64
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	9	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	18	1.63
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	12	1.63
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	19	1.63
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	17	1.63
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD12	18	1.63
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	4	1.63
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	17	1.63
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	14	1.63
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	11	1.62
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	1	1.62
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	3	1.62
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	9	1.62
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	18	1.62
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	8	1.61
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	17	1.61
(2,47)	1:144:A:GLU:H	1:146:A:THR:HG21	7	1.61
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	19	1.61
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	11	1.61
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	14	1.61
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	6	1.61
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	19	1.61
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	3	1.6
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	5	1.6
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	6	1.6
(2,69)	1:159:A:PHE:H	1:156:A:ARG:HB2	2	1.6
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	16	1.6
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	13	1.6
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	2	1.6
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	10	1.6
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD11	6	1.6
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	20	1.59
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	16	1.59
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	18	1.59
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	9	1.59
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	20	1.59
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	9	1.59
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG22	6	1.59
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	2	1.58
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	14	1.58
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	18	1.58
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	10	1.58
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	9	1.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	12	1.58
(1,1510)	1:129:A:GLU:HG2	1:126:A:LYS:HD3	2	1.58
(1,1477)	1:186:A:MET:HE1	1:170:A:ARG:HD2	17	1.58
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	7	1.58
(2,201)	1:111:A:VAL:HG11	1:130:A:ALA:HB3	12	1.57
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG23	13	1.57
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD2	18	1.57
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	7	1.57
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	15	1.57
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	14	1.57
(1,76)	1:139:A:MET:H	1:136:A:VAL:HG13	1	1.57
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	1	1.56
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	3	1.56
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD12	15	1.56
(1,1436)	1:136:A:VAL:HG21	1:144:A:GLU:HB2	8	1.56
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	19	1.56
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	4	1.56
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	5	1.56
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	10	1.56
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	20	1.56
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG23	16	1.55
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	1	1.55
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	11	1.55
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG22	14	1.55
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	14	1.54
(1,1436)	1:136:A:VAL:HG21	1:144:A:GLU:HB2	4	1.54
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	14	1.54
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	16	1.54
(1,1052)	1:173:A:LEU:HB3	1:180:A:LEU:HD13	2	1.54
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	15	1.54
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	5	1.53
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD12	3	1.53
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	3	1.53
(1,1255)	1:179:A:HIS:HB2	1:178:A:ASP:HB3	9	1.53
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	13	1.53
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	17	1.53
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	7	1.53
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	9	1.53
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	15	1.52
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	7	1.52
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	4	1.52
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	9	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	10	1.52
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	4	1.51
(1,1477)	1:186:A:MET:HE3	1:170:A:ARG:HD2	14	1.51
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	18	1.51
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	5	1.51
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	17	1.51
(1,76)	1:139:A:MET:H	1:136:A:VAL:HG13	9	1.51
(2,198)	1:169:A:VAL:HG11	1:170:A:ARG:HB3	17	1.5
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	7	1.5
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	3	1.5
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG23	15	1.5
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	13	1.5
(1,608)	1:188:A:ASN:H	1:190:A:ARG:HG2	14	1.5
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	13	1.5
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	7	1.49
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	5	1.49
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	8	1.49
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	9	1.49
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	13	1.49
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	8	1.49
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	12	1.49
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	9	1.49
(1,1477)	1:186:A:MET:HE2	1:170:A:ARG:HD2	5	1.49
(1,1436)	1:136:A:VAL:HG22	1:144:A:GLU:HB2	19	1.49
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	12	1.49
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	8	1.49
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	17	1.49
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	19	1.49
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	10	1.49
(2,198)	1:141:A:ARG:HB3	1:140:A:THR:HG23	19	1.48
(2,169)	1:163:A:ASP:HB2	1:162:A:PRO:HB3	1	1.48
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	6	1.48
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD11	11	1.48
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	20	1.48
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	7	1.48
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG12	10	1.47
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD2	15	1.47
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	2	1.47
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	10	1.47
(1,1503)	1:122:A:ASN:HB3	1:123:A:GLU:HB2	1	1.47
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD22	2	1.47
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	10	1.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	3	1.47
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	10	1.47
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	7	1.47
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	15	1.46
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	5	1.46
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	10	1.46
(2,11)	1:195:A:PHE:H	1:171:A:ALA:HB1	18	1.46
(1,1477)	1:186:A:MET:HE1	1:170:A:ARG:HD2	12	1.46
(1,1476)	1:119:A:ILE:HG23	1:117:A:MET:HG3	17	1.46
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	7	1.46
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	10	1.46
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	17	1.46
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD12	1	1.46
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	6	1.45
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	13	1.45
(1,1476)	1:119:A:ILE:HG23	1:117:A:MET:HG3	10	1.45
(1,1049)	1:156:A:ARG:HD3	1:197:A:LEU:HA	1	1.45
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	7	1.45
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	16	1.44
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	18	1.44
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD13	1	1.44
(1,1373)	1:128:A:LEU:HD21	1:154:A:MET:HB2	4	1.44
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	17	1.44
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	18	1.44
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	17	1.44
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	10	1.43
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	18	1.43
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	20	1.43
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	15	1.43
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	7	1.43
(1,1384)	1:127:A:LEU:HD21	1:127:A:LEU:HA	8	1.43
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	17	1.43
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	11	1.43
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	1	1.42
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD21	12	1.42
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	12	1.42
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	17	1.42
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	2	1.42
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	9	1.42
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	17	1.42
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	6	1.42
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	4	1.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	4	1.41
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	6	1.41
(1,1578)	1:140:A:THR:HG23	1:138:A:LYS:HE3	8	1.41
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	7	1.41
(2,201)	1:111:A:VAL:HG12	1:130:A:ALA:HB2	5	1.4
(2,53)	1:134:A:ARG:H	1:141:A:ARG:HG3	13	1.4
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG22	18	1.4
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	7	1.4
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	16	1.4
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	1	1.4
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	18	1.39
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG22	5	1.39
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	10	1.39
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG13	4	1.39
(1,1436)	1:136:A:VAL:HG21	1:144:A:GLU:HB2	3	1.39
(1,1373)	1:128:A:LEU:HD23	1:154:A:MET:HB2	2	1.39
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	10	1.39
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	7	1.39
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	10	1.38
(2,198)	1:169:A:VAL:HG11	1:170:A:ARG:HB3	8	1.38
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	9	1.38
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	11	1.38
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG22	9	1.38
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	13	1.38
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	19	1.38
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	14	1.38
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	20	1.38
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	9	1.37
(2,198)	1:169:A:VAL:HG11	1:170:A:ARG:HB3	12	1.37
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	11	1.37
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	10	1.37
(1,1655)	1:195:A:PHE:HZ	1:156:A:ARG:HD2	6	1.37
(1,1477)	1:186:A:MET:HE1	1:170:A:ARG:HD2	11	1.37
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	16	1.37
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	1	1.37
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	2	1.37
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	1	1.37
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	2	1.36
(2,93)	1:188:A:ASN:H	1:186:A:MET:HB3	14	1.36
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	12	1.36
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG22	14	1.36
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD12	14	1.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	20	1.36
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	4	1.36
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	11	1.36
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	18	1.36
(1,529)	1:145:A:PHE:H	1:136:A:VAL:HG13	1	1.36
(1,340)	1:172:A:ARG:H	1:186:A:MET:HG2	5	1.36
(2,186)	1:173:A:LEU:HD13	1:195:A:PHE:HB2	12	1.35
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	12	1.35
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	2	1.35
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	18	1.35
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	17	1.35
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	19	1.35
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	2	1.35
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	8	1.35
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	10	1.35
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	17	1.35
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	15	1.34
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	19	1.34
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB1	8	1.34
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	11	1.34
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD22	1	1.34
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	3	1.34
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD22	18	1.34
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	5	1.34
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	15	1.34
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD13	15	1.34
(1,529)	1:145:A:PHE:H	1:136:A:VAL:HG12	4	1.34
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	11	1.34
(1,76)	1:139:A:MET:H	1:136:A:VAL:HG12	4	1.34
(2,201)	1:111:A:VAL:HG12	1:130:A:ALA:HB3	2	1.33
(2,201)	1:111:A:VAL:HG11	1:130:A:ALA:HB3	7	1.33
(2,201)	1:111:A:VAL:HG12	1:130:A:ALA:HB3	8	1.33
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	2	1.33
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	10	1.33
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	4	1.33
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	9	1.33
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	6	1.33
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	2	1.33
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	17	1.33
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	15	1.33
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	6	1.33
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG22	17	1.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,132)	1:167:A:GLY:HA3	1:168:A:GLN:HG2	12	1.32
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	16	1.32
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	12	1.32
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	17	1.32
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	1	1.32
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	12	1.32
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	9	1.32
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD12	7	1.31
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	2	1.31
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	20	1.31
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	8	1.31
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	19	1.31
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD22	10	1.31
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	7	1.31
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	8	1.31
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	15	1.31
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD11	2	1.31
(1,1088)	1:133:A:TYR:HB3	1:128:A:LEU:HB2	15	1.31
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	7	1.31
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	9	1.3
(2,199)	1:140:A:THR:HG22	1:138:A:LYS:HG2	4	1.3
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	4	1.3
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	9	1.3
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	15	1.3
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD12	8	1.3
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	9	1.3
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD22	5	1.3
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	13	1.3
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	1	1.3
(1,1233)	1:186:A:MET:HG2	1:185:A:ASN:HA	13	1.3
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	14	1.3
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	7	1.3
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	8	1.3
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	2	1.3
(1,723)	1:115:A:PRO:HA	1:180:A:LEU:HD21	2	1.3
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	20	1.3
(1,529)	1:145:A:PHE:H	1:136:A:VAL:HG13	9	1.3
(2,201)	1:111:A:VAL:HG13	1:130:A:ALA:HB2	17	1.29
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	17	1.29
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	1	1.29
(2,49)	1:134:A:ARG:H	1:135:A:GLN:HB3	2	1.29
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG22	8	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	17	1.29
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	6	1.29
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD22	9	1.29
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD22	10	1.29
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	12	1.29
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	14	1.29
(1,1373)	1:128:A:LEU:HD21	1:154:A:MET:HB2	14	1.29
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	3	1.29
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	7	1.29
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	7	1.29
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	15	1.29
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	10	1.29
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD12	15	1.29
(1,76)	1:139:A:MET:H	1:136:A:VAL:HG13	2	1.29
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	2	1.28
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	16	1.28
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB2	16	1.28
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	12	1.28
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	4	1.28
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	11	1.28
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	2	1.28
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	4	1.28
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	20	1.28
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	6	1.28
(1,529)	1:145:A:PHE:H	1:136:A:VAL:HG13	2	1.28
(1,340)	1:172:A:ARG:H	1:186:A:MET:HG2	14	1.28
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	6	1.28
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	15	1.27
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	20	1.27
(1,1373)	1:128:A:LEU:HD23	1:154:A:MET:HB2	12	1.27
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	3	1.27
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	7	1.27
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	14	1.27
(1,1233)	1:186:A:MET:HG2	1:185:A:ASN:HA	18	1.27
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	11	1.27
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	1	1.27
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	11	1.27
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	8	1.27
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	1	1.26
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	6	1.26
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	11	1.26
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	13	1.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	1	1.26
(2,53)	1:134:A:ARG:H	1:135:A:GLN:HB3	2	1.26
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	9	1.26
(1,1578)	1:140:A:THR:HG22	1:138:A:LYS:HE3	9	1.26
(1,1419)	1:113:A:LEU:HA	1:113:A:LEU:HD11	6	1.26
(1,1401)	1:180:A:LEU:HD12	1:180:A:LEU:HB2	2	1.26
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	12	1.26
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	17	1.26
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	4	1.26
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	13	1.26
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	5	1.25
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	11	1.25
(1,1658)	1:131:A:THR:HB	1:127:A:LEU:HD21	6	1.25
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	7	1.25
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	16	1.25
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD21	20	1.25
(1,1395)	1:197:A:LEU:HD23	1:156:A:ARG:HG3	15	1.25
(1,1233)	1:186:A:MET:HG2	1:185:A:ASN:HA	14	1.25
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	10	1.25
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD13	6	1.25
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	3	1.24
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	1	1.24
(1,1420)	1:113:A:LEU:HD23	1:154:A:MET:HG2	4	1.24
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	6	1.24
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD13	3	1.24
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	8	1.24
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	3	1.24
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	9	1.24
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	14	1.24
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	16	1.24
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB3	14	1.23
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	8	1.23
(1,1740)	1:138:A:LYS:HB3	1:138:A:LYS:HE2	8	1.23
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG22	16	1.23
(1,1490)	1:119:A:ILE:HD11	1:119:A:ILE:HA	14	1.23
(1,1476)	1:119:A:ILE:HG21	1:117:A:MET:HG3	14	1.23
(1,1373)	1:128:A:LEU:HD23	1:154:A:MET:HB2	8	1.23
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	19	1.23
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG12	7	1.23
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG23	6	1.23
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG21	9	1.23
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	3	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	20	1.23
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	2	1.23
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	11	1.22
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	2	1.22
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG21	15	1.22
(1,1427)	1:128:A:LEU:HB2	1:128:A:LEU:HD23	11	1.22
(1,1373)	1:128:A:LEU:HD23	1:154:A:MET:HB2	13	1.22
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	8	1.22
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	19	1.22
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	3	1.22
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG13	19	1.22
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	11	1.22
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	7	1.22
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	11	1.22
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG23	3	1.21
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	14	1.21
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	19	1.21
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	20	1.21
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	9	1.21
(1,1510)	1:129:A:GLU:HG2	1:126:A:LYS:HD3	17	1.21
(1,1421)	1:113:A:LEU:HD11	1:113:A:LEU:HB3	15	1.21
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	11	1.21
(1,1231)	1:186:A:MET:HB3	1:170:A:ARG:HD2	12	1.21
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	17	1.21
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG13	18	1.21
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	2	1.21
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG23	7	1.21
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	19	1.21
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	9	1.21
(2,201)	1:111:A:VAL:HG13	1:130:A:ALA:HB2	19	1.2
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	6	1.2
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	20	1.2
(1,1468)	1:152:A:ILE:HG23	1:145:A:PHE:HB3	2	1.2
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB3	10	1.2
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	16	1.2
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	9	1.2
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	11	1.2
(1,1144)	1:185:A:ASN:HB3	1:190:A:ARG:HB3	2	1.2
(1,1144)	1:185:A:ASN:HB3	1:190:A:ARG:HB3	11	1.2
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG23	19	1.2
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	18	1.2
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG22	4	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	3	1.2
(1,631)	1:167:A:GLY:H	1:158:A:PRO:HA	19	1.2
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	3	1.19
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	4	1.19
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD22	16	1.19
(1,1400)	1:180:A:LEU:HD13	1:173:A:LEU:HG	2	1.19
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	7	1.19
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	6	1.19
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	2	1.19
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	4	1.19
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	6	1.19
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	11	1.19
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	17	1.19
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	20	1.19
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	12	1.19
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	16	1.19
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	7	1.19
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	20	1.19
(1,698)	1:161:A:PHE:H	1:165:A:LYS:HB2	5	1.19
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD13	2	1.19
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE1	9	1.18
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	6	1.18
(1,1421)	1:113:A:LEU:HD13	1:113:A:LEU:HB3	5	1.18
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	7	1.18
(1,1421)	1:113:A:LEU:HD11	1:113:A:LEU:HB3	10	1.18
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	2	1.18
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	3	1.18
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	12	1.18
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	8	1.18
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	4	1.18
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	2	1.18
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG22	8	1.18
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD23	5	1.18
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD21	5	1.17
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD22	18	1.17
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	2	1.17
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	12	1.17
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	20	1.17
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	11	1.17
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	17	1.17
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	20	1.17
(1,1233)	1:186:A:MET:HG2	1:185:A:ASN:HA	5	1.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	9	1.17
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG21	14	1.17
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	5	1.17
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	3	1.17
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	14	1.17
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	3	1.17
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	8	1.17
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD21	19	1.17
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD22	7	1.16
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	9	1.16
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	10	1.16
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG23	13	1.16
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	20	1.16
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	5	1.16
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	13	1.16
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG23	2	1.16
(1,1080)	1:192:A:PHE:HB3	1:184:A:VAL:H	11	1.16
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG21	4	1.16
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	12	1.16
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	8	1.16
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	14	1.16
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG12	10	1.16
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	1	1.15
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	4	1.15
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	8	1.15
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB3	19	1.15
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	18	1.15
(1,1579)	1:184:A:VAL:HG11	1:183:A:ILE:HG23	7	1.15
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	4	1.15
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	8	1.15
(1,1421)	1:113:A:LEU:HD13	1:113:A:LEU:HB3	9	1.15
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	14	1.15
(1,1373)	1:128:A:LEU:HD21	1:154:A:MET:HB2	20	1.15
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	10	1.15
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	17	1.15
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	10	1.15
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG22	11	1.15
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	16	1.15
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	4	1.15
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	6	1.15
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	13	1.15
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	19	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	13	1.15
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG21	3	1.15
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD11	3	1.14
(1,1490)	1:119:A:ILE:HD11	1:119:A:ILE:HA	7	1.14
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	8	1.14
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB2	8	1.14
(1,1421)	1:113:A:LEU:HD11	1:113:A:LEU:HB3	3	1.14
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	16	1.14
(1,1373)	1:128:A:LEU:HD23	1:154:A:MET:HB2	15	1.14
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	5	1.14
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG23	3	1.14
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG21	5	1.14
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	18	1.14
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	8	1.14
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG22	1	1.14
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG22	9	1.14
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	1	1.14
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	2	1.14
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	5	1.14
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	8	1.14
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	9	1.14
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	17	1.14
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG12	9	1.14
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD13	5	1.13
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	16	1.13
(1,1578)	1:140:A:THR:HG21	1:138:A:LYS:HE3	7	1.13
(1,1490)	1:119:A:ILE:HD13	1:119:A:ILE:HA	11	1.13
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD23	6	1.13
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	3	1.13
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	8	1.13
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	9	1.13
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG23	1	1.13
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG22	18	1.13
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	10	1.13
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	14	1.13
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	15	1.13
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	16	1.13
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	18	1.13
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	5	1.13
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	11	1.12
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	3	1.12
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	1	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	16	1.12
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	4	1.12
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	11	1.12
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD22	12	1.12
(1,1532)	1:190:A:ARG:HB3	1:188:A:ASN:HB3	14	1.12
(1,1421)	1:113:A:LEU:HD12	1:113:A:LEU:HB3	12	1.12
(1,1373)	1:128:A:LEU:HD21	1:154:A:MET:HB2	3	1.12
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	8	1.12
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	1	1.12
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	7	1.12
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	12	1.12
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	15	1.12
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	17	1.12
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	13	1.12
(1,734)	1:174:A:THR:HA	1:175:A:PHE:HB3	11	1.12
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG21	2	1.12
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	2	1.11
(2,126)	1:112:A:ASN:HA	1:197:A:LEU:HG	7	1.11
(2,69)	1:159:A:PHE:H	1:166:A:GLU:HB3	13	1.11
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	3	1.11
(2,1)	1:170:A:ARG:H	1:154:A:MET:HG2	14	1.11
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	1	1.11
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	3	1.11
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	13	1.11
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	14	1.11
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	10	1.11
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	3	1.11
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	4	1.11
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	9	1.11
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	10	1.11
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	13	1.11
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	16	1.11
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	18	1.11
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	18	1.11
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	7	1.11
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG22	20	1.11
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	1	1.11
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	16	1.11
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	3	1.11
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	8	1.11
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	19	1.11
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG13	3	1.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	4	1.1
(2,136)	1:172:A:ARG:HD2	1:172:A:ARG:HB2	8	1.1
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	16	1.1
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	20	1.1
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG21	11	1.1
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	2	1.1
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	15	1.1
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	11	1.1
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	14	1.1
(1,1310)	1:126:A:LYS:HD3	1:126:A:LYS:HB2	14	1.1
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG21	12	1.1
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	6	1.1
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	13	1.1
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	16	1.1
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	20	1.1
(1,316)	1:147:A:VAL:H	1:136:A:VAL:HG11	1	1.1
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	2	1.1
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	16	1.1
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	16	1.09
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG21	5	1.09
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	3	1.09
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	4	1.09
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	7	1.09
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	17	1.09
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG21	10	1.09
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	19	1.09
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	17	1.09
(1,614)	1:132:A:GLN:H	1:132:A:GLN:HG3	7	1.09
(1,419)	1:190:A:ARG:H	1:190:A:ARG:HG2	14	1.09
(2,199)	1:140:A:THR:HG22	1:138:A:LYS:HG2	15	1.08
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD13	12	1.08
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	3	1.08
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	13	1.08
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	4	1.08
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD11	11	1.08
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG22	6	1.08
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG22	17	1.08
(1,1510)	1:129:A:GLU:HG2	1:126:A:LYS:HD3	13	1.08
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	1	1.08
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	9	1.08
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	6	1.08
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	18	1.08

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	3	1.08
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	10	1.08
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD13	4	1.08
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	9	1.08
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	18	1.08
(1,316)	1:147:A:VAL:H	1:136:A:VAL:HG11	9	1.08
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HG2	11	1.07
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	3	1.07
(2,137)	1:156:A:ARG:HD3	1:169:A:VAL:HG21	4	1.07
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD11	17	1.07
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	19	1.07
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	20	1.07
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	14	1.07
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	12	1.07
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	5	1.07
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	7	1.07
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	12	1.07
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	16	1.07
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	15	1.07
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG23	5	1.07
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG21	14	1.07
(1,1049)	1:156:A:ARG:HD3	1:197:A:LEU:HA	10	1.07
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	15	1.07
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	7	1.07
(1,316)	1:147:A:VAL:H	1:136:A:VAL:HG13	4	1.07
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	8	1.06
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	20	1.06
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	18	1.06
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG22	4	1.06
(1,1490)	1:119:A:ILE:HD11	1:119:A:ILE:HA	3	1.06
(1,1373)	1:128:A:LEU:HD21	1:154:A:MET:HB2	7	1.06
(1,1373)	1:128:A:LEU:HD23	1:154:A:MET:HB2	11	1.06
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	17	1.06
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	13	1.06
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	2	1.06
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	5	1.06
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	17	1.06
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG22	2	1.06
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	1	1.06
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	13	1.06
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	3	1.06
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	4	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG13	8	1.06
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD21	14	1.05
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD21	15	1.05
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	17	1.05
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD23	19	1.05
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	3	1.05
(1,1579)	1:184:A:VAL:HG11	1:183:A:ILE:HG22	20	1.05
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	3	1.05
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	5	1.05
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	2	1.05
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	19	1.05
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	15	1.05
(1,1028)	1:141:A:ARG:HD3	1:140:A:THR:HG23	16	1.05
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	16	1.05
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG23	5	1.05
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	17	1.05
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	11	1.05
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	5	1.05
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	1	1.05
(2,201)	1:111:A:VAL:HG22	1:130:A:ALA:HB2	15	1.04
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	17	1.04
(2,186)	1:173:A:LEU:HD13	1:195:A:PHE:HB2	20	1.04
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	14	1.04
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	8	1.04
(2,1)	1:170:A:ARG:H	1:154:A:MET:HG2	13	1.04
(2,1)	1:170:A:ARG:H	1:154:A:MET:HG2	18	1.04
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD23	20	1.04
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	20	1.04
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	20	1.04
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	4	1.04
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	9	1.04
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG22	12	1.04
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	2	1.04
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	17	1.04
(2,199)	1:140:A:THR:HG22	1:138:A:LYS:HG2	12	1.03
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	7	1.03
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	20	1.03
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	11	1.03
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD21	1	1.03
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG22	10	1.03
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	2	1.03
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	12	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	9	1.03
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	14	1.03
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG23	13	1.03
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG21	14	1.03
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	7	1.03
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD12	14	1.03
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	7	1.03
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	2	1.03
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	12	1.03
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG22	11	1.03
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	20	1.03
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	18	1.03
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD13	11	1.02
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	7	1.02
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG21	1	1.02
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG21	14	1.02
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	17	1.02
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	1	1.02
(1,1329)	1:115:A:PRO:HG2	1:115:A:PRO:HA	19	1.02
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	12	1.02
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	8	1.02
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG21	9	1.02
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG21	16	1.02
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG22	10	1.02
(1,340)	1:172:A:ARG:H	1:186:A:MET:HG2	13	1.02
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	8	1.01
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	7	1.01
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG22	12	1.01
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG22	15	1.01
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	1	1.01
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	5	1.01
(1,1373)	1:128:A:LEU:HD22	1:154:A:MET:HB2	19	1.01
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	9	1.01
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	6	1.01
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG12	4	1.01
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	6	1.01
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD11	11	1.01
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	10	1.01
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	8	1.0
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	11	1.0
(1,1579)	1:184:A:VAL:HG11	1:183:A:ILE:HG22	2	1.0
(1,1579)	1:184:A:VAL:HG11	1:183:A:ILE:HG22	8	1.0

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG22	18	1.0
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG21	19	1.0
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	15	1.0
(1,1384)	1:127:A:LEU:HD23	1:127:A:LEU:HA	18	1.0
(1,1383)	1:127:A:LEU:HB3	1:127:A:LEU:HD21	3	1.0
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	8	1.0
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	13	1.0
(1,974)	1:158:A:PRO:HD3	1:158:A:PRO:HA	12	1.0
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG21	11	1.0
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG22	17	1.0
(1,678)	1:124:A:MET:H	1:120:A:SER:H	7	1.0
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	18	1.0
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	4	1.0
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	8	1.0
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	4	1.0
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	3	0.99
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE3	7	0.99
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	10	0.99
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	11	0.99
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD12	9	0.99
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	17	0.99
(1,1579)	1:184:A:VAL:HG11	1:183:A:ILE:HG22	3	0.99
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	6	0.99
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD11	16	0.99
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	1	0.99
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD11	14	0.99
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	14	0.99
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	7	0.99
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	8	0.99
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	10	0.99
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	17	0.99
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	9	0.99
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD11	13	0.99
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	2	0.99
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	9	0.99
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	15	0.99
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG22	14	0.99
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	15	0.99
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	19	0.99
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	14	0.98
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG13	8	0.98
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	13	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,166)	1:122:A:ASN:HB3	1:125:A:VAL:HB	8	0.98
(2,132)	1:167:A:GLY:HA3	1:168:A:GLN:HG2	3	0.98
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	1	0.98
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD12	9	0.98
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD12	5	0.98
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	7	0.98
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	5	0.98
(2,49)	1:118:A:THR:H	1:119:A:ILE:HG13	6	0.98
(1,1740)	1:138:A:LYS:HB3	1:138:A:LYS:HE2	9	0.98
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG21	7	0.98
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG21	13	0.98
(1,1579)	1:184:A:VAL:HG12	1:183:A:ILE:HG21	9	0.98
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	16	0.98
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	19	0.98
(1,1384)	1:127:A:LEU:HD21	1:127:A:LEU:HA	1	0.98
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG21	4	0.98
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	3	0.98
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD13	17	0.98
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG21	19	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	1	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	2	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	4	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	7	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	9	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	11	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	12	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	14	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	15	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	16	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	18	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	19	0.98
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	20	0.98
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	18	0.98
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	6	0.98
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD13	1	0.98
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD13	16	0.98
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	11	0.98
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG22	16	0.98
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	5	0.98
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	7	0.98
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG13	17	0.98
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD11	18	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD13	16	0.97
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	9	0.97
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	18	0.97
(1,1579)	1:184:A:VAL:HG13	1:183:A:ILE:HG22	16	0.97
(1,1570)	1:127:A:LEU:HD13	1:127:A:LEU:HB2	6	0.97
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD1	15	0.97
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	15	0.97
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	1	0.97
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	18	0.97
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	3	0.97
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	6	0.97
(1,614)	1:132:A:GLN:H	1:132:A:GLN:HG3	17	0.97
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	2	0.97
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG12	18	0.97
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD13	3	0.96
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD11	17	0.96
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD11	6	0.96
(2,1)	1:170:A:ARG:H	1:154:A:MET:HG2	16	0.96
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	5	0.96
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	8	0.96
(1,1384)	1:127:A:LEU:HD22	1:127:A:LEU:HA	16	0.96
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD13	15	0.96
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	18	0.96
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	4	0.96
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	16	0.96
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	5	0.96
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	2	0.96
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD13	7	0.96
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG22	15	0.96
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG22	20	0.96
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	13	0.96
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	17	0.96
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	11	0.96
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	17	0.96
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	20	0.96
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	14	0.96
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD13	19	0.96
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	2	0.96
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	18	0.96
(2,199)	1:140:A:THR:HG22	1:138:A:LYS:HG2	5	0.95
(2,199)	1:140:A:THR:HG22	1:138:A:LYS:HG2	14	0.95
(2,198)	1:169:A:VAL:HG11	1:170:A:ARG:HB3	3	0.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD12	3	0.95
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	5	0.95
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	19	0.95
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	5	0.95
(2,53)	1:118:A:THR:H	1:119:A:ILE:HG13	6	0.95
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB3	12	0.95
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	19	0.95
(1,1468)	1:152:A:ILE:HG23	1:145:A:PHE:HB3	9	0.95
(1,1384)	1:127:A:LEU:HD21	1:127:A:LEU:HA	9	0.95
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	6	0.95
(1,1049)	1:156:A:ARG:HD3	1:197:A:LEU:HA	9	0.95
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	6	0.95
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG21	6	0.95
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG21	10	0.95
(1,717)	1:162:A:PRO:HA	1:162:A:PRO:HG2	5	0.95
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	19	0.95
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	1	0.95
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD12	10	0.95
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD11	18	0.95
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	19	0.95
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG21	6	0.95
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	7	0.95
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD22	4	0.95
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	14	0.95
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	14	0.94
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	19	0.94
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	9	0.94
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	4	0.94
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD12	12	0.94
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD22	20	0.94
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG13	15	0.94
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	15	0.94
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD12	6	0.94
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	15	0.94
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	18	0.94
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	20	0.94
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD12	18	0.94
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	15	0.94
(1,1384)	1:127:A:LEU:HD23	1:127:A:LEU:HA	13	0.94
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	13	0.94
(1,1049)	1:156:A:ARG:HD3	1:197:A:LEU:HA	3	0.94
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	16	0.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	19	0.94
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	1	0.94
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	19	0.94
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	20	0.94
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	12	0.94
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD12	20	0.94
(1,719)	1:138:A:LYS:H	1:137:A:SER:HB2	16	0.94
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	17	0.94
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	3	0.94
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	4	0.94
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	13	0.94
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	17	0.94
(1,592)	1:131:A:THR:H	1:127:A:LEU:HD11	9	0.94
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	14	0.94
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	16	0.94
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG23	9	0.94
(1,340)	1:172:A:ARG:H	1:186:A:MET:HG2	18	0.94
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	7	0.93
(2,132)	1:167:A:GLY:HA3	1:168:A:GLN:HG2	14	0.93
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	15	0.93
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	20	0.93
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD12	19	0.93
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	9	0.93
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	12	0.93
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	6	0.93
(1,1660)	1:156:A:ARG:HB3	1:195:A:PHE:HZ	2	0.93
(1,1648)	1:195:A:PHE:HE1	1:183:A:ILE:HG23	12	0.93
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	17	0.93
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD13	7	0.93
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	4	0.93
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	12	0.93
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	14	0.93
(1,1510)	1:129:A:GLU:HG2	1:126:A:LYS:HD3	10	0.93
(1,1483)	1:183:A:ILE:HD11	1:195:A:PHE:HD2	2	0.93
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	2	0.93
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	1	0.93
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	15	0.93
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	1	0.93
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	11	0.93
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	18	0.93
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	17	0.93
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	2	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	12	0.93
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	15	0.93
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	2	0.93
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG23	3	0.93
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG23	8	0.93
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD11	2	0.92
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD13	11	0.92
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	7	0.92
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG13	3	0.92
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG12	9	0.92
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	10	0.92
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	5	0.92
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD11	13	0.92
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG11	6	0.92
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG13	13	0.92
(1,1521)	1:138:A:LYS:HB3	1:138:A:LYS:HD2	11	0.92
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD2	9	0.92
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	1	0.92
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	4	0.92
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	5	0.92
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	8	0.92
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	18	0.92
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	20	0.92
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	9	0.92
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	10	0.92
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	16	0.92
(1,764)	1:146:A:THR:HA	1:136:A:VAL:HG22	7	0.92
(1,719)	1:138:A:LYS:H	1:137:A:SER:HB2	6	0.92
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	4	0.92
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	5	0.92
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	8	0.92
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD12	14	0.92
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG21	1	0.92
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG22	6	0.92
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD13	7	0.91
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD12	18	0.91
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD12	20	0.91
(2,198)	1:169:A:VAL:HG12	1:170:A:ARG:HB3	13	0.91
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	1	0.91
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD12	14	0.91
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD11	16	0.91
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	7	0.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	8	0.91
(1,1510)	1:129:A:GLU:HG2	1:126:A:LYS:HD3	1	0.91
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	6	0.91
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	16	0.91
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	4	0.91
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	13	0.91
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	17	0.91
(1,1029)	1:190:A:ARG:HD2	1:188:A:ASN:HB2	19	0.91
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	4	0.91
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD13	19	0.91
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	2	0.91
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	13	0.91
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	18	0.91
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG21	15	0.91
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	11	0.91
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	15	0.91
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HG2	18	0.9
(2,166)	1:122:A:ASN:HB3	1:125:A:VAL:HB	5	0.9
(2,166)	1:122:A:ASN:HB3	1:125:A:VAL:HB	12	0.9
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	15	0.9
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD21	7	0.9
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	18	0.9
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	5	0.9
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD11	5	0.9
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	4	0.9
(1,1431)	1:146:A:THR:HG21	1:139:A:MET:HE3	20	0.9
(1,1395)	1:197:A:LEU:HD21	1:156:A:ARG:HG3	6	0.9
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	20	0.9
(1,1312)	1:126:A:LYS:HD3	1:109:A:ARG:HB3	18	0.9
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	8	0.9
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	2	0.9
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	9	0.9
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	14	0.9
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	8	0.9
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	11	0.9
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	13	0.9
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	2	0.9
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD12	5	0.9
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD12	7	0.9
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	20	0.9
(1,506)	1:189:A:ASN:H	1:190:A:ARG:HG2	14	0.9
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG23	14	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG22	16	0.9
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	1	0.9
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG13	5	0.9
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG12	19	0.9
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	7	0.9
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	5	0.89
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	12	0.89
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HG2	20	0.89
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	16	0.89
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG12	20	0.89
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	11	0.89
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	20	0.89
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	15	0.89
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD11	2	0.89
(1,1384)	1:127:A:LEU:HD22	1:127:A:LEU:HA	14	0.89
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	14	0.89
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	17	0.89
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	10	0.89
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	12	0.89
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	3	0.89
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	15	0.89
(1,429)	1:190:A:ARG:H	1:190:A:ARG:HB3	14	0.89
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	1	0.89
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	20	0.89
(1,316)	1:147:A:VAL:H	1:136:A:VAL:HG11	2	0.89
(1,105)	1:112:A:ASN:H	1:113:A:LEU:HD11	13	0.89
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD11	5	0.88
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG12	6	0.88
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	3	0.88
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	20	0.88
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	5	0.88
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB2	10	0.88
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD13	14	0.88
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	9	0.88
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	2	0.88
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	6	0.88
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	10	0.88
(1,1468)	1:152:A:ILE:HG23	1:145:A:PHE:HB3	1	0.88
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	2	0.88
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	20	0.88
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	7	0.88
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	9	0.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	16	0.88
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	18	0.88
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	10	0.88
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	14	0.88
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	2	0.88
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG23	19	0.88
(1,974)	1:158:A:PRO:HD3	1:158:A:PRO:HA	2	0.88
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	7	0.88
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	5	0.88
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	10	0.88
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	9	0.88
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	14	0.88
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG23	12	0.88
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD21	16	0.88
(1,121)	1:175:A:PHE:H	1:180:A:LEU:HD11	2	0.88
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	7	0.88
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG12	20	0.88
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD11	4	0.87
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD12	9	0.87
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD12	19	0.87
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD12	18	0.87
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	11	0.87
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	11	0.87
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	10	0.87
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	6	0.87
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	4	0.87
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	8	0.87
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD11	10	0.87
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD22	15	0.87
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG12	2	0.87
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD2	6	0.87
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	16	0.87
(1,1456)	1:130:A:ALA:HB3	1:132:A:GLN:HG3	18	0.87
(1,1431)	1:146:A:THR:HG21	1:139:A:MET:HE1	14	0.87
(1,1395)	1:197:A:LEU:HD21	1:156:A:ARG:HG3	8	0.87
(1,1395)	1:197:A:LEU:HD22	1:156:A:ARG:HG3	12	0.87
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	3	0.87
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	10	0.87
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	11	0.87
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	19	0.87
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	17	0.87
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG22	7	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	3	0.87
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	7	0.87
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	16	0.87
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	11	0.87
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	20	0.87
(1,719)	1:138:A:LYS:H	1:137:A:SER:HB2	8	0.87
(1,719)	1:138:A:LYS:H	1:137:A:SER:HB2	20	0.87
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	12	0.87
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	13	0.87
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	9	0.87
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG23	18	0.87
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	20	0.87
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	12	0.87
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	1	0.86
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	10	0.86
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	8	0.86
(2,69)	1:159:A:PHE:H	1:156:A:ARG:HB2	17	0.86
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	13	0.86
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG12	10	0.86
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG11	4	0.86
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD13	13	0.86
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	5	0.86
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	8	0.86
(1,1350)	1:135:A:GLN:HB3	1:145:A:PHE:HZ	1	0.86
(1,1277)	1:190:A:ARG:HB3	1:190:A:ARG:HD2	14	0.86
(1,1231)	1:186:A:MET:HB3	1:170:A:ARG:HD2	11	0.86
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	12	0.86
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	15	0.86
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	19	0.86
(1,1158)	1:144:A:GLU:HG2	1:141:A:ARG:HG3	13	0.86
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG12	8	0.86
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	17	0.86
(1,678)	1:124:A:MET:H	1:120:A:SER:H	3	0.86
(1,678)	1:124:A:MET:H	1:120:A:SER:H	8	0.86
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	11	0.86
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	12	0.86
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	15	0.86
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	19	0.86
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	3	0.86
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG11	17	0.86
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG21	18	0.86
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	8	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD12	13	0.85
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	1	0.85
(2,166)	1:122:A:ASN:HB3	1:125:A:VAL:HB	14	0.85
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	18	0.85
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	18	0.85
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD11	4	0.85
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD11	11	0.85
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	10	0.85
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG11	5	0.85
(1,1740)	1:138:A:LYS:HB3	1:138:A:LYS:HE2	7	0.85
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD12	17	0.85
(1,1570)	1:127:A:LEU:HD12	1:127:A:LEU:HB2	2	0.85
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD2	10	0.85
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	18	0.85
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	6	0.85
(1,1384)	1:127:A:LEU:HD22	1:127:A:LEU:HA	11	0.85
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	2	0.85
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	6	0.85
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	20	0.85
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	13	0.85
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	3	0.85
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	5	0.85
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	1	0.85
(1,678)	1:124:A:MET:H	1:120:A:SER:H	20	0.85
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	2	0.85
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	5	0.85
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	7	0.85
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	12	0.85
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	16	0.85
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	20	0.85
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	1	0.85
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	19	0.85
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG22	7	0.85
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG23	3	0.85
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	18	0.85
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	19	0.85
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD13	14	0.84
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD12	16	0.84
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	13	0.84
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	3	0.84
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	13	0.84
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	16	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	12	0.84
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB1	9	0.84
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	18	0.84
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	2	0.84
(1,1570)	1:127:A:LEU:HD11	1:127:A:LEU:HB2	7	0.84
(1,1510)	1:129:A:GLU:HG2	1:126:A:LYS:HD3	14	0.84
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	20	0.84
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	12	0.84
(1,1367)	1:141:A:ARG:HA	1:141:A:ARG:HG3	12	0.84
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG22	10	0.84
(1,1218)	1:185:A:ASN:HA	1:186:A:MET:HB3	6	0.84
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	7	0.84
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	15	0.84
(1,957)	1:112:A:ASN:HA	1:113:A:LEU:HB3	20	0.84
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	11	0.84
(1,719)	1:138:A:LYS:H	1:137:A:SER:HB2	9	0.84
(1,719)	1:138:A:LYS:H	1:137:A:SER:HB2	12	0.84
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	10	0.84
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	1	0.84
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	4	0.84
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG23	11	0.84
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG23	20	0.84
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD11	9	0.84
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	16	0.84
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	2	0.84
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD11	8	0.83
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	11	0.83
(2,201)	1:111:A:VAL:HG11	1:130:A:ALA:HB2	4	0.83
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD11	9	0.83
(2,186)	1:173:A:LEU:HD12	1:195:A:PHE:HB2	4	0.83
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG23	15	0.83
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	4	0.83
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	19	0.83
(2,132)	1:167:A:GLY:HA3	1:168:A:GLN:HG2	10	0.83
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	4	0.83
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	17	0.83
(2,103)	1:125:A:VAL:HA	1:152:A:ILE:HD13	13	0.83
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	7	0.83
(2,81)	1:140:A:THR:H	1:136:A:VAL:HG11	13	0.83
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	2	0.83
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	11	0.83
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	14	0.83

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD11	13	0.83
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD13	1	0.83
(2,5)	1:196:A:ARG:H	1:111:A:VAL:HG11	3	0.83
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	7	0.83
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	16	0.83
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	13	0.83
(1,1570)	1:127:A:LEU:HD12	1:127:A:LEU:HB2	12	0.83
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	13	0.83
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD11	2	0.83
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	9	0.83
(1,1456)	1:130:A:ALA:HB3	1:132:A:GLN:HG3	15	0.83
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG11	16	0.83
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	19	0.83
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	6	0.83
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	14	0.83
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	19	0.83
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	8	0.83
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	11	0.83
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	17	0.83
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	19	0.83
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD13	9	0.83
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	10	0.83
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	7	0.83
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG23	8	0.83
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	15	0.83
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG22	10	0.83
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD23	1	0.83
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	16	0.83
(2,208)	1:152:A:ILE:HD13	1:124:A:MET:HB2	7	0.82
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	19	0.82
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD13	8	0.82
(1,1570)	1:127:A:LEU:HD11	1:127:A:LEU:HB2	19	0.82
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	7	0.82
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	13	0.82
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	19	0.82
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	7	0.82
(1,1420)	1:113:A:LEU:HD22	1:154:A:MET:HG2	16	0.82
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG23	18	0.82
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	4	0.82
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	8	0.82
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	17	0.82
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	3	0.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	1	0.82
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	2	0.82
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	14	0.82
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	18	0.82
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	20	0.82
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD11	20	0.82
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	1	0.82
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	4	0.82
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	13	0.82
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	13	0.82
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD13	18	0.82
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	8	0.81
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	11	0.81
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	1	0.81
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	2	0.81
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	11	0.81
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD2	8	0.81
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	19	0.81
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB2	9	0.81
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	8	0.81
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	13	0.81
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB1	15	0.81
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB1	18	0.81
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG13	9	0.81
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	4	0.81
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	17	0.81
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	8	0.81
(1,1607)	1:155:A:ILE:HD13	1:170:A:ARG:HG2	13	0.81
(1,1570)	1:127:A:LEU:HD13	1:127:A:LEU:HB2	20	0.81
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD11	13	0.81
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD12	17	0.81
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	10	0.81
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD22	16	0.81
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD22	18	0.81
(1,1403)	1:180:A:LEU:HD13	1:183:A:ILE:HD12	17	0.81
(1,1384)	1:127:A:LEU:HD21	1:127:A:LEU:HA	10	0.81
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	10	0.81
(1,1061)	1:176:A:ASP:HB3	1:181:A:ALA:H	10	0.81
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	18	0.81
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	8	0.81
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	19	0.81
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	17	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD12	14	0.81
(1,583)	1:131:A:THR:H	1:132:A:GLN:HG3	7	0.81
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	6	0.81
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	10	0.81
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	11	0.81
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	2	0.81
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	8	0.81
(2,221)	1:172:A:ARG:HD2	1:173:A:LEU:HD13	1	0.8
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	16	0.8
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG23	2	0.8
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	16	0.8
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB1	3	0.8
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	12	0.8
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD11	14	0.8
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	18	0.8
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD11	4	0.8
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG11	1	0.8
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG11	19	0.8
(2,2)	1:170:A:ARG:H	1:186:A:MET:HG3	5	0.8
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD13	4	0.8
(1,1570)	1:127:A:LEU:HD13	1:127:A:LEU:HB2	5	0.8
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	14	0.8
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD23	3	0.8
(1,1416)	1:147:A:VAL:HG11	1:147:A:VAL:HA	1	0.8
(1,1416)	1:147:A:VAL:HG11	1:147:A:VAL:HA	5	0.8
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	9	0.8
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	14	0.8
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	15	0.8
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	15	0.8
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	9	0.8
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	13	0.8
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	6	0.8
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	13	0.8
(1,609)	1:146:A:THR:H	1:154:A:MET:HB2	16	0.8
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB2	8	0.8
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	7	0.8
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG11	8	0.8
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	19	0.8
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	18	0.8
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	17	0.8
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE1	19	0.8
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD11	6	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	16	0.79
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD13	13	0.79
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	16	0.79
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	17	0.79
(2,151)	1:112:A:ASN:HB2	1:111:A:VAL:HG11	3	0.79
(2,132)	1:167:A:GLY:HA3	1:168:A:GLN:HG2	7	0.79
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	3	0.79
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	4	0.79
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	1	0.79
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD11	18	0.79
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	3	0.79
(1,1468)	1:152:A:ILE:HG23	1:145:A:PHE:HB3	13	0.79
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	1	0.79
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	10	0.79
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	6	0.79
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	3	0.79
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	17	0.79
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	18	0.79
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	3	0.79
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	16	0.79
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	12	0.79
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	16	0.79
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD13	17	0.79
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	18	0.79
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	16	0.79
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	6	0.79
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	6	0.79
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	1	0.79
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	11	0.79
(1,614)	1:132:A:GLN:H	1:132:A:GLN:HG3	12	0.79
(1,572)	1:179:A:HIS:H	1:177:A:GLY:HA2	14	0.79
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	12	0.79
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	1	0.79
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	9	0.79
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	6	0.79
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	10	0.79
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	20	0.79
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	11	0.79
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	16	0.79
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	7	0.78
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	18	0.78
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	12	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD11	1	0.78
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG12	18	0.78
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	9	0.78
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	9	0.78
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	11	0.78
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	17	0.78
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG12	3	0.78
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG13	8	0.78
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	9	0.78
(1,1607)	1:155:A:ILE:HD13	1:170:A:ARG:HG2	3	0.78
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	4	0.78
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD23	9	0.78
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	11	0.78
(1,1431)	1:146:A:THR:HG23	1:139:A:MET:HE2	17	0.78
(1,1416)	1:147:A:VAL:HG11	1:147:A:VAL:HA	2	0.78
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	8	0.78
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	11	0.78
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG11	15	0.78
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG12	5	0.78
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	14	0.78
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD11	2	0.78
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD11	5	0.78
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD12	12	0.78
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	14	0.78
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	9	0.78
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	7	0.78
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD22	8	0.78
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD23	9	0.78
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD22	18	0.78
(1,999)	1:143:A:GLY:HA3	1:159:A:PHE:HZ	13	0.78
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	15	0.78
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	17	0.78
(1,761)	1:129:A:GLU:HA	1:129:A:GLU:HG3	1	0.78
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG22	10	0.78
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD11	8	0.78
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	4	0.78
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	16	0.78
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG21	3	0.78
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG21	5	0.78
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG21	8	0.78
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG23	15	0.78
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG22	19	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	12	0.78
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	15	0.78
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	15	0.78
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	17	0.78
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	12	0.77
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	15	0.77
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD12	4	0.77
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD13	14	0.77
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG11	7	0.77
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	4	0.77
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	7	0.77
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB3	16	0.77
(2,54)	1:129:A:GLU:H	1:129:A:GLU:HG2	15	0.77
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD11	13	0.77
(1,1570)	1:127:A:LEU:HD11	1:127:A:LEU:HB2	17	0.77
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD2	18	0.77
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG22	5	0.77
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	3	0.77
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	4	0.77
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	12	0.77
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	16	0.77
(1,1416)	1:147:A:VAL:HG11	1:147:A:VAL:HA	20	0.77
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	3	0.77
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	4	0.77
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	1	0.77
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	18	0.77
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	1	0.77
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD11	6	0.77
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD11	15	0.77
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD23	12	0.77
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	17	0.77
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD22	20	0.77
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	10	0.77
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	9	0.77
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	14	0.77
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	11	0.77
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	12	0.77
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	13	0.77
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	10	0.77
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD23	14	0.77
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	1	0.77
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	11	0.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE3	9	0.77
(2,214)	1:112:A:ASN:HB3	1:111:A:VAL:HA	9	0.76
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	7	0.76
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	16	0.76
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	7	0.76
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	12	0.76
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	19	0.76
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	2	0.76
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	17	0.76
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	12	0.76
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	11	0.76
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	17	0.76
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	9	0.76
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	11	0.76
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	7	0.76
(1,1416)	1:147:A:VAL:HG12	1:147:A:VAL:HA	10	0.76
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	17	0.76
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	13	0.76
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	7	0.76
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG12	3	0.76
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	4	0.76
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD12	19	0.76
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	2	0.76
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	5	0.76
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	18	0.76
(1,761)	1:129:A:GLU:HA	1:129:A:GLU:HG3	13	0.76
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	5	0.76
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD11	18	0.76
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	1	0.76
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD22	18	0.76
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	2	0.76
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	14	0.76
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG21	16	0.76
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	18	0.76
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG21	7	0.76
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	7	0.76
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	14	0.76
(1,72)	1:139:A:MET:H	1:139:A:MET:HE1	11	0.76
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	16	0.76
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	6	0.76
(2,214)	1:112:A:ASN:HB3	1:111:A:VAL:HA	2	0.75
(2,214)	1:112:A:ASN:HB3	1:111:A:VAL:HA	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	6	0.75
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	10	0.75
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	20	0.75
(2,186)	1:173:A:LEU:HD13	1:195:A:PHE:HB2	13	0.75
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	6	0.75
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	19	0.75
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG21	16	0.75
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	1	0.75
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD2	20	0.75
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	4	0.75
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	2	0.75
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD23	5	0.75
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG12	9	0.75
(1,1481)	1:152:A:ILE:HD13	1:128:A:LEU:HD21	18	0.75
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	20	0.75
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG22	17	0.75
(1,1416)	1:147:A:VAL:HG11	1:147:A:VAL:HA	6	0.75
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG13	10	0.75
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	2	0.75
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG11	5	0.75
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG13	6	0.75
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG11	4	0.75
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	15	0.75
(1,1061)	1:176:A:ASP:HB3	1:181:A:ALA:H	8	0.75
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	17	0.75
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	1	0.75
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	3	0.75
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD23	5	0.75
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD22	10	0.75
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	12	0.75
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	2	0.75
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	7	0.75
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD12	17	0.75
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG13	20	0.75
(1,761)	1:129:A:GLU:HA	1:129:A:GLU:HG3	10	0.75
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	2	0.75
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	15	0.75
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD12	3	0.75
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD11	16	0.75
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD11	14	0.75
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	7	0.75
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	5	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,287)	1:136:A:VAL:H	1:136:A:VAL:HG22	17	0.75
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	5	0.75
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	17	0.75
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	7	0.75
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE1	10	0.75
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD13	10	0.74
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	13	0.74
(2,198)	1:169:A:VAL:HG13	1:170:A:ARG:HB3	5	0.74
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	8	0.74
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG23	1	0.74
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	20	0.74
(2,63)	1:133:A:TYR:H	1:130:A:ALA:HB2	20	0.74
(2,54)	1:129:A:GLU:H	1:129:A:GLU:HG2	7	0.74
(2,54)	1:129:A:GLU:H	1:129:A:GLU:HG2	8	0.74
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD23	20	0.74
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	4	0.74
(1,1570)	1:127:A:LEU:HD12	1:127:A:LEU:HB2	3	0.74
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG21	7	0.74
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG23	4	0.74
(1,1452)	1:181:A:ALA:HB1	1:180:A:LEU:HD21	15	0.74
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	16	0.74
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	19	0.74
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	9	0.74
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	10	0.74
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	14	0.74
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	17	0.74
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG22	14	0.74
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD22	5	0.74
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	19	0.74
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG11	1	0.74
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG12	20	0.74
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE2	5	0.74
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE2	6	0.74
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	19	0.74
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD11	8	0.74
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	10	0.74
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	10	0.74
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	18	0.74
(1,628)	1:167:A:GLY:H	1:169:A:VAL:HG21	5	0.74
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	13	0.74
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG21	13	0.74
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	13	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD21	17	0.74
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD22	20	0.74
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB1	4	0.74
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	17	0.74
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	4	0.74
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	9	0.74
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	18	0.74
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	19	0.73
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD11	10	0.73
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD11	12	0.73
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	2	0.73
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	13	0.73
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	1	0.73
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	2	0.73
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG12	14	0.73
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	7	0.73
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	3	0.73
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD12	6	0.73
(1,1452)	1:181:A:ALA:HB1	1:180:A:LEU:HD22	8	0.73
(1,1416)	1:147:A:VAL:HG13	1:147:A:VAL:HA	13	0.73
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD13	1	0.73
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	14	0.73
(1,1384)	1:127:A:LEU:HD22	1:127:A:LEU:HA	4	0.73
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	6	0.73
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	8	0.73
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	16	0.73
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	18	0.73
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	12	0.73
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	9	0.73
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE2	12	0.73
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE2	13	0.73
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	7	0.73
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	8	0.73
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	11	0.73
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	11	0.73
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	17	0.73
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD11	10	0.73
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	16	0.73
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD12	20	0.73
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD13	3	0.73
(1,80)	1:186:A:MET:H	1:186:A:MET:HG2	14	0.73
(1,72)	1:139:A:MET:H	1:139:A:MET:HE2	14	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	1	0.73
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	19	0.72
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG13	17	0.72
(2,166)	1:122:A:ASN:HB2	1:125:A:VAL:HB	2	0.72
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	14	0.72
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	1	0.72
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	1	0.72
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	19	0.72
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	17	0.72
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	11	0.72
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD23	1	0.72
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	12	0.72
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	10	0.72
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	15	0.72
(1,1456)	1:130:A:ALA:HB3	1:132:A:GLN:HG3	3	0.72
(1,1456)	1:130:A:ALA:HB1	1:132:A:GLN:HG3	5	0.72
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB2	18	0.72
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	2	0.72
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	5	0.72
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	7	0.72
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	11	0.72
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	12	0.72
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	19	0.72
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	20	0.72
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	1	0.72
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG23	17	0.72
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	3	0.72
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	12	0.72
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	4	0.72
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	17	0.72
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG12	7	0.72
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG11	17	0.72
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG11	19	0.72
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE2	4	0.72
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	3	0.72
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	19	0.72
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD12	5	0.72
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	18	0.72
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	4	0.72
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	12	0.72
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	9	0.72
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	3	0.72

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	7	0.72
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	18	0.72
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG12	13	0.72
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	11	0.72
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	12	0.72
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD11	19	0.72
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	6	0.72
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	10	0.72
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	13	0.72
(1,504)	1:194:A:PHE:H	1:192:A:PHE:HB2	15	0.72
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	6	0.72
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD12	11	0.72
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	3	0.72
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG11	3	0.72
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	14	0.72
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD13	14	0.72
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	16	0.72
(1,72)	1:139:A:MET:H	1:139:A:MET:HE3	17	0.72
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD11	15	0.71
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	4	0.71
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	4	0.71
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	6	0.71
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG12	4	0.71
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	14	0.71
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	1	0.71
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	17	0.71
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	1	0.71
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	17	0.71
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	16	0.71
(2,54)	1:129:A:GLU:H	1:129:A:GLU:HG2	3	0.71
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	6	0.71
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD11	13	0.71
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	11	0.71
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	13	0.71
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	14	0.71
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	16	0.71
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	18	0.71
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD11	12	0.71
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	4	0.71
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	7	0.71
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD23	6	0.71
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG23	3	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG21	13	0.71
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG23	4	0.71
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	6	0.71
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	1	0.71
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	1	0.71
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	10	0.71
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD13	11	0.71
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD22	6	0.71
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD23	11	0.71
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	2	0.71
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	3	0.71
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	7	0.71
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	14	0.71
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	16	0.71
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	4	0.71
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	9	0.71
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	10	0.71
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	13	0.71
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	14	0.71
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	16	0.71
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	17	0.71
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG11	18	0.71
(1,745)	1:131:A:THR:HA	1:132:A:GLN:HG3	7	0.71
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	18	0.71
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	16	0.71
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	18	0.71
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	5	0.71
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	1	0.71
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	9	0.71
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD12	14	0.71
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	18	0.71
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD13	4	0.71
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	2	0.71
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB1	8	0.71
(1,80)	1:186:A:MET:H	1:186:A:MET:HG2	13	0.71
(1,80)	1:186:A:MET:H	1:186:A:MET:HG2	18	0.71
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	4	0.71
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	1	0.71
(2,221)	1:172:A:ARG:HD3	1:173:A:LEU:HD12	12	0.7
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	1	0.7
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	11	0.7
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	12	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	4	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	3	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	7	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	9	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	10	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	12	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	15	0.7
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	18	0.7
(1,1648)	1:195:A:PHE:HE1	1:183:A:ILE:HG23	20	0.7
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	20	0.7
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	9	0.7
(1,1483)	1:183:A:ILE:HD11	1:195:A:PHE:HD1	1	0.7
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD1	8	0.7
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD22	15	0.7
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE2	10	0.7
(1,1475)	1:119:A:ILE:HG23	1:119:A:ILE:HA	5	0.7
(1,1456)	1:130:A:ALA:HB2	1:132:A:GLN:HG3	8	0.7
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD21	2	0.7
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD22	12	0.7
(1,1452)	1:181:A:ALA:HB1	1:180:A:LEU:HD23	13	0.7
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD11	11	0.7
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	18	0.7
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG22	20	0.7
(1,1275)	1:141:A:ARG:HB3	1:141:A:ARG:HD3	3	0.7
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	11	0.7
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	5	0.7
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG13	20	0.7
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG12	2	0.7
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	11	0.7
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	15	0.7
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	17	0.7
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	9	0.7
(1,942)	1:133:A:TYR:HD1	1:145:A:PHE:HB2	13	0.7
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	5	0.7
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	18	0.7
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	5	0.7
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	14	0.7
(1,812)	1:192:A:PHE:HA	1:193:A:GLY:HA2	8	0.7
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG12	11	0.7
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG13	14	0.7
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	16	0.7
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	14	0.7

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	6	0.7
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG22	19	0.7
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	5	0.7
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	13	0.7
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	17	0.7
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	19	0.7
(1,225)	1:128:A:LEU:H	1:127:A:LEU:HD21	6	0.7
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD22	18	0.7
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	16	0.7
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	12	0.7
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD11	17	0.7
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE3	20	0.7
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	19	0.69
(2,201)	1:111:A:VAL:HG12	1:130:A:ALA:HB3	16	0.69
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	12	0.69
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	19	0.69
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB2	1	0.69
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	5	0.69
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	3	0.69
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	14	0.69
(2,4)	1:135:A:GLN:H	1:147:A:VAL:HG11	20	0.69
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG22	11	0.69
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	18	0.69
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	8	0.69
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	17	0.69
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	10	0.69
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	18	0.69
(1,1562)	1:173:A:LEU:HD12	1:174:A:THR:H	13	0.69
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	11	0.69
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	4	0.69
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD13	19	0.69
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	1	0.69
(1,1475)	1:119:A:ILE:HG23	1:119:A:ILE:HA	12	0.69
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	16	0.69
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD21	5	0.69
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD22	7	0.69
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD22	10	0.69
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD23	11	0.69
(1,1431)	1:146:A:THR:HG22	1:139:A:MET:HE3	11	0.69
(1,1420)	1:113:A:LEU:HD22	1:154:A:MET:HG2	14	0.69
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	6	0.69
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	15	0.69

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	16	0.69
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	18	0.69
(1,1029)	1:190:A:ARG:HD2	1:188:A:ASN:HB2	15	0.69
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	20	0.69
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	10	0.69
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	3	0.69
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	4	0.69
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	10	0.69
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD12	4	0.69
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	5	0.69
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	20	0.69
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	14	0.69
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	5	0.69
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	3	0.69
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	19	0.69
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD11	16	0.69
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	8	0.69
(1,244)	1:183:A:ILE:H	1:180:A:LEU:HD22	2	0.69
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD21	5	0.69
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	6	0.69
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB2	20	0.69
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	18	0.69
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	11	0.69
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	2	0.69
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	3	0.68
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	8	0.68
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	9	0.68
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	16	0.68
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	17	0.68
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	18	0.68
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	1	0.68
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	3	0.68
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	12	0.68
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	3	0.68
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	7	0.68
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG13	3	0.68
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	12	0.68
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD21	17	0.68
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	14	0.68
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	7	0.68
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	14	0.68
(1,1735)	1:190:A:ARG:HD2	1:185:A:ASN:HB2	19	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	2	0.68
(1,1701)	1:133:A:TYR:HE1	1:134:A:ARG:H	9	0.68
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	6	0.68
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	5	0.68
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	6	0.68
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	14	0.68
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	16	0.68
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	4	0.68
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	14	0.68
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	19	0.68
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	20	0.68
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	15	0.68
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	19	0.68
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD1	16	0.68
(1,1475)	1:119:A:ILE:HG23	1:119:A:ILE:HA	6	0.68
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	8	0.68
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	10	0.68
(1,1475)	1:119:A:ILE:HG23	1:119:A:ILE:HA	17	0.68
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD23	4	0.68
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	20	0.68
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	2	0.68
(1,1397)	1:125:A:VAL:HG12	1:122:A:ASN:HB3	16	0.68
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	19	0.68
(1,1366)	1:173:A:LEU:HD13	1:171:A:ALA:HB1	9	0.68
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB1	14	0.68
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	13	0.68
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	12	0.68
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	14	0.68
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD12	20	0.68
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD12	11	0.68
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	19	0.68
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	9	0.68
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	19	0.68
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	10	0.68
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG12	17	0.68
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	12	0.68
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	17	0.68
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD12	10	0.68
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	6	0.68
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG23	17	0.68
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG13	3	0.68
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD22	16	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,72)	1:139:A:MET:H	1:139:A:MET:HE1	20	0.68
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	13	0.68
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	5	0.67
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD3	6	0.67
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	11	0.67
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD3	14	0.67
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	14	0.67
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	15	0.67
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	15	0.67
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD11	8	0.67
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG23	3	0.67
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG23	4	0.67
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	7	0.67
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG23	15	0.67
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	15	0.67
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	2	0.67
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	15	0.67
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD13	6	0.67
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	4	0.67
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	13	0.67
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	5	0.67
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	1	0.67
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	4	0.67
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	8	0.67
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	20	0.67
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD12	18	0.67
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	7	0.67
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	1	0.67
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	3	0.67
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG23	8	0.67
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	12	0.67
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	13	0.67
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE1	12	0.67
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	9	0.67
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	13	0.67
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	15	0.67
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	18	0.67
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	19	0.67
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	2	0.67
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD21	1	0.67
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	10	0.67
(1,1420)	1:113:A:LEU:HD22	1:154:A:MET:HG2	20	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1403)	1:180:A:LEU:HD13	1:183:A:ILE:HD12	19	0.67
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD23	11	0.67
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	17	0.67
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	3	0.67
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	8	0.67
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	9	0.67
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	10	0.67
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	10	0.67
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD22	1	0.67
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	15	0.67
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	9	0.67
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	7	0.67
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	11	0.67
(1,1049)	1:156:A:ARG:HD3	1:197:A:LEU:HA	11	0.67
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	14	0.67
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	11	0.67
(1,761)	1:129:A:GLU:HA	1:129:A:GLU:HG3	2	0.67
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	10	0.67
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	9	0.67
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	19	0.67
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	13	0.67
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	18	0.67
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	5	0.67
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB2	17	0.67
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	19	0.67
(1,505)	1:194:A:PHE:H	1:183:A:ILE:HD11	8	0.67
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG23	6	0.67
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	11	0.67
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	10	0.67
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD12	12	0.67
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD22	9	0.67
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD11	13	0.67
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	18	0.67
(1,199)	1:191:A:GLN:H	1:190:A:ARG:HG2	20	0.67
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD21	7	0.67
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	6	0.67
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD22	8	0.67
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	12	0.67
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB1	3	0.67
(1,80)	1:186:A:MET:H	1:186:A:MET:HG2	5	0.67
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	14	0.67
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD13	11	0.67

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD13	3	0.67
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	7	0.66
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD3	10	0.66
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	13	0.66
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	17	0.66
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	16	0.66
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	9	0.66
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	2	0.66
(2,52)	1:134:A:ARG:H	1:128:A:LEU:HB3	13	0.66
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	6	0.66
(2,34)	1:166:A:GLU:H	1:159:A:PHE:HB2	19	0.66
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	19	0.66
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD1	19	0.66
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG22	1	0.66
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	10	0.66
(1,1623)	1:133:A:TYR:HD1	1:136:A:VAL:HG11	2	0.66
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	6	0.66
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	19	0.66
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	15	0.66
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG23	1	0.66
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	9	0.66
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	16	0.66
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG13	8	0.66
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	2	0.66
(1,1461)	1:183:A:ILE:HG23	1:183:A:ILE:HG13	4	0.66
(1,1461)	1:183:A:ILE:HG22	1:183:A:ILE:HG13	11	0.66
(1,1461)	1:183:A:ILE:HG23	1:183:A:ILE:HG13	17	0.66
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG22	7	0.66
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD23	19	0.66
(1,1452)	1:181:A:ALA:HB2	1:180:A:LEU:HD23	20	0.66
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	1	0.66
(1,1403)	1:180:A:LEU:HD12	1:183:A:ILE:HD11	7	0.66
(1,1403)	1:180:A:LEU:HD12	1:183:A:ILE:HD11	15	0.66
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	8	0.66
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	9	0.66
(1,1395)	1:197:A:LEU:HD22	1:156:A:ARG:HG3	4	0.66
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	16	0.66
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	9	0.66
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	13	0.66
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	2	0.66
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	20	0.66
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG13	3	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG11	10	0.66
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	13	0.66
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	19	0.66
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG11	13	0.66
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG22	12	0.66
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	2	0.66
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG11	7	0.66
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	5	0.66
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD11	20	0.66
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	1	0.66
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD11	12	0.66
(1,583)	1:131:A:THR:H	1:132:A:GLN:HG3	17	0.66
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	4	0.66
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG21	8	0.66
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	15	0.66
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG22	5	0.66
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD11	13	0.66
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	3	0.66
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD11	20	0.66
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	6	0.66
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	9	0.66
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	10	0.66
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	10	0.66
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	4	0.66
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD22	7	0.66
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	13	0.66
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	12	0.66
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	10	0.66
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	10	0.66
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	2	0.65
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	4	0.65
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	12	0.65
(2,201)	1:111:A:VAL:HG11	1:130:A:ALA:HB3	1	0.65
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	19	0.65
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD11	5	0.65
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD13	17	0.65
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	11	0.65
(2,183)	1:158:A:PRO:HG2	1:158:A:PRO:HA	14	0.65
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	10	0.65
(2,131)	1:115:A:PRO:HD2	1:193:A:GLY:HA3	4	0.65
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	20	0.65
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	10	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	20	0.65
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	12	0.65
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	18	0.65
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	11	0.65
(2,54)	1:129:A:GLU:H	1:129:A:GLU:HG2	5	0.65
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD12	13	0.65
(2,5)	1:196:A:ARG:H	1:171:A:ALA:HB3	16	0.65
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD13	4	0.65
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	10	0.65
(1,1654)	1:195:A:PHE:HZ	1:195:A:PHE:HD2	2	0.65
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	6	0.65
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	8	0.65
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	19	0.65
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG23	4	0.65
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	5	0.65
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	6	0.65
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	15	0.65
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	14	0.65
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	6	0.65
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD12	17	0.65
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD11	12	0.65
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	3	0.65
(1,1475)	1:119:A:ILE:HG23	1:119:A:ILE:HA	11	0.65
(1,1475)	1:119:A:ILE:HG21	1:119:A:ILE:HA	20	0.65
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG22	10	0.65
(1,1452)	1:181:A:ALA:HB3	1:180:A:LEU:HD21	14	0.65
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG21	17	0.65
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG22	2	0.65
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG21	10	0.65
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG21	19	0.65
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	2	0.65
(1,1403)	1:180:A:LEU:HD13	1:183:A:ILE:HD12	20	0.65
(1,1397)	1:125:A:VAL:HG12	1:122:A:ASN:HB3	7	0.65
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD13	6	0.65
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	7	0.65
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	10	0.65
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	20	0.65
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	16	0.65
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	18	0.65
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	9	0.65
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	6	0.65
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG13	8	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG11	9	0.65
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	5	0.65
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD11	13	0.65
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD12	6	0.65
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG11	3	0.65
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD12	6	0.65
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD11	7	0.65
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	18	0.65
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	20	0.65
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	3	0.65
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	19	0.65
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	4	0.65
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD12	6	0.65
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	8	0.65
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	11	0.65
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG13	15	0.65
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD13	18	0.65
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	13	0.65
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	14	0.65
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD23	2	0.65
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	19	0.65
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD21	1	0.65
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	9	0.65
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	17	0.65
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	15	0.65
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD2	1	0.64
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD11	19	0.64
(2,186)	1:173:A:LEU:HD11	1:195:A:PHE:HB2	10	0.64
(2,183)	1:158:A:PRO:HG2	1:158:A:PRO:HA	6	0.64
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	8	0.64
(2,183)	1:158:A:PRO:HG2	1:158:A:PRO:HA	11	0.64
(2,183)	1:158:A:PRO:HG2	1:158:A:PRO:HA	18	0.64
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	20	0.64
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG23	8	0.64
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG21	12	0.64
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	4	0.64
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	11	0.64
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	7	0.64
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	17	0.64
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	5	0.64
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	7	0.64
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	18	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	20	0.64
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	11	0.64
(2,56)	1:110:A:MET:H	1:109:A:ARG:HB3	17	0.64
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	18	0.64
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	5	0.64
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	10	0.64
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	17	0.64
(1,1655)	1:195:A:PHE:HZ	1:156:A:ARG:HD2	8	0.64
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	5	0.64
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	17	0.64
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	17	0.64
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	12	0.64
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	20	0.64
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG22	2	0.64
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	17	0.64
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD13	13	0.64
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	19	0.64
(1,1478)	1:120:A:SER:H	1:152:A:ILE:HD11	5	0.64
(1,1461)	1:183:A:ILE:HG22	1:183:A:ILE:HG13	7	0.64
(1,1461)	1:183:A:ILE:HG21	1:183:A:ILE:HG13	13	0.64
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	3	0.64
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG22	11	0.64
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG23	20	0.64
(1,1424)	1:128:A:LEU:HD21	1:127:A:LEU:HB2	14	0.64
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	7	0.64
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD22	8	0.64
(1,1403)	1:180:A:LEU:HD13	1:183:A:ILE:HD11	12	0.64
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD13	12	0.64
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	20	0.64
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	18	0.64
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	14	0.64
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	17	0.64
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	12	0.64
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD22	15	0.64
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	19	0.64
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	9	0.64
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG23	1	0.64
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	19	0.64
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD23	15	0.64
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	3	0.64
(1,1029)	1:190:A:ARG:HD2	1:188:A:ASN:HB2	9	0.64
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	12	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD22	13	0.64
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	4	0.64
(1,934)	1:141:A:ARG:HA	1:141:A:ARG:HD3	17	0.64
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	2	0.64
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	15	0.64
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD12	8	0.64
(1,666)	1:156:A:ARG:H	1:155:A:ILE:HD13	12	0.64
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD12	13	0.64
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	3	0.64
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG21	13	0.64
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD13	4	0.64
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	15	0.64
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD13	7	0.64
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	14	0.64
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD22	10	0.64
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD23	3	0.64
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	19	0.64
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	19	0.64
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	20	0.64
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD11	8	0.64
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	19	0.63
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD11	15	0.63
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	15	0.63
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	17	0.63
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	15	0.63
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	14	0.63
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	13	0.63
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	16	0.63
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	14	0.63
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	15	0.63
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD12	2	0.63
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD11	12	0.63
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	13	0.63
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	18	0.63
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	19	0.63
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	9	0.63
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG13	2	0.63
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	7	0.63
(1,1575)	1:118:A:THR:H	1:118:A:THR:HG21	11	0.63
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	10	0.63
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG12	10	0.63
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	10	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE2	4	0.63
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	2	0.63
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD12	18	0.63
(1,1424)	1:128:A:LEU:HD21	1:127:A:LEU:HB2	10	0.63
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	12	0.63
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	11	0.63
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	1	0.63
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	8	0.63
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	7	0.63
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	11	0.63
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG12	16	0.63
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	4	0.63
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD11	9	0.63
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	14	0.63
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	16	0.63
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	5	0.63
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	1	0.63
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG23	5	0.63
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD12	18	0.63
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	15	0.63
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD11	10	0.63
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD11	14	0.63
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD23	13	0.63
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	18	0.63
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	11	0.63
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD21	15	0.63
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	19	0.63
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	10	0.63
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD23	5	0.63
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD13	13	0.63
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	20	0.63
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	3	0.63
(2,214)	1:112:A:ASN:HB3	1:111:A:VAL:HA	20	0.62
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD11	6	0.62
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	3	0.62
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	13	0.62
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG21	16	0.62
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	18	0.62
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	20	0.62
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	16	0.62
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	18	0.62
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	9	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	11	0.62
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	11	0.62
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	9	0.62
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	12	0.62
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	13	0.62
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	15	0.62
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	19	0.62
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	10	0.62
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	16	0.62
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	8	0.62
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG21	5	0.62
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	20	0.62
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	4	0.62
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	5	0.62
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG21	4	0.62
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG22	12	0.62
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD12	4	0.62
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	13	0.62
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD13	18	0.62
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	1	0.62
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	8	0.62
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	20	0.62
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG11	18	0.62
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG22	2	0.62
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	2	0.62
(1,1053)	1:173:A:LEU:HB3	1:173:A:LEU:HD12	10	0.62
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	7	0.62
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	1	0.62
(1,745)	1:131:A:THR:HA	1:132:A:GLN:HG3	17	0.62
(1,699)	1:182:A:THR:HB	1:191:A:GLN:HG3	8	0.62
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	14	0.62
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	15	0.62
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD11	17	0.62
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	9	0.62
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	12	0.62
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB2	13	0.62
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB2	15	0.62
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	19	0.62
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	6	0.62
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	12	0.62
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG22	14	0.62
(1,475)	1:116:A:ASP:H	1:182:A:THR:HG23	5	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	4	0.62
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD22	5	0.62
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	19	0.62
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	9	0.62
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	16	0.62
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG21	5	0.62
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	9	0.62
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	17	0.62
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	5	0.62
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	6	0.62
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD13	14	0.62
(2,201)	1:111:A:VAL:HG21	1:127:A:LEU:HB3	3	0.61
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG3	8	0.61
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG11	3	0.61
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	13	0.61
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	4	0.61
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	9	0.61
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	15	0.61
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG21	19	0.61
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	12	0.61
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	4	0.61
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	6	0.61
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	14	0.61
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	11	0.61
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	15	0.61
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	20	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	1	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	3	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	4	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	6	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	8	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	11	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	17	0.61
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	18	0.61
(2,55)	1:123:A:GLU:H	1:124:A:MET:HA	8	0.61
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	13	0.61
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD13	6	0.61
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	18	0.61
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD23	3	0.61
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	9	0.61
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	8	0.61
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG22	19	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	19	0.61
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	8	0.61
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	12	0.61
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD12	1	0.61
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	15	0.61
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	15	0.61
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	4	0.61
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	5	0.61
(1,1420)	1:113:A:LEU:HD22	1:154:A:MET:HG2	8	0.61
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	13	0.61
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	9	0.61
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD13	20	0.61
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	18	0.61
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	13	0.61
(1,1137)	1:189:A:ASN:HB2	1:184:A:VAL:HG13	6	0.61
(1,1029)	1:190:A:ARG:HD2	1:188:A:ASN:HB2	11	0.61
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	18	0.61
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG12	10	0.61
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	11	0.61
(1,746)	1:119:A:ILE:HA	1:117:A:MET:HG3	14	0.61
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	4	0.61
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	11	0.61
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD11	10	0.61
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	2	0.61
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	9	0.61
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG23	11	0.61
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG22	16	0.61
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD11	16	0.61
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD13	18	0.61
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	6	0.61
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	1	0.61
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD11	4	0.61
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD11	16	0.61
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD12	9	0.61
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG13	7	0.61
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	13	0.61
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	20	0.61
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	17	0.61
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	4	0.6
(2,214)	1:112:A:ASN:HB2	1:111:A:VAL:HA	17	0.6
(2,194)	1:180:A:LEU:HD11	1:119:A:ILE:HD11	20	0.6
(2,192)	1:125:A:VAL:HG11	1:109:A:ARG:H	8	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	1	0.6
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	10	0.6
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG23	3	0.6
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	1	0.6
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	12	0.6
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	16	0.6
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	7	0.6
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	10	0.6
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	16	0.6
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG11	14	0.6
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	11	0.6
(1,1735)	1:190:A:ARG:HD2	1:185:A:ASN:HB2	9	0.6
(1,1735)	1:190:A:ARG:HD2	1:185:A:ASN:HB2	15	0.6
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD22	8	0.6
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	1	0.6
(1,1634)	1:195:A:PHE:HE1	1:195:A:PHE:HB2	5	0.6
(1,1623)	1:133:A:TYR:HD1	1:136:A:VAL:HG11	9	0.6
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	2	0.6
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	19	0.6
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	18	0.6
(1,1531)	1:126:A:LYS:HB2	1:126:A:LYS:HE3	3	0.6
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	17	0.6
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD11	4	0.6
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	13	0.6
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG21	2	0.6
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	6	0.6
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG23	16	0.6
(1,1420)	1:113:A:LEU:HD21	1:154:A:MET:HG2	17	0.6
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG22	9	0.6
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	4	0.6
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	3	0.6
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	5	0.6
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD13	14	0.6
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	6	0.6
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	4	0.6
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	17	0.6
(1,1045)	1:180:A:LEU:HB2	1:117:A:MET:HG3	14	0.6
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	10	0.6
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	17	0.6
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	12	0.6
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG22	1	0.6
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG21	7	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:174:A:THR:H	1:174:A:THR:HG21	14	0.6
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG22	3	0.6
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	12	0.6
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	16	0.6
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD12	13	0.6
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	11	0.6
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	7	0.6
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	14	0.6
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	5	0.6
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	6	0.6
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	13	0.6
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	5	0.6
(2,202)	1:184:A:VAL:HG13	1:172:A:ARG:HG2	15	0.59
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	7	0.59
(2,170)	1:110:A:MET:H	1:109:A:ARG:HB3	16	0.59
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG23	9	0.59
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	8	0.59
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG21	8	0.59
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	6	0.59
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD13	14	0.59
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	2	0.59
(2,70)	1:191:A:GLN:H	1:190:A:ARG:H	5	0.59
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	2	0.59
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	4	0.59
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	1	0.59
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	4	0.59
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	3	0.59
(1,1531)	1:126:A:LYS:HB2	1:126:A:LYS:HE3	15	0.59
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	6	0.59
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	5	0.59
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	18	0.59
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG12	19	0.59
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	4	0.59
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD13	12	0.59
(1,1468)	1:152:A:ILE:HG22	1:145:A:PHE:HB3	17	0.59
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG23	13	0.59
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	15	0.59
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG23	1	0.59
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD23	15	0.59
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB3	17	0.59
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG21	6	0.59
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG21	8	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:117:A:MET:H	1:117:A:MET:HG3	17	0.59
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	9	0.59
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	16	0.59
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	14	0.59
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	19	0.59
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	8	0.59
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG21	12	0.59
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	11	0.59
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD11	4	0.59
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG13	8	0.59
(1,761)	1:129:A:GLU:HA	1:129:A:GLU:HG3	14	0.59
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	1	0.59
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB1	7	0.59
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG22	11	0.59
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD23	5	0.59
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	6	0.59
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	20	0.59
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG11	12	0.59
(1,352)	1:172:A:ARG:H	1:169:A:VAL:HG12	13	0.59
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	15	0.59
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG22	3	0.59
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD21	14	0.59
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	6	0.59
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG11	8	0.59
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	12	0.59
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG11	20	0.59
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	4	0.59
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	14	0.59
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	4	0.59
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD12	11	0.58
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG12	18	0.58
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG11	4	0.58
(2,173)	1:124:A:MET:HB3	1:123:A:GLU:HB3	15	0.58
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG23	1	0.58
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG23	16	0.58
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	20	0.58
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	19	0.58
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	16	0.58
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	4	0.58
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	14	0.58
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	8	0.58
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD12	17	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	2	0.58
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	17	0.58
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	9	0.58
(2,52)	1:134:A:ARG:H	1:128:A:LEU:HB3	20	0.58
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	4	0.58
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	9	0.58
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	19	0.58
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD13	2	0.58
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	19	0.58
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD23	4	0.58
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	13	0.58
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	16	0.58
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	12	0.58
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD12	14	0.58
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	20	0.58
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG11	19	0.58
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	2	0.58
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	7	0.58
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	9	0.58
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD12	5	0.58
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	7	0.58
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD12	13	0.58
(1,1475)	1:119:A:ILE:HG22	1:119:A:ILE:HA	14	0.58
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	8	0.58
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	16	0.58
(1,1452)	1:181:A:ALA:HB1	1:180:A:LEU:HD23	17	0.58
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG23	7	0.58
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	12	0.58
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	12	0.58
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	9	0.58
(1,1420)	1:113:A:LEU:HD22	1:154:A:MET:HG2	5	0.58
(1,1406)	1:180:A:LEU:HD12	1:175:A:PHE:HD1	20	0.58
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD12	5	0.58
(1,1397)	1:125:A:VAL:HG12	1:122:A:ASN:HB3	10	0.58
(1,1397)	1:125:A:VAL:HG11	1:122:A:ASN:HB3	19	0.58
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	4	0.58
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD13	11	0.58
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG23	18	0.58
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	2	0.58
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	7	0.58
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	13	0.58
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	7	0.58

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	12	0.58
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD23	20	0.58
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	1	0.58
(1,926)	1:173:A:LEU:HA	1:180:A:LEU:HD13	2	0.58
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	19	0.58
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	2	0.58
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	15	0.58
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	2	0.58
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	11	0.58
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	20	0.58
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD12	14	0.58
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD13	9	0.58
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	6	0.58
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	6	0.58
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	15	0.58
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	5	0.58
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD11	18	0.58
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	17	0.58
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG22	20	0.58
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	2	0.58
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	3	0.58
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	1	0.58
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	4	0.58
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	9	0.58
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD23	10	0.58
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE2	10	0.58
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	17	0.58
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	15	0.58
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	13	0.57
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	5	0.57
(2,143)	1:138:A:LYS:HE3	1:138:A:LYS:HG3	5	0.57
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	11	0.57
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	15	0.57
(2,143)	1:138:A:LYS:HE3	1:138:A:LYS:HG3	18	0.57
(2,143)	1:138:A:LYS:HE3	1:138:A:LYS:HG3	20	0.57
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	8	0.57
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	11	0.57
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG2	20	0.57
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	3	0.57
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	1	0.57
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	16	0.57
(2,85)	1:145:A:PHE:H	1:141:A:ARG:HG2	10	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	17	0.57
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	20	0.57
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	18	0.57
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	12	0.57
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	19	0.57
(1,1734)	1:195:A:PHE:HD1	1:195:A:PHE:HB2	5	0.57
(1,1701)	1:133:A:TYR:HE1	1:134:A:ARG:H	1	0.57
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	12	0.57
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD23	15	0.57
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	18	0.57
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG13	7	0.57
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	11	0.57
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	14	0.57
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD13	15	0.57
(1,1468)	1:152:A:ILE:HG23	1:145:A:PHE:HB3	11	0.57
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	4	0.57
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG22	20	0.57
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG21	3	0.57
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	20	0.57
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	1	0.57
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	14	0.57
(1,1431)	1:146:A:THR:HG23	1:139:A:MET:HE2	13	0.57
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG22	8	0.57
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	12	0.57
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	5	0.57
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	5	0.57
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	2	0.57
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	8	0.57
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD12	10	0.57
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG21	16	0.57
(1,1241)	1:117:A:MET:H	1:117:A:MET:HG3	14	0.57
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	3	0.57
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	4	0.57
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG11	14	0.57
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	17	0.57
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	2	0.57
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	7	0.57
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	11	0.57
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	15	0.57
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	14	0.57
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	1	0.57
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	7	0.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD12	2	0.57
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG23	7	0.57
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD13	4	0.57
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD11	18	0.57
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG13	6	0.57
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG12	19	0.57
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	3	0.57
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD12	20	0.57
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	7	0.57
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG23	20	0.57
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	11	0.57
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	13	0.57
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	18	0.57
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD11	12	0.57
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	4	0.57
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD21	3	0.57
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	3	0.57
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD21	20	0.57
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	15	0.57
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE2	19	0.57
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD13	12	0.57
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	3	0.57
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD3	15	0.56
(2,218)	1:115:A:PRO:HB3	1:115:A:PRO:HD3	20	0.56
(2,201)	1:111:A:VAL:HG12	1:130:A:ALA:HB3	11	0.56
(2,192)	1:125:A:VAL:HG12	1:109:A:ARG:H	1	0.56
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	12	0.56
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	6	0.56
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	7	0.56
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HB3	14	0.56
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	3	0.56
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	2	0.56
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	17	0.56
(2,38)	1:176:A:ASP:H	1:179:A:HIS:HB3	14	0.56
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD13	17	0.56
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD22	11	0.56
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	1	0.56
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG22	14	0.56
(1,1648)	1:195:A:PHE:HE1	1:183:A:ILE:HG22	19	0.56
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	16	0.56
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	13	0.56
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD13	10	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG21	9	0.56
(1,1531)	1:126:A:LYS:HB2	1:126:A:LYS:HE3	7	0.56
(1,1490)	1:119:A:ILE:HD13	1:119:A:ILE:HA	16	0.56
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE2	5	0.56
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	1	0.56
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	16	0.56
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG21	13	0.56
(1,1461)	1:183:A:ILE:HG21	1:183:A:ILE:HG13	20	0.56
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	6	0.56
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	7	0.56
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	8	0.56
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG23	5	0.56
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG22	11	0.56
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	8	0.56
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	11	0.56
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG23	20	0.56
(1,1366)	1:173:A:LEU:HD13	1:171:A:ALA:HB1	10	0.56
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE2	7	0.56
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	8	0.56
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD21	4	0.56
(1,1188)	1:117:A:MET:HB2	1:180:A:LEU:HD23	18	0.56
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG22	13	0.56
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG23	9	0.56
(1,1019)	1:196:A:ARG:HD2	1:195:A:PHE:HB2	6	0.56
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	16	0.56
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	19	0.56
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	5	0.56
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	17	0.56
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD13	5	0.56
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG23	4	0.56
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	10	0.56
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD12	13	0.56
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG11	15	0.56
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG22	10	0.56
(1,537)	1:122:A:ASN:H	1:121:A:LYS:HB2	14	0.56
(1,528)	1:145:A:PHE:H	1:136:A:VAL:HG21	3	0.56
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	13	0.56
(1,450)	1:174:A:THR:H	1:174:A:THR:HG21	5	0.56
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG23	4	0.56
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG23	12	0.56
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG22	18	0.56
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD13	12	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	17	0.56
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG21	6	0.56
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	12	0.56
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG22	17	0.56
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG13	8	0.56
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	2	0.56
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	2	0.56
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	9	0.56
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	16	0.56
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD11	6	0.56
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD11	14	0.56
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	18	0.56
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	5	0.56
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	7	0.56
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	2	0.55
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	6	0.55
(2,197)	1:184:A:VAL:HG22	1:172:A:ARG:HG2	2	0.55
(2,194)	1:180:A:LEU:HD12	1:119:A:ILE:HD13	3	0.55
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG11	10	0.55
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG11	16	0.55
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	14	0.55
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	18	0.55
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	6	0.55
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	14	0.55
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	12	0.55
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	4	0.55
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	17	0.55
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	20	0.55
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	10	0.55
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	5	0.55
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	11	0.55
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	15	0.55
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	6	0.55
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	8	0.55
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD13	19	0.55
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	5	0.55
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	7	0.55
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	11	0.55
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	20	0.55
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	15	0.55
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	4	0.55
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	3	0.55

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	15	0.55
(1,1485)	1:183:A:ILE:HD12	1:115:A:PRO:HA	5	0.55
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	20	0.55
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	9	0.55
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG13	14	0.55
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD11	16	0.55
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	4	0.55
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	20	0.55
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	10	0.55
(1,1371)	1:128:A:LEU:H	1:128:A:LEU:HD11	15	0.55
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG23	3	0.55
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	10	0.55
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	15	0.55
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	20	0.55
(1,1105)	1:128:A:LEU:HB3	1:127:A:LEU:HD21	3	0.55
(1,1007)	1:167:A:GLY:HA2	1:168:A:GLN:HB2	19	0.55
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	3	0.55
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	8	0.55
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD12	4	0.55
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD12	13	0.55
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG21	9	0.55
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD11	11	0.55
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	17	0.55
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	7	0.55
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	10	0.55
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG21	1	0.55
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	19	0.55
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	20	0.55
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD13	2	0.55
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	1	0.55
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	4	0.55
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG11	7	0.55
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	10	0.55
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	14	0.55
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	19	0.55
(1,84)	1:186:A:MET:H	1:171:A:ALA:HB3	9	0.55
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	1	0.55
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	2	0.55
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD13	5	0.55
(2,202)	1:184:A:VAL:HG11	1:172:A:ARG:HG2	12	0.54
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG12	6	0.54
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	17	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	9	0.54
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	10	0.54
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	17	0.54
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	15	0.54
(2,133)	1:167:A:GLY:HA2	1:168:A:GLN:HG2	19	0.54
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE3	6	0.54
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HG3	3	0.54
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	9	0.54
(2,54)	1:129:A:GLU:H	1:129:A:GLU:HG2	11	0.54
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	20	0.54
(2,34)	1:166:A:GLU:H	1:159:A:PHE:HB2	5	0.54
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD12	8	0.54
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	6	0.54
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	5	0.54
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	7	0.54
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	16	0.54
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	1	0.54
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD23	14	0.54
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	17	0.54
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	14	0.54
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	2	0.54
(1,1623)	1:133:A:TYR:HD1	1:136:A:VAL:HG13	4	0.54
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	3	0.54
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	13	0.54
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	16	0.54
(1,1531)	1:126:A:LYS:HB2	1:126:A:LYS:HE3	17	0.54
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	5	0.54
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG11	12	0.54
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG13	3	0.54
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE1	13	0.54
(1,1469)	1:128:A:LEU:HD22	1:152:A:ILE:HG21	2	0.54
(1,1462)	1:195:A:PHE:HD1	1:183:A:ILE:HG23	12	0.54
(1,1461)	1:183:A:ILE:HG21	1:183:A:ILE:HG13	15	0.54
(1,1461)	1:183:A:ILE:HG23	1:183:A:ILE:HG13	19	0.54
(1,1459)	1:183:A:ILE:HG23	1:172:A:ARG:HB3	13	0.54
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	8	0.54
(1,1454)	1:130:A:ALA:HB1	1:128:A:LEU:H	3	0.54
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	10	0.54
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	13	0.54
(1,1454)	1:130:A:ALA:HB1	1:128:A:LEU:H	18	0.54
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG21	4	0.54
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG23	18	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	16	0.54
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG13	17	0.54
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	19	0.54
(1,1424)	1:128:A:LEU:HD21	1:127:A:LEU:HB2	3	0.54
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB3	8	0.54
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	5	0.54
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	6	0.54
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	13	0.54
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	14	0.54
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	17	0.54
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	20	0.54
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	1	0.54
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	5	0.54
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	16	0.54
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	13	0.54
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG21	13	0.54
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	19	0.54
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG11	5	0.54
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG12	12	0.54
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG13	16	0.54
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	11	0.54
(1,579)	1:179:A:HIS:H	1:181:A:ALA:HB3	2	0.54
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	4	0.54
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	6	0.54
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD13	2	0.54
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD13	15	0.54
(1,450)	1:174:A:THR:H	1:174:A:THR:HG23	9	0.54
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	20	0.54
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	8	0.54
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	9	0.54
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	1	0.54
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	15	0.54
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	4	0.54
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	8	0.54
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	11	0.54
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD11	13	0.54
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG21	5	0.54
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG21	10	0.54
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG23	12	0.54
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	2	0.54
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD12	3	0.54
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD11	11	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	2	0.54
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG23	4	0.54
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG22	11	0.54
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	1	0.54
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	13	0.54
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	19	0.54
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	7	0.54
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	8	0.54
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	2	0.54
(2,202)	1:184:A:VAL:HG13	1:172:A:ARG:HG2	6	0.53
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	16	0.53
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	5	0.53
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	10	0.53
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	15	0.53
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	6	0.53
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	1	0.53
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	9	0.53
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	20	0.53
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	10	0.53
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	13	0.53
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	19	0.53
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB3	15	0.53
(2,52)	1:134:A:ARG:H	1:128:A:LEU:HB3	11	0.53
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	12	0.53
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	15	0.53
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	19	0.53
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD13	11	0.53
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD11	16	0.53
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	3	0.53
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	12	0.53
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	14	0.53
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	7	0.53
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	14	0.53
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	9	0.53
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	3	0.53
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	4	0.53
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	7	0.53
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	10	0.53
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	15	0.53
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	2	0.53
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	11	0.53
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG23	2	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG22	12	0.53
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG12	6	0.53
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	17	0.53
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	18	0.53
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	20	0.53
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	3	0.53
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	1	0.53
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	5	0.53
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD13	6	0.53
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG21	7	0.53
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG23	17	0.53
(1,1461)	1:183:A:ILE:HG23	1:183:A:ILE:HG13	1	0.53
(1,1461)	1:183:A:ILE:HG21	1:183:A:ILE:HG13	12	0.53
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	11	0.53
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG22	14	0.53
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	4	0.53
(1,1454)	1:130:A:ALA:HB1	1:128:A:LEU:H	9	0.53
(1,1454)	1:130:A:ALA:HB1	1:128:A:LEU:H	15	0.53
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG23	2	0.53
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG22	9	0.53
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	7	0.53
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	16	0.53
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG22	7	0.53
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG23	11	0.53
(1,1424)	1:128:A:LEU:HD21	1:127:A:LEU:HB2	16	0.53
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	17	0.53
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE1	1	0.53
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	1	0.53
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	8	0.53
(1,1150)	1:192:A:PHE:HE2	1:185:A:ASN:HB2	11	0.53
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	2	0.53
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG23	20	0.53
(1,1045)	1:180:A:LEU:HB2	1:117:A:MET:HG3	17	0.53
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD12	14	0.53
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	15	0.53
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD13	15	0.53
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD2	10	0.53
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	12	0.53
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG21	2	0.53
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG21	13	0.53
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	4	0.53
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD21	12	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD13	17	0.53
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	16	0.53
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD13	19	0.53
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	16	0.53
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	10	0.53
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD12	11	0.53
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG23	1	0.53
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD11	19	0.53
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	10	0.53
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD13	7	0.53
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG11	3	0.53
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	9	0.53
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	11	0.53
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	16	0.53
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	4	0.53
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	18	0.52
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HG2	2	0.52
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HG2	6	0.52
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	4	0.52
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	2	0.52
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	2	0.52
(2,143)	1:138:A:LYS:HE3	1:138:A:LYS:HG3	16	0.52
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE1	10	0.52
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE1	18	0.52
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	12	0.52
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	19	0.52
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	1	0.52
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	8	0.52
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	16	0.52
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	4	0.52
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG12	10	0.52
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	15	0.52
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD13	8	0.52
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD11	10	0.52
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	6	0.52
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	19	0.52
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	3	0.52
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	16	0.52
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	3	0.52
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	7	0.52
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	3	0.52
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD13	5	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	9	0.52
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	15	0.52
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD23	20	0.52
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	2	0.52
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	4	0.52
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	15	0.52
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	12	0.52
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	16	0.52
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	9	0.52
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	5	0.52
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	4	0.52
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD23	14	0.52
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	15	0.52
(1,1585)	1:136:A:VAL:HG21	1:136:A:VAL:HG11	19	0.52
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	10	0.52
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	8	0.52
(1,1490)	1:119:A:ILE:HD11	1:119:A:ILE:HA	17	0.52
(1,1485)	1:183:A:ILE:HD12	1:115:A:PRO:HA	20	0.52
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	12	0.52
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	17	0.52
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	19	0.52
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	20	0.52
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG22	6	0.52
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	13	0.52
(1,1392)	1:197:A:LEU:HD22	1:195:A:PHE:HE1	5	0.52
(1,1231)	1:186:A:MET:HB3	1:170:A:ARG:HD2	17	0.52
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	3	0.52
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	4	0.52
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	13	0.52
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	3	0.52
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	4	0.52
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	9	0.52
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB2	15	0.52
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB2	19	0.52
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	20	0.52
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD2	4	0.52
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD2	8	0.52
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	2	0.52
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG21	18	0.52
(1,776)	1:136:A:VAL:HA	1:136:A:VAL:HG11	10	0.52
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	3	0.52
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	10	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	15	0.52
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD21	7	0.52
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD23	15	0.52
(1,450)	1:174:A:THR:H	1:174:A:THR:HG23	13	0.52
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	14	0.52
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	7	0.52
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG23	9	0.52
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD13	15	0.52
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	1	0.52
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG21	7	0.52
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG11	2	0.52
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	16	0.52
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG13	17	0.52
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	18	0.52
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	5	0.52
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	20	0.52
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	17	0.51
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	7	0.51
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG23	6	0.51
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	11	0.51
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	13	0.51
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	3	0.51
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	13	0.51
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	13	0.51
(2,133)	1:167:A:GLY:HA2	1:166:A:GLU:HG3	16	0.51
(2,110)	1:126:A:LYS:HA	1:109:A:ARG:HA	18	0.51
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	11	0.51
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	7	0.51
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	7	0.51
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	14	0.51
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	8	0.51
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	11	0.51
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	10	0.51
(1,1655)	1:195:A:PHE:HZ	1:156:A:ARG:HD2	5	0.51
(1,1623)	1:133:A:TYR:HD1	1:136:A:VAL:HG11	1	0.51
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG22	15	0.51
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG12	8	0.51
(1,1531)	1:126:A:LYS:HB2	1:126:A:LYS:HE3	8	0.51
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	16	0.51
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	11	0.51
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	6	0.51
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	15	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG23	13	0.51
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	16	0.51
(1,1485)	1:183:A:ILE:HD13	1:115:A:PRO:HA	2	0.51
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD2	6	0.51
(1,1483)	1:183:A:ILE:HD11	1:195:A:PHE:HD1	14	0.51
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD11	17	0.51
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD11	20	0.51
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG23	2	0.51
(1,1459)	1:183:A:ILE:HG23	1:172:A:ARG:HB3	7	0.51
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	6	0.51
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	11	0.51
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG23	13	0.51
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	18	0.51
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	13	0.51
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD22	15	0.51
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB2	15	0.51
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	17	0.51
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	11	0.51
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	2	0.51
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	9	0.51
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	12	0.51
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	18	0.51
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG22	17	0.51
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	9	0.51
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	13	0.51
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG13	3	0.51
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	9	0.51
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	12	0.51
(1,890)	1:135:A:GLN:HA	1:136:A:VAL:HG13	4	0.51
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	19	0.51
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	11	0.51
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	20	0.51
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	11	0.51
(1,796)	1:186:A:MET:HA	1:186:A:MET:HG2	18	0.51
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD12	14	0.51
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	8	0.51
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG22	4	0.51
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG22	5	0.51
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	3	0.51
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	20	0.51
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG22	13	0.51
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	11	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD12	17	0.51
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG21	16	0.51
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD13	12	0.51
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	6	0.51
(1,136)	1:157:A:ARG:H	1:156:A:ARG:HG3	1	0.51
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	6	0.51
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	15	0.51
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	8	0.51
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	9	0.51
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	12	0.51
(2,202)	1:184:A:VAL:HG11	1:172:A:ARG:HG2	4	0.5
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG11	5	0.5
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG12	14	0.5
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	20	0.5
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	17	0.5
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	10	0.5
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	15	0.5
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	19	0.5
(2,143)	1:138:A:LYS:HE2	1:138:A:LYS:HG3	3	0.5
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	10	0.5
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	14	0.5
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	13	0.5
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	3	0.5
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	3	0.5
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	5	0.5
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	12	0.5
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	14	0.5
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	5	0.5
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	9	0.5
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	18	0.5
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	10	0.5
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	3	0.5
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	13	0.5
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	13	0.5
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	1	0.5
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD12	3	0.5
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG21	1	0.5
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG21	11	0.5
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	10	0.5
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG23	19	0.5
(1,1483)	1:183:A:ILE:HD11	1:195:A:PHE:HD1	3	0.5
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	17	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG23	15	0.5
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG23	18	0.5
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG23	10	0.5
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG22	14	0.5
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG22	3	0.5
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	17	0.5
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB3	16	0.5
(1,1241)	1:117:A:MET:H	1:117:A:MET:HG3	10	0.5
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	15	0.5
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG22	10	0.5
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	19	0.5
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	7	0.5
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	16	0.5
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG13	5	0.5
(1,1018)	1:170:A:ARG:HD3	1:155:A:ILE:HD12	12	0.5
(1,985)	1:177:A:GLY:HA2	1:178:A:ASP:HB2	12	0.5
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	18	0.5
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG12	9	0.5
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	6	0.5
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	16	0.5
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG21	17	0.5
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	2	0.5
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	19	0.5
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	2	0.5
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	3	0.5
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD11	19	0.5
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG21	17	0.5
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	9	0.5
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD2	11	0.5
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG22	15	0.5
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	11	0.5
(1,81)	1:186:A:MET:H	1:186:A:MET:HE3	9	0.5
(1,72)	1:139:A:MET:H	1:139:A:MET:HE3	7	0.5
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	15	0.5
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HG2	16	0.49
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	4	0.49
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG23	7	0.49
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	8	0.49
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	11	0.49
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	1	0.49
(2,143)	1:138:A:LYS:HE3	1:138:A:LYS:HG3	6	0.49
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE1	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HG3	13	0.49
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	19	0.49
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	8	0.49
(2,56)	1:110:A:MET:H	1:109:A:ARG:HB3	9	0.49
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	10	0.49
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	16	0.49
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	14	0.49
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	20	0.49
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	18	0.49
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	16	0.49
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	17	0.49
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG22	17	0.49
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG22	20	0.49
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	9	0.49
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	18	0.49
(1,1487)	1:183:A:ILE:HD13	1:183:A:ILE:HB	8	0.49
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD13	7	0.49
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD1	2	0.49
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	18	0.49
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	9	0.49
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	14	0.49
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG22	12	0.49
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG21	9	0.49
(1,1397)	1:125:A:VAL:HG13	1:122:A:ASN:HB3	6	0.49
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD22	10	0.49
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	4	0.49
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB3	4	0.49
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	4	0.49
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE1	17	0.49
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	4	0.49
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	11	0.49
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG12	16	0.49
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	7	0.49
(1,1140)	1:189:A:ASN:HB3	1:184:A:VAL:HG13	11	0.49
(1,1049)	1:156:A:ARG:HD3	1:197:A:LEU:HA	13	0.49
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	16	0.49
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	5	0.49
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	3	0.49
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	10	0.49
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG23	11	0.49
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG23	15	0.49
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	7	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	16	0.49
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD12	7	0.49
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	8	0.49
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	11	0.49
(1,614)	1:132:A:GLN:H	1:132:A:GLN:HG3	9	0.49
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	9	0.49
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	11	0.49
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	2	0.49
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	20	0.49
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	9	0.49
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	18	0.49
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG23	13	0.49
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	6	0.49
(1,229)	1:200:A:ARG:H	1:200:A:ARG:HG2	20	0.49
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD2	3	0.49
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	18	0.49
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG21	8	0.49
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	1	0.49
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	12	0.49
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD11	20	0.49
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	9	0.49
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	13	0.49
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HG2	3	0.48
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG22	8	0.48
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG23	19	0.48
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	4	0.48
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	5	0.48
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG21	14	0.48
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	5	0.48
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB2	10	0.48
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD23	10	0.48
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD22	13	0.48
(2,105)	1:115:A:PRO:HA	1:181:A:ALA:HA	5	0.48
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	6	0.48
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	9	0.48
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG12	18	0.48
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG12	2	0.48
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	14	0.48
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	16	0.48
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD11	19	0.48
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	9	0.48
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	7	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	11	0.48
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	13	0.48
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD13	15	0.48
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	18	0.48
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG22	18	0.48
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	20	0.48
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	5	0.48
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	1	0.48
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	13	0.48
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	5	0.48
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG13	17	0.48
(1,1487)	1:183:A:ILE:HD11	1:183:A:ILE:HB	14	0.48
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD13	12	0.48
(1,1463)	1:183:A:ILE:HG23	1:195:A:PHE:HB3	6	0.48
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG23	19	0.48
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	1	0.48
(1,1454)	1:130:A:ALA:HB3	1:128:A:LEU:H	2	0.48
(1,1454)	1:130:A:ALA:HB2	1:128:A:LEU:H	5	0.48
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG22	19	0.48
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	18	0.48
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	11	0.48
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	17	0.48
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	19	0.48
(1,1403)	1:180:A:LEU:HD11	1:183:A:ILE:HD11	6	0.48
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG22	18	0.48
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	10	0.48
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	18	0.48
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG23	3	0.48
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG22	5	0.48
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD13	6	0.48
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	14	0.48
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG21	5	0.48
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	14	0.48
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	9	0.48
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	3	0.48
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	19	0.48
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD11	12	0.48
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD23	1	0.48
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD22	17	0.48
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	5	0.48
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	7	0.48
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	16	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	14	0.48
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD13	11	0.48
(1,424)	1:190:A:ARG:H	1:185:A:ASN:HB3	2	0.48
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	8	0.48
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD22	10	0.48
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	1	0.48
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD13	8	0.48
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	8	0.48
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD11	20	0.48
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	19	0.48
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	10	0.48
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD11	3	0.48
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	7	0.48
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	19	0.48
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	2	0.48
(2,192)	1:110:A:MET:H	1:125:A:VAL:HG13	9	0.47
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	18	0.47
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	16	0.47
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	14	0.47
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	20	0.47
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	12	0.47
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	5	0.47
(2,93)	1:188:A:ASN:H	1:190:A:ARG:HB3	2	0.47
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD13	19	0.47
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	13	0.47
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	4	0.47
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	18	0.47
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG12	7	0.47
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	12	0.47
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	10	0.47
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	20	0.47
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD13	15	0.47
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	12	0.47
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	17	0.47
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD11	10	0.47
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG11	20	0.47
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	15	0.47
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	15	0.47
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	4	0.47
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	15	0.47
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD12	1	0.47
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD11	19	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG23	4	0.47
(1,1461)	1:183:A:ILE:HG21	1:183:A:ILE:HG13	2	0.47
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG23	1	0.47
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	17	0.47
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	8	0.47
(1,1433)	1:191:A:GLN:HG3	1:184:A:VAL:HG23	10	0.47
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG23	6	0.47
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG23	18	0.47
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB3	18	0.47
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	5	0.47
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	20	0.47
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	4	0.47
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	12	0.47
(1,1183)	1:191:A:GLN:H	1:191:A:GLN:HG2	17	0.47
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	8	0.47
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD23	16	0.47
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD13	8	0.47
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	8	0.47
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	2	0.47
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB1	10	0.47
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB1	12	0.47
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD12	20	0.47
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD12	1	0.47
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD11	20	0.47
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	9	0.47
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD11	16	0.47
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD12	16	0.47
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	12	0.47
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD13	5	0.47
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD12	18	0.47
(1,450)	1:174:A:THR:H	1:174:A:THR:HG21	6	0.47
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	19	0.47
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	8	0.47
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	2	0.47
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD12	14	0.47
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD12	14	0.47
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	12	0.47
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG22	17	0.47
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD13	17	0.47
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	20	0.47
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	6	0.47
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	10	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	14	0.46
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	2	0.46
(2,170)	1:110:A:MET:H	1:109:A:ARG:HB3	9	0.46
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	20	0.46
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG23	17	0.46
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	6	0.46
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	7	0.46
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	15	0.46
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	18	0.46
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	7	0.46
(2,145)	1:194:A:PHE:HB3	1:114:A:GLU:HG3	6	0.46
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	13	0.46
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	20	0.46
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE1	14	0.46
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	7	0.46
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG13	8	0.46
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD12	3	0.46
(2,62)	1:120:A:SER:H	1:123:A:GLU:HA	17	0.46
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	1	0.46
(2,51)	1:136:A:VAL:H	1:144:A:GLU:HA	7	0.46
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	1	0.46
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB2	20	0.46
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD12	18	0.46
(1,1735)	1:190:A:ARG:HD2	1:185:A:ASN:HB2	2	0.46
(1,1701)	1:133:A:TYR:HE2	1:134:A:ARG:H	6	0.46
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD22	2	0.46
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD22	12	0.46
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	9	0.46
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	8	0.46
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	18	0.46
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	7	0.46
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD11	1	0.46
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	13	0.46
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	10	0.46
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	17	0.46
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	5	0.46
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG11	11	0.46
(1,1527)	1:117:A:MET:HG3	1:180:A:LEU:HD23	2	0.46
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	20	0.46
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	3	0.46
(1,1487)	1:183:A:ILE:HD11	1:183:A:ILE:HB	3	0.46
(1,1487)	1:183:A:ILE:HD13	1:183:A:ILE:HB	16	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1479)	1:152:A:ILE:HD12	1:175:A:PHE:HE1	17	0.46
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	6	0.46
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	9	0.46
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	18	0.46
(1,1420)	1:113:A:LEU:HD22	1:154:A:MET:HG2	11	0.46
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE3	19	0.46
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	6	0.46
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	9	0.46
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	12	0.46
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	14	0.46
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG22	16	0.46
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG22	7	0.46
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	20	0.46
(1,1045)	1:180:A:LEU:HB2	1:117:A:MET:HG3	10	0.46
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	7	0.46
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	4	0.46
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	3	0.46
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	1	0.46
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	10	0.46
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	15	0.46
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	17	0.46
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD12	10	0.46
(1,797)	1:175:A:PHE:HA	1:175:A:PHE:HD2	8	0.46
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	2	0.46
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	3	0.46
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	5	0.46
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	2	0.46
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	6	0.46
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG22	11	0.46
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	10	0.46
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	15	0.46
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	14	0.46
(1,407)	1:168:A:GLN:H	1:158:A:PRO:HD2	12	0.46
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	7	0.46
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD12	10	0.46
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	7	0.46
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG21	14	0.46
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	16	0.46
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG23	18	0.46
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG23	2	0.46
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG12	1	0.46
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	15	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG12	6	0.46
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	8	0.46
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	10	0.46
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD13	8	0.46
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	1	0.46
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	5	0.46
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE2	13	0.46
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	11	0.45
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	12	0.45
(2,175)	1:119:A:ILE:HA	1:123:A:GLU:HB3	3	0.45
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	17	0.45
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	12	0.45
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB2	4	0.45
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	19	0.45
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	20	0.45
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	13	0.45
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	20	0.45
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD13	8	0.45
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD11	10	0.45
(1,1694)	1:111:A:VAL:HA	1:111:A:VAL:HG23	3	0.45
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	18	0.45
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	17	0.45
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	16	0.45
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	3	0.45
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	14	0.45
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	10	0.45
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	2	0.45
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG11	4	0.45
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	2	0.45
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	9	0.45
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	12	0.45
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	13	0.45
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB2	3	0.45
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	19	0.45
(1,1487)	1:183:A:ILE:HD13	1:183:A:ILE:HB	18	0.45
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	15	0.45
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	18	0.45
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	8	0.45
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD21	10	0.45
(1,1474)	1:119:A:ILE:HG21	1:175:A:PHE:HD1	18	0.45
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	4	0.45
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	17	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	16	0.45
(1,1451)	1:181:A:ALA:HB3	1:182:A:THR:HG21	8	0.45
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	11	0.45
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB1	8	0.45
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD22	11	0.45
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	13	0.45
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	17	0.45
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	10	0.45
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	17	0.45
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	5	0.45
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	3	0.45
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	3	0.45
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	4	0.45
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	14	0.45
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB1	2	0.45
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB2	4	0.45
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB1	18	0.45
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	20	0.45
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	9	0.45
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	15	0.45
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	8	0.45
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	18	0.45
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	1	0.45
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	19	0.45
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	3	0.45
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	9	0.45
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	16	0.45
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD11	19	0.45
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	15	0.45
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	11	0.45
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	16	0.45
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	5	0.45
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	8	0.45
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	11	0.45
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	15	0.45
(1,336)	1:110:A:MET:H	1:111:A:VAL:HG23	3	0.45
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG22	10	0.45
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	5	0.45
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	12	0.45
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG11	5	0.45
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG13	20	0.45
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	1	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE3	11	0.45
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	19	0.45
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	18	0.45
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	19	0.45
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	9	0.44
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	15	0.44
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG13	19	0.44
(2,199)	1:140:A:THR:HG22	1:138:A:LYS:HG2	10	0.44
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	10	0.44
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG21	20	0.44
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	11	0.44
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	3	0.44
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	20	0.44
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	2	0.44
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	7	0.44
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	18	0.44
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	8	0.44
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	6	0.44
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	10	0.44
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	14	0.44
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	16	0.44
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	20	0.44
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD12	11	0.44
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	15	0.44
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD11	17	0.44
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	3	0.44
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	5	0.44
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	13	0.44
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	20	0.44
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	11	0.44
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD23	1	0.44
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD23	11	0.44
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	9	0.44
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	1	0.44
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	6	0.44
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	15	0.44
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	18	0.44
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	13	0.44
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	8	0.44
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	14	0.44
(1,1487)	1:183:A:ILE:HD13	1:183:A:ILE:HB	10	0.44
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD13	11	0.44
(1,1463)	1:183:A:ILE:HG23	1:195:A:PHE:HB3	2	0.44
(1,1451)	1:181:A:ALA:HB2	1:182:A:THR:HG23	16	0.44
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD11	1	0.44
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	1	0.44
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD23	9	0.44
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	2	0.44
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	3	0.44
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE1	12	0.44
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	13	0.44
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	19	0.44
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	6	0.44
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG22	14	0.44
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	20	0.44
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	14	0.44
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	17	0.44
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	17	0.44
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	6	0.44
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD12	14	0.44
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD13	16	0.44
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	20	0.44
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	8	0.44
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	17	0.44
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	2	0.44
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	20	0.44
(1,678)	1:124:A:MET:H	1:120:A:SER:H	14	0.44
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	8	0.44
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD12	5	0.44
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	4	0.44
(1,450)	1:174:A:THR:H	1:174:A:THR:HG22	8	0.44
(1,450)	1:174:A:THR:H	1:174:A:THR:HG21	17	0.44
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	1	0.44
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	6	0.44
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	12	0.44
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD13	15	0.44
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	12	0.44
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	8	0.44
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG22	4	0.44
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	14	0.44
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	8	0.44
(1,256)	1:192:A:PHE:H	1:184:A:VAL:HG13	2	0.44
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	16	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD13	4	0.44
(1,5)	1:170:A:ARG:H	1:186:A:MET:HE3	14	0.44
(2,175)	1:119:A:ILE:HA	1:123:A:GLU:HB3	20	0.43
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	5	0.43
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	13	0.43
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	10	0.43
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB2	3	0.43
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	13	0.43
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	12	0.43
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	19	0.43
(2,86)	1:164:A:SER:H	1:164:A:SER:HB3	9	0.43
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	18	0.43
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	19	0.43
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG12	3	0.43
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	4	0.43
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	7	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	1	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	3	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	6	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	7	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	8	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	9	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	12	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	15	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	16	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	17	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	18	0.43
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	20	0.43
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	5	0.43
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	3	0.43
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	15	0.43
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	1	0.43
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD21	10	0.43
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD13	19	0.43
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD13	10	0.43
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG22	6	0.43
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG22	10	0.43
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	8	0.43
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	14	0.43
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	9	0.43
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	4	0.43
(1,1562)	1:173:A:LEU:HD12	1:174:A:THR:H	12	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	8	0.43
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG12	14	0.43
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	14	0.43
(1,1490)	1:119:A:ILE:HD11	1:119:A:ILE:HA	13	0.43
(1,1487)	1:183:A:ILE:HD12	1:183:A:ILE:HB	9	0.43
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	10	0.43
(1,1481)	1:152:A:ILE:HD13	1:128:A:LEU:HD21	5	0.43
(1,1468)	1:152:A:ILE:HG21	1:145:A:PHE:HB3	14	0.43
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG23	10	0.43
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	5	0.43
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD11	15	0.43
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	15	0.43
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	10	0.43
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	1	0.43
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	2	0.43
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	10	0.43
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	16	0.43
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	19	0.43
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	7	0.43
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	8	0.43
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	15	0.43
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	17	0.43
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	9	0.43
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG23	17	0.43
(1,1029)	1:190:A:ARG:HD2	1:188:A:ASN:HB2	2	0.43
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	17	0.43
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	3	0.43
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD22	7	0.43
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG23	19	0.43
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	7	0.43
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD2	20	0.43
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	5	0.43
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	10	0.43
(1,678)	1:124:A:MET:H	1:120:A:SER:H	5	0.43
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	10	0.43
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	12	0.43
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	18	0.43
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	18	0.43
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	6	0.43
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB3	3	0.43
(1,450)	1:174:A:THR:H	1:174:A:THR:HG21	1	0.43
(1,450)	1:174:A:THR:H	1:174:A:THR:HG21	10	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	7	0.43
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	12	0.43
(1,424)	1:190:A:ARG:H	1:185:A:ASN:HB3	11	0.43
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	1	0.43
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	3	0.43
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	18	0.43
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	20	0.43
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	17	0.43
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	3	0.43
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	20	0.43
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD2	2	0.43
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	19	0.43
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB3	12	0.43
(1,95)	1:184:A:VAL:H	1:184:A:VAL:HG12	11	0.43
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	3	0.43
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	15	0.43
(2,194)	1:180:A:LEU:HD13	1:119:A:ILE:HD13	7	0.42
(2,173)	1:124:A:MET:HB3	1:123:A:GLU:HB3	18	0.42
(2,168)	1:139:A:MET:HG2	1:146:A:THR:HG22	11	0.42
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	7	0.42
(2,157)	1:122:A:ASN:HB3	1:125:A:VAL:HB	14	0.42
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	5	0.42
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	5	0.42
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE1	2	0.42
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	11	0.42
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	13	0.42
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	20	0.42
(2,66)	1:168:A:GLN:H	1:142:A:PRO:HA	5	0.42
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG12	5	0.42
(2,52)	1:134:A:ARG:H	1:128:A:LEU:HB3	18	0.42
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG22	19	0.42
(2,38)	1:176:A:ASP:H	1:179:A:HIS:HB3	10	0.42
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	12	0.42
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG22	5	0.42
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	19	0.42
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	2	0.42
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	4	0.42
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	10	0.42
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	11	0.42
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	14	0.42
(1,1682)	1:162:A:PRO:HA	1:162:A:PRO:HB2	19	0.42
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	6	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD22	10	0.42
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	19	0.42
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG13	11	0.42
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG13	13	0.42
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	18	0.42
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG21	19	0.42
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG11	17	0.42
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB2	4	0.42
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	4	0.42
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	20	0.42
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	16	0.42
(1,1485)	1:183:A:ILE:HD12	1:115:A:PRO:HA	19	0.42
(1,1479)	1:152:A:ILE:HD13	1:175:A:PHE:HE1	19	0.42
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD2	19	0.42
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG23	5	0.42
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD11	10	0.42
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD12	13	0.42
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB1	3	0.42
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	14	0.42
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	11	0.42
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB2	16	0.42
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE1	15	0.42
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	15	0.42
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	18	0.42
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	3	0.42
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	8	0.42
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	14	0.42
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	16	0.42
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	17	0.42
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	5	0.42
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	5	0.42
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	9	0.42
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	5	0.42
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	9	0.42
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	7	0.42
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	11	0.42
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD12	16	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	1	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	2	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	3	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	4	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	5	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	6	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	7	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	8	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	9	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	10	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	11	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	12	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	13	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	14	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	15	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	16	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	17	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	18	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	19	0.42
(1,846)	1:116:A:ASP:HA	1:116:A:ASP:HB3	20	0.42
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	3	0.42
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	8	0.42
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	12	0.42
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	16	0.42
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD12	3	0.42
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	8	0.42
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	11	0.42
(1,761)	1:129:A:GLU:HA	1:129:A:GLU:HG3	17	0.42
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	10	0.42
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	16	0.42
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	19	0.42
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	14	0.42
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	7	0.42
(1,678)	1:124:A:MET:H	1:120:A:SER:H	12	0.42
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	20	0.42
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD21	18	0.42
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	20	0.42
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD11	3	0.42
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	17	0.42
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	4	0.42
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	7	0.42
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	9	0.42
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	13	0.42
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	15	0.42
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD13	9	0.42
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	12	0.42
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	20	0.42
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	5	0.42
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	4	0.42
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	5	0.42
(1,327)	1:123:A:GLU:H	1:119:A:ILE:HD12	7	0.42
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	3	0.42
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD13	14	0.42
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	17	0.42
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG21	17	0.42
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD11	20	0.42
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD13	16	0.42
(2,212)	1:120:A:SER:HB2	1:121:A:LYS:HB2	10	0.41
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	2	0.41
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	13	0.41
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	16	0.41
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	6	0.41
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	2	0.41
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	5	0.41
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	7	0.41
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	12	0.41
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	15	0.41
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE3	17	0.41
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG23	13	0.41
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	3	0.41
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	8	0.41
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	17	0.41
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	15	0.41
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	15	0.41
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	12	0.41
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	4	0.41
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG12	19	0.41
(2,64)	1:133:A:TYR:H	1:131:A:THR:HA	1	0.41
(2,55)	1:123:A:GLU:H	1:109:A:ARG:HA	3	0.41
(2,52)	1:134:A:ARG:H	1:128:A:LEU:HB3	15	0.41
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG13	2	0.41
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	10	0.41
(2,35)	1:166:A:GLU:H	1:165:A:LYS:HG3	5	0.41
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD12	15	0.41
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG13	1	0.41
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	19	0.41
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	20	0.41
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD11	20	0.41
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	19	0.41
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	20	0.41
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	9	0.41
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD22	13	0.41
(1,1641)	1:145:A:PHE:HE2	1:145:A:PHE:H	20	0.41
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	7	0.41
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	10	0.41
(1,1607)	1:155:A:ILE:HD11	1:170:A:ARG:HG2	14	0.41
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	17	0.41
(1,1590)	1:171:A:ALA:HB2	1:183:A:ILE:HG22	4	0.41
(1,1590)	1:171:A:ALA:HB1	1:183:A:ILE:HG22	16	0.41
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	3	0.41
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG11	14	0.41
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG21	6	0.41
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	10	0.41
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB1	16	0.41
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	11	0.41
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	13	0.41
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	19	0.41
(1,1485)	1:183:A:ILE:HD13	1:115:A:PRO:HA	9	0.41
(1,1483)	1:183:A:ILE:HD11	1:195:A:PHE:HD1	13	0.41
(1,1476)	1:119:A:ILE:HG21	1:117:A:MET:HG3	9	0.41
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG23	1	0.41
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	3	0.41
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG22	1	0.41
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	3	0.41
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	12	0.41
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	4	0.41
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	19	0.41
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	17	0.41
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD12	7	0.41
(1,1384)	1:127:A:LEU:HD22	1:127:A:LEU:HA	15	0.41
(1,1358)	1:197:A:LEU:HG	1:197:A:LEU:H	2	0.41
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE2	9	0.41
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	8	0.41
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	6	0.41
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	11	0.41
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	14	0.41
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	2	0.41
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	3	0.41
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	10	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG11	12	0.41
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG23	15	0.41
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG21	19	0.41
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD22	7	0.41
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	3	0.41
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	3	0.41
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	17	0.41
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	19	0.41
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	16	0.41
(1,952)	1:150:A:ASN:HA	1:150:A:ASN:HB3	1	0.41
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	6	0.41
(1,890)	1:135:A:GLN:HA	1:136:A:VAL:HG11	2	0.41
(1,875)	1:154:A:MET:HA	1:131:A:THR:HG23	20	0.41
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	6	0.41
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	2	0.41
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	18	0.41
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	2	0.41
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	18	0.41
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG23	3	0.41
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	3	0.41
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	15	0.41
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG23	17	0.41
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG21	20	0.41
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	3	0.41
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	13	0.41
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	7	0.41
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	12	0.41
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD12	20	0.41
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	16	0.41
(1,407)	1:168:A:GLN:H	1:158:A:PRO:HD2	2	0.41
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD12	20	0.41
(1,387)	1:133:A:TYR:H	1:128:A:LEU:HD11	2	0.41
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD21	4	0.41
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	8	0.41
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	3	0.41
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	20	0.41
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	8	0.41
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	12	0.41
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE1	20	0.41
(1,40)	1:153:A:GLU:H	1:152:A:ILE:HD12	7	0.41
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	13	0.41
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	16	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	10	0.4
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	13	0.4
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	17	0.4
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	9	0.4
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	20	0.4
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	4	0.4
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	12	0.4
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	9	0.4
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	19	0.4
(2,125)	1:185:A:ASN:HA	1:186:A:MET:HB2	14	0.4
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	12	0.4
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	3	0.4
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	20	0.4
(2,38)	1:176:A:ASP:H	1:179:A:HIS:HB3	16	0.4
(2,38)	1:176:A:ASP:H	1:179:A:HIS:HB3	18	0.4
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	11	0.4
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	18	0.4
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	1	0.4
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	5	0.4
(1,1735)	1:190:A:ARG:HD2	1:185:A:ASN:HB2	11	0.4
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG22	14	0.4
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	2	0.4
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD23	9	0.4
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	10	0.4
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	11	0.4
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	18	0.4
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD13	14	0.4
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG23	7	0.4
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG21	11	0.4
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG13	17	0.4
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	1	0.4
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	9	0.4
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	6	0.4
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	12	0.4
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	6	0.4
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG22	18	0.4
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	14	0.4
(1,1490)	1:119:A:ILE:HD13	1:119:A:ILE:HA	18	0.4
(1,1489)	1:183:A:ILE:HD13	1:183:A:ILE:HG22	5	0.4
(1,1485)	1:183:A:ILE:HD13	1:115:A:PRO:HA	1	0.4
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	8	0.4
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	12	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD12	2	0.4
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	16	0.4
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD1	5	0.4
(1,1476)	1:119:A:ILE:HG22	1:117:A:MET:HG3	19	0.4
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	12	0.4
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	19	0.4
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	10	0.4
(1,1457)	1:144:A:GLU:H	1:155:A:ILE:HG21	13	0.4
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD11	9	0.4
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	8	0.4
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	2	0.4
(1,1406)	1:180:A:LEU:HD12	1:175:A:PHE:HD1	8	0.4
(1,1395)	1:197:A:LEU:HD22	1:156:A:ARG:HG3	17	0.4
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE2	20	0.4
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	7	0.4
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	7	0.4
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	11	0.4
(1,1242)	1:117:A:MET:HG3	1:118:A:THR:H	10	0.4
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	3	0.4
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG11	6	0.4
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG22	11	0.4
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	16	0.4
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	1	0.4
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	13	0.4
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	3	0.4
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	4	0.4
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	6	0.4
(1,890)	1:135:A:GLN:HA	1:136:A:VAL:HG11	1	0.4
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG12	20	0.4
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG22	1	0.4
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG22	8	0.4
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	14	0.4
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	15	0.4
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	16	0.4
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	15	0.4
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	8	0.4
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	15	0.4
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	16	0.4
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD12	16	0.4
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD21	16	0.4
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	1	0.4
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG23	2	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	7	0.4
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	19	0.4
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	10	0.4
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	7	0.4
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	2	0.4
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	17	0.4
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	20	0.4
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG22	9	0.4
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	7	0.4
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	19	0.4
(1,160)	1:141:A:ARG:H	1:141:A:ARG:HD2	15	0.4
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD13	10	0.4
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG13	12	0.4
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	6	0.4
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	8	0.4
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	18	0.4
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	13	0.39
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	17	0.39
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	4	0.39
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	16	0.39
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	17	0.39
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	4	0.39
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	10	0.39
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	18	0.39
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	12	0.39
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG21	14	0.39
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG23	19	0.39
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG13	17	0.39
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG3	12	0.39
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	19	0.39
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	5	0.39
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG13	8	0.39
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG13	20	0.39
(2,36)	1:176:A:ASP:H	1:180:A:LEU:HD21	2	0.39
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG12	6	0.39
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB3	6	0.39
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	13	0.39
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD12	9	0.39
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	10	0.39
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	2	0.39
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	3	0.39
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	17	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	19	0.39
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD23	4	0.39
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	1	0.39
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	8	0.39
(1,1612)	1:145:A:PHE:HD2	1:128:A:LEU:HB2	6	0.39
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG23	13	0.39
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG21	1	0.39
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	1	0.39
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	5	0.39
(1,1485)	1:183:A:ILE:HD13	1:115:A:PRO:HA	3	0.39
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD12	3	0.39
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD23	4	0.39
(1,1481)	1:152:A:ILE:HD13	1:128:A:LEU:HD22	12	0.39
(1,1481)	1:152:A:ILE:HD11	1:128:A:LEU:HD21	17	0.39
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD2	7	0.39
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	16	0.39
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	2	0.39
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	6	0.39
(1,1424)	1:128:A:LEU:HD22	1:127:A:LEU:HB2	6	0.39
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	5	0.39
(1,1382)	1:127:A:LEU:HD22	1:124:A:MET:HB2	1	0.39
(1,1382)	1:127:A:LEU:HD22	1:124:A:MET:HB2	10	0.39
(1,1368)	1:141:A:ARG:HD3	1:141:A:ARG:HG3	15	0.39
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	15	0.39
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	16	0.39
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	18	0.39
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	5	0.39
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	6	0.39
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	8	0.39
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	10	0.39
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	12	0.39
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	9	0.39
(1,1150)	1:192:A:PHE:HE2	1:185:A:ASN:HB2	2	0.39
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG23	16	0.39
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	1	0.39
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	2	0.39
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	4	0.39
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	6	0.39
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	9	0.39
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	15	0.39
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	15	0.39
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG12	18	0.39
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	6	0.39
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG23	7	0.39
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	19	0.39
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	13	0.39
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	1	0.39
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	18	0.39
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	19	0.39
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	3	0.39
(1,678)	1:124:A:MET:H	1:120:A:SER:H	11	0.39
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	6	0.39
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	2	0.39
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	6	0.39
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	7	0.39
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	19	0.39
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	6	0.39
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	9	0.39
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	4	0.39
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD13	8	0.39
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD12	9	0.39
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	18	0.39
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD12	18	0.39
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	17	0.39
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	5	0.39
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	6	0.39
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	15	0.39
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	1	0.39
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	15	0.39
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	14	0.39
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	12	0.39
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	15	0.39
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD12	11	0.39
(1,49)	1:195:A:PHE:H	1:183:A:ILE:HG23	6	0.39
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	6	0.39
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD11	7	0.39
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	18	0.38
(2,171)	1:141:A:ARG:HB3	1:140:A:THR:HG21	12	0.38
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	3	0.38
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	8	0.38
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	17	0.38
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	18	0.38
(2,166)	1:122:A:ASN:HB3	1:125:A:VAL:HB	1	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	14	0.38
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	17	0.38
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	19	0.38
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD23	4	0.38
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	9	0.38
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	10	0.38
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG12	9	0.38
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG12	20	0.38
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	5	0.38
(2,31)	1:166:A:GLU:H	1:167:A:GLY:H	19	0.38
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB2	2	0.38
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB3	5	0.38
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	4	0.38
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	11	0.38
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	16	0.38
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	11	0.38
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD11	13	0.38
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD11	14	0.38
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	8	0.38
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	5	0.38
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	6	0.38
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	10	0.38
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	15	0.38
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	3	0.38
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	16	0.38
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	2	0.38
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	9	0.38
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	3	0.38
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	7	0.38
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	13	0.38
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	12	0.38
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG13	10	0.38
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG12	16	0.38
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	3	0.38
(1,1562)	1:173:A:LEU:HD12	1:174:A:THR:H	19	0.38
(1,1528)	1:172:A:ARG:HB2	1:171:A:ALA:HB3	1	0.38
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	7	0.38
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG21	2	0.38
(1,1490)	1:119:A:ILE:HD13	1:119:A:ILE:HA	4	0.38
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD11	18	0.38
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD1	17	0.38
(1,1476)	1:119:A:ILE:HG23	1:117:A:MET:HG3	4	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	4	0.38
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	5	0.38
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	8	0.38
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	20	0.38
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	20	0.38
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG13	10	0.38
(1,1451)	1:181:A:ALA:HB1	1:182:A:THR:HG21	15	0.38
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG11	17	0.38
(1,1414)	1:147:A:VAL:HG11	1:145:A:PHE:HZ	6	0.38
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	8	0.38
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD23	1	0.38
(1,1368)	1:141:A:ARG:HD3	1:141:A:ARG:HG3	1	0.38
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB1	5	0.38
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE1	8	0.38
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	9	0.38
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	11	0.38
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	3	0.38
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	3	0.38
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	15	0.38
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	18	0.38
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	20	0.38
(1,1242)	1:117:A:MET:HG3	1:118:A:THR:H	14	0.38
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	20	0.38
(1,1220)	1:186:A:MET:HG2	1:172:A:ARG:HB3	5	0.38
(1,1220)	1:186:A:MET:HG2	1:172:A:ARG:HB3	18	0.38
(1,1158)	1:144:A:GLU:HG2	1:141:A:ARG:HG3	20	0.38
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG22	6	0.38
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD22	16	0.38
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	11	0.38
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	7	0.38
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	12	0.38
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	20	0.38
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	5	0.38
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	2	0.38
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	5	0.38
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	6	0.38
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	1	0.38
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD2	17	0.38
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	9	0.38
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	12	0.38
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	6	0.38
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	17	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	13	0.38
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	5	0.38
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	12	0.38
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	13	0.38
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	15	0.38
(1,678)	1:124:A:MET:H	1:120:A:SER:H	19	0.38
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	9	0.38
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	11	0.38
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	20	0.38
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	11	0.38
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	9	0.38
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG21	19	0.38
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	6	0.38
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	8	0.38
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD12	3	0.38
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	11	0.38
(1,450)	1:174:A:THR:H	1:174:A:THR:HG23	18	0.38
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD13	5	0.38
(1,440)	1:114:A:GLU:H	1:113:A:LEU:HD11	15	0.38
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	6	0.38
(1,361)	1:152:A:ILE:H	1:173:A:LEU:HD13	17	0.38
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	10	0.38
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	13	0.38
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	18	0.38
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	13	0.38
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD13	6	0.38
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD13	6	0.38
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD13	1	0.38
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD11	17	0.38
(1,81)	1:186:A:MET:H	1:186:A:MET:HE2	18	0.38
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	10	0.38
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD3	4	0.37
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	10	0.37
(2,202)	1:184:A:VAL:HG13	1:172:A:ARG:HG2	5	0.37
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG23	8	0.37
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	7	0.37
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	15	0.37
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	20	0.37
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	1	0.37
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	9	0.37
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	15	0.37
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	5	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,141)	1:126:A:LYS:HE3	1:109:A:ARG:HA	6	0.37
(2,128)	1:115:A:PRO:HD3	1:192:A:PHE:HB2	15	0.37
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	5	0.37
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	8	0.37
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	8	0.37
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	3	0.37
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	17	0.37
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	11	0.37
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	7	0.37
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	1	0.37
(2,33)	1:166:A:GLU:H	1:165:A:LYS:HE2	14	0.37
(2,32)	1:166:A:GLU:H	1:164:A:SER:HB3	7	0.37
(2,32)	1:166:A:GLU:H	1:164:A:SER:HB3	17	0.37
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	7	0.37
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB2	19	0.37
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	8	0.37
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	12	0.37
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	15	0.37
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	8	0.37
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG22	10	0.37
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG21	13	0.37
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	1	0.37
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG23	19	0.37
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD13	6	0.37
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD11	16	0.37
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	1	0.37
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	4	0.37
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	18	0.37
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	13	0.37
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	16	0.37
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG23	1	0.37
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	14	0.37
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	20	0.37
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	3	0.37
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD12	20	0.37
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD11	16	0.37
(1,1590)	1:171:A:ALA:HB2	1:183:A:ILE:HG22	3	0.37
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG21	7	0.37
(1,1578)	1:140:A:THR:HG21	1:138:A:LYS:HE3	3	0.37
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	15	0.37
(1,1535)	1:154:A:MET:HG3	1:173:A:LEU:HD13	13	0.37
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG21	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG22	4	0.37
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG21	16	0.37
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	2	0.37
(1,1485)	1:183:A:ILE:HD13	1:115:A:PRO:HA	6	0.37
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD13	15	0.37
(1,1476)	1:119:A:ILE:HG21	1:117:A:MET:HG3	15	0.37
(1,1469)	1:128:A:LEU:HD22	1:152:A:ILE:HG23	15	0.37
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	8	0.37
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	9	0.37
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	14	0.37
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	7	0.37
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	14	0.37
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG13	5	0.37
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG11	7	0.37
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	8	0.37
(1,1424)	1:128:A:LEU:HD23	1:127:A:LEU:HB2	15	0.37
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	4	0.37
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	6	0.37
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	15	0.37
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	7	0.37
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB3	9	0.37
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	13	0.37
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD21	1	0.37
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	5	0.37
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	10	0.37
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	12	0.37
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	12	0.37
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	1	0.37
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	9	0.37
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	14	0.37
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	16	0.37
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG11	13	0.37
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	4	0.37
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	11	0.37
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG21	6	0.37
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	18	0.37
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	8	0.37
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	14	0.37
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	18	0.37
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB1	9	0.37
(1,875)	1:154:A:MET:HA	1:131:A:THR:HG22	17	0.37
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	19	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD11	19	0.37
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG22	20	0.37
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	13	0.37
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	16	0.37
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	18	0.37
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	3	0.37
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	6	0.37
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	7	0.37
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	9	0.37
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	15	0.37
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	16	0.37
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	7	0.37
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	13	0.37
(1,683)	1:143:A:GLY:H	1:131:A:THR:HG21	15	0.37
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	9	0.37
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	11	0.37
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG22	15	0.37
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG21	18	0.37
(1,583)	1:131:A:THR:H	1:132:A:GLN:HG3	12	0.37
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG22	4	0.37
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG21	5	0.37
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	3	0.37
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	11	0.37
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	14	0.37
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	1	0.37
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	13	0.37
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	14	0.37
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	20	0.37
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	1	0.37
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	2	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	1	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	2	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	3	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	5	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	11	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	16	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	17	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	19	0.37
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	20	0.37
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	14	0.37
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD12	6	0.37
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	3	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	15	0.37
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	16	0.37
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD21	8	0.37
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	6	0.37
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	15	0.37
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	17	0.37
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	12	0.37
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	16	0.37
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	19	0.37
(1,160)	1:141:A:ARG:H	1:141:A:ARG:HD2	1	0.37
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB2	19	0.37
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	5	0.37
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	20	0.37
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	16	0.37
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	6	0.36
(2,197)	1:184:A:VAL:HG22	1:172:A:ARG:HG2	9	0.36
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	3	0.36
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	13	0.36
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG23	19	0.36
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	7	0.36
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	12	0.36
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	19	0.36
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	20	0.36
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	10	0.36
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	14	0.36
(2,145)	1:194:A:PHE:HB3	1:114:A:GLU:HG3	5	0.36
(2,133)	1:167:A:GLY:HA2	1:158:A:PRO:HB2	6	0.36
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	17	0.36
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	18	0.36
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	11	0.36
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	16	0.36
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	6	0.36
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	2	0.36
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	16	0.36
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	17	0.36
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	17	0.36
(2,56)	1:110:A:MET:H	1:109:A:ARG:HB3	6	0.36
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	16	0.36
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG11	6	0.36
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	13	0.36
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	7	0.36
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	6	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	17	0.36
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	2	0.36
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	15	0.36
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG22	17	0.36
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	1	0.36
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD12	11	0.36
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	2	0.36
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	17	0.36
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	12	0.36
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	10	0.36
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	14	0.36
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	1	0.36
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	11	0.36
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	9	0.36
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG23	11	0.36
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG23	18	0.36
(1,1591)	1:183:A:ILE:HG22	1:173:A:LEU:HD12	13	0.36
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	3	0.36
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	7	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	2	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	3	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	4	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	5	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	6	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	7	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	8	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	11	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	12	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	14	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	15	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	16	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	18	0.36
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	20	0.36
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG23	4	0.36
(1,1484)	1:114:A:GLU:HA	1:183:A:ILE:HD13	9	0.36
(1,1481)	1:152:A:ILE:HD11	1:128:A:LEU:HD23	3	0.36
(1,1476)	1:119:A:ILE:HG23	1:117:A:MET:HG3	12	0.36
(1,1463)	1:183:A:ILE:HG22	1:195:A:PHE:HB3	1	0.36
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG23	3	0.36
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD13	3	0.36
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	7	0.36
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	8	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:131:A:THR:HG22	1:127:A:LEU:HD22	14	0.36
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	15	0.36
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	18	0.36
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	5	0.36
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	6	0.36
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	16	0.36
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	2	0.36
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	4	0.36
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	14	0.36
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG21	3	0.36
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	7	0.36
(1,1280)	1:154:A:MET:H	1:154:A:MET:HG2	15	0.36
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	5	0.36
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	12	0.36
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	2	0.36
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	4	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	1	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	4	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	5	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	7	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	8	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	9	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	13	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	15	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	17	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	18	0.36
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	19	0.36
(1,1166)	1:153:A:GLU:HG3	1:172:A:ARG:HB2	8	0.36
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG21	9	0.36
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	15	0.36
(1,1065)	1:175:A:PHE:HB2	1:175:A:PHE:HE1	14	0.36
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	11	0.36
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	15	0.36
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	10	0.36
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	20	0.36
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD12	8	0.36
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD13	10	0.36
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG12	14	0.36
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	12	0.36
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	18	0.36
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	2	0.36
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	5	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	8	0.36
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	10	0.36
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	12	0.36
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	13	0.36
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	19	0.36
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	20	0.36
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	5	0.36
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	1	0.36
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	15	0.36
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	17	0.36
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	6	0.36
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	2	0.36
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	14	0.36
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG21	12	0.36
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	4	0.36
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	7	0.36
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	12	0.36
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	17	0.36
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	3	0.36
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	4	0.36
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	7	0.36
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	10	0.36
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	3	0.36
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	12	0.36
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	17	0.36
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	7	0.36
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	9	0.36
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	10	0.36
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	12	0.36
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	13	0.36
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	15	0.36
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	18	0.36
(1,450)	1:174:A:THR:H	1:174:A:THR:HG23	12	0.36
(1,359)	1:152:A:ILE:H	1:174:A:THR:HG22	8	0.36
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG11	1	0.36
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG11	7	0.36
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG22	5	0.36
(1,265)	1:197:A:LEU:H	1:197:A:LEU:HD13	1	0.36
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	17	0.36
(1,72)	1:139:A:MET:H	1:139:A:MET:HE2	13	0.36
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	11	0.36
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	12	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	19	0.35
(2,172)	1:170:A:ARG:HB3	1:155:A:ILE:HG12	12	0.35
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	1	0.35
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	13	0.35
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	1	0.35
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	12	0.35
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	7	0.35
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	12	0.35
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	3	0.35
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	11	0.35
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	7	0.35
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	18	0.35
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	9	0.35
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	16	0.35
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG11	8	0.35
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG13	12	0.35
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG13	17	0.35
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG11	6	0.35
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	17	0.35
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	11	0.35
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG21	9	0.35
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	2	0.35
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	3	0.35
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	4	0.35
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD23	14	0.35
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	10	0.35
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	8	0.35
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	17	0.35
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG23	2	0.35
(1,1578)	1:140:A:THR:HG23	1:138:A:LYS:HE3	13	0.35
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	8	0.35
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD11	9	0.35
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD12	12	0.35
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD11	19	0.35
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	13	0.35
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	17	0.35
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	7	0.35
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD2	1	0.35
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD2	11	0.35
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG22	11	0.35
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG11	12	0.35
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	16	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	11	0.35
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG22	1	0.35
(1,1425)	1:128:A:LEU:HD23	1:131:A:THR:HG21	13	0.35
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	10	0.35
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	6	0.35
(1,1392)	1:197:A:LEU:HD22	1:195:A:PHE:HE1	16	0.35
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	6	0.35
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	11	0.35
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	15	0.35
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	17	0.35
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB2	2	0.35
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	7	0.35
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG21	8	0.35
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	9	0.35
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	13	0.35
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	2	0.35
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	13	0.35
(1,1242)	1:117:A:MET:HG3	1:118:A:THR:H	17	0.35
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	18	0.35
(1,1235)	1:142:A:PRO:HB2	1:155:A:ILE:HG21	4	0.35
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	18	0.35
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	3	0.35
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	16	0.35
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	11	0.35
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	12	0.35
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	14	0.35
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	20	0.35
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG23	15	0.35
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG21	4	0.35
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD23	4	0.35
(1,1044)	1:180:A:LEU:HB3	1:180:A:LEU:HD23	2	0.35
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD11	20	0.35
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	16	0.35
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	19	0.35
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD23	6	0.35
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD22	14	0.35
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG13	17	0.35
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	1	0.35
(1,908)	1:180:A:LEU:HA	1:180:A:LEU:HD11	18	0.35
(1,890)	1:135:A:GLN:HA	1:136:A:VAL:HG11	9	0.35
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	3	0.35
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	13	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	8	0.35
(1,827)	1:194:A:PHE:HA	1:194:A:PHE:HD1	7	0.35
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	6	0.35
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	8	0.35
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	20	0.35
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG21	8	0.35
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	20	0.35
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	1	0.35
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	4	0.35
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	11	0.35
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	14	0.35
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	20	0.35
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	19	0.35
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	16	0.35
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	5	0.35
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	9	0.35
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	11	0.35
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG21	16	0.35
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	1	0.35
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	8	0.35
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	9	0.35
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	18	0.35
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	2	0.35
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	4	0.35
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	3	0.35
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG21	5	0.35
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	4	0.35
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	9	0.35
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	16	0.35
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	18	0.35
(1,416)	1:159:A:PHE:H	1:158:A:PRO:HD3	19	0.35
(1,404)	1:168:A:GLN:H	1:169:A:VAL:HG22	19	0.35
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	7	0.35
(1,400)	1:117:A:MET:H	1:119:A:ILE:HG21	8	0.35
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	11	0.35
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	3	0.35
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG23	15	0.35
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB1	18	0.35
(1,279)	1:134:A:ARG:H	1:136:A:VAL:HG22	1	0.35
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG22	15	0.35
(1,227)	1:200:A:ARG:H	1:199:A:PRO:HB2	1	0.35
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	6	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	19	0.35
(1,108)	1:185:A:ASN:H	1:169:A:VAL:HG11	15	0.35
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	6	0.35
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	1	0.35
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	4	0.35
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	17	0.35
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	1	0.35
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	14	0.35
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD11	19	0.35
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	13	0.34
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	14	0.34
(2,192)	1:125:A:VAL:HG11	1:109:A:ARG:H	5	0.34
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	1	0.34
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	9	0.34
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	12	0.34
(2,175)	1:119:A:ILE:HA	1:123:A:GLU:HB3	8	0.34
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	10	0.34
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	14	0.34
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	16	0.34
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	1	0.34
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG13	14	0.34
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	13	0.34
(2,81)	1:140:A:THR:H	1:155:A:ILE:HD13	7	0.34
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB2	12	0.34
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	3	0.34
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG21	18	0.34
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD13	4	0.34
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD13	18	0.34
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	12	0.34
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	16	0.34
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	9	0.34
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	15	0.34
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	13	0.34
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	4	0.34
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD11	7	0.34
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	14	0.34
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	16	0.34
(1,1529)	1:139:A:MET:HG2	1:136:A:VAL:HG13	7	0.34
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	11	0.34
(1,1517)	1:132:A:GLN:HG3	1:131:A:THR:HG23	10	0.34
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG12	18	0.34
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1485)	1:183:A:ILE:HD12	1:115:A:PRO:HA	4	0.34
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD1	11	0.34
(1,1482)	1:183:A:ILE:H	1:183:A:ILE:HD12	2	0.34
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	13	0.34
(1,1414)	1:147:A:VAL:HG11	1:145:A:PHE:HZ	19	0.34
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	17	0.34
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD21	9	0.34
(1,1409)	1:131:A:THR:HG21	1:127:A:LEU:HD23	13	0.34
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	3	0.34
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	4	0.34
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	12	0.34
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	14	0.34
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	18	0.34
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	7	0.34
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	16	0.34
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	20	0.34
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG21	10	0.34
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG22	14	0.34
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG21	16	0.34
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	1	0.34
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	9	0.34
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	12	0.34
(1,1215)	1:197:A:LEU:HB3	1:111:A:VAL:HB	7	0.34
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	6	0.34
(1,1201)	1:138:A:LYS:HA	1:138:A:LYS:HB3	16	0.34
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	11	0.34
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG22	17	0.34
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD22	20	0.34
(1,1010)	1:168:A:GLN:H	1:167:A:GLY:HA3	5	0.34
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	7	0.34
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD11	13	0.34
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD11	2	0.34
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	14	0.34
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB3	13	0.34
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG11	17	0.34
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD13	12	0.34
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD12	6	0.34
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	20	0.34
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	12	0.34
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	14	0.34
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	15	0.34
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	5	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	14	0.34
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	17	0.34
(1,697)	1:154:A:MET:H	1:145:A:PHE:HA	6	0.34
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	4	0.34
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	2	0.34
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	13	0.34
(1,678)	1:124:A:MET:H	1:120:A:SER:H	4	0.34
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	4	0.34
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	7	0.34
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	13	0.34
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	17	0.34
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG21	17	0.34
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	3	0.34
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	2	0.34
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	10	0.34
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	16	0.34
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	19	0.34
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	13	0.34
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	20	0.34
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	4	0.34
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	7	0.34
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	8	0.34
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	16	0.34
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	20	0.34
(1,495)	1:126:A:LYS:H	1:126:A:LYS:HB3	14	0.34
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	13	0.34
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	19	0.34
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD21	10	0.34
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	13	0.34
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD12	3	0.34
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD13	9	0.34
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	15	0.34
(1,331)	1:110:A:MET:H	1:122:A:ASN:HB3	20	0.34
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	9	0.34
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	19	0.34
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	3	0.34
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	10	0.34
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG22	17	0.34
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	3	0.34
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	13	0.34
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	16	0.34
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG21	2	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD13	3	0.34
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	12	0.33
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	10	0.33
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	11	0.33
(2,170)	1:110:A:MET:H	1:109:A:ARG:HB3	6	0.33
(2,167)	1:126:A:LYS:H	1:125:A:VAL:HB	5	0.33
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	16	0.33
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HG3	19	0.33
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	9	0.33
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD21	2	0.33
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	15	0.33
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	2	0.33
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	7	0.33
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	14	0.33
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	14	0.33
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG11	16	0.33
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	3	0.33
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD12	10	0.33
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG22	6	0.33
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	7	0.33
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	16	0.33
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD11	2	0.33
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	13	0.33
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	14	0.33
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	7	0.33
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	18	0.33
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD21	13	0.33
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD21	18	0.33
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	16	0.33
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD13	9	0.33
(1,1607)	1:155:A:ILE:HD13	1:170:A:ARG:HG2	4	0.33
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	4	0.33
(1,1597)	1:180:A:LEU:HD13	1:152:A:ILE:HD13	1	0.33
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	5	0.33
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	3	0.33
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	18	0.33
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	14	0.33
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	18	0.33
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	19	0.33
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD23	7	0.33
(1,1476)	1:119:A:ILE:HG21	1:117:A:MET:HG3	2	0.33
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD2	9	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	16	0.33
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD12	12	0.33
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD13	17	0.33
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD11	19	0.33
(1,1425)	1:128:A:LEU:HD22	1:131:A:THR:HG23	9	0.33
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	9	0.33
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	1	0.33
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG22	6	0.33
(1,1395)	1:197:A:LEU:HD22	1:156:A:ARG:HG3	16	0.33
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	12	0.33
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	20	0.33
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	3	0.33
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE1	11	0.33
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	6	0.33
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	14	0.33
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	4	0.33
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	19	0.33
(1,1271)	1:139:A:MET:HG2	1:140:A:THR:HA	13	0.33
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	1	0.33
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	8	0.33
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG21	11	0.33
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG21	8	0.33
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	2	0.33
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	19	0.33
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	2	0.33
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	11	0.33
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD22	14	0.33
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD13	4	0.33
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	11	0.33
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	1	0.33
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	7	0.33
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	2	0.33
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	18	0.33
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	8	0.33
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	7	0.33
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG13	8	0.33
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	14	0.33
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	6	0.33
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	3	0.33
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	13	0.33
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	5	0.33
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	12	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG21	7	0.33
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	9	0.33
(1,782)	1:126:A:LYS:HA	1:126:A:LYS:HB2	18	0.33
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	20	0.33
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	11	0.33
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	12	0.33
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	19	0.33
(1,690)	1:195:A:PHE:H	1:113:A:LEU:HB3	7	0.33
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	4	0.33
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	9	0.33
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	13	0.33
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	17	0.33
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	12	0.33
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	19	0.33
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	6	0.33
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	3	0.33
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	15	0.33
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	1	0.33
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	1	0.33
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	14	0.33
(1,577)	1:179:A:HIS:H	1:118:A:THR:HG23	17	0.33
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	17	0.33
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	1	0.33
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	6	0.33
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	5	0.33
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	12	0.33
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	19	0.33
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	18	0.33
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	3	0.33
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG21	8	0.33
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	18	0.33
(1,470)	1:116:A:ASP:H	1:180:A:LEU:HD21	2	0.33
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	8	0.33
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD12	1	0.33
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	12	0.33
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	14	0.33
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	13	0.33
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	12	0.33
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	5	0.33
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	13	0.33
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	1	0.33
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	7	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	8	0.33
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	10	0.33
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	12	0.33
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG23	10	0.33
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	8	0.33
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	14	0.33
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD22	13	0.33
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	15	0.33
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	2	0.33
(2,197)	1:184:A:VAL:HG21	1:172:A:ARG:HG2	20	0.32
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	4	0.32
(2,173)	1:124:A:MET:HB3	1:123:A:GLU:HB3	7	0.32
(2,173)	1:124:A:MET:HB2	1:123:A:GLU:HB3	9	0.32
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	10	0.32
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	2	0.32
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	9	0.32
(2,132)	1:167:A:GLY:HA3	1:158:A:PRO:HB2	5	0.32
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	7	0.32
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	2	0.32
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	10	0.32
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	15	0.32
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	16	0.32
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG12	10	0.32
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	5	0.32
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	17	0.32
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	8	0.32
(1,1719)	1:154:A:MET:HA	1:173:A:LEU:HD12	7	0.32
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG23	13	0.32
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	14	0.32
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	19	0.32
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	9	0.32
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	10	0.32
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG23	6	0.32
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG23	12	0.32
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	18	0.32
(1,1607)	1:155:A:ILE:HD12	1:170:A:ARG:HG2	5	0.32
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG11	12	0.32
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG12	20	0.32
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	1	0.32
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	5	0.32
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	11	0.32
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD12	18	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	12	0.32
(1,1485)	1:183:A:ILE:HD12	1:115:A:PRO:HA	14	0.32
(1,1479)	1:152:A:ILE:HD11	1:175:A:PHE:HE1	11	0.32
(1,1477)	1:186:A:MET:HE1	1:170:A:ARG:HD2	3	0.32
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	5	0.32
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	18	0.32
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG13	19	0.32
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	7	0.32
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	18	0.32
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	11	0.32
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	12	0.32
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	5	0.32
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD12	9	0.32
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	15	0.32
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	18	0.32
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD11	11	0.32
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG23	9	0.32
(1,1348)	1:183:A:ILE:HG12	1:183:A:ILE:HG21	18	0.32
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	19	0.32
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	2	0.32
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	6	0.32
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	11	0.32
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	5	0.32
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	18	0.32
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	5	0.32
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD13	3	0.32
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG22	19	0.32
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	6	0.32
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	14	0.32
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG22	1	0.32
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG22	4	0.32
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG22	8	0.32
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	13	0.32
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	16	0.32
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG21	13	0.32
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD11	12	0.32
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB2	8	0.32
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	3	0.32
(1,861)	1:166:A:GLU:HA	1:166:A:GLU:HG3	12	0.32
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	11	0.32
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	14	0.32
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	3	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	3	0.32
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG21	5	0.32
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG21	8	0.32
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	18	0.32
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	6	0.32
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	13	0.32
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	2	0.32
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	3	0.32
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	12	0.32
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	16	0.32
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	18	0.32
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	16	0.32
(1,643)	1:173:A:LEU:H	1:171:A:ALA:HB1	10	0.32
(1,628)	1:167:A:GLY:H	1:169:A:VAL:HG22	19	0.32
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	5	0.32
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG21	10	0.32
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG22	20	0.32
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	4	0.32
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	17	0.32
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	11	0.32
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	13	0.32
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	15	0.32
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	16	0.32
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	1	0.32
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	12	0.32
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	1	0.32
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	5	0.32
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	15	0.32
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	1	0.32
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	2	0.32
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	15	0.32
(1,483)	1:187:A:GLU:H	1:169:A:VAL:HG12	10	0.32
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	2	0.32
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	10	0.32
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB3	8	0.32
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	9	0.32
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	9	0.32
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	2	0.32
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	19	0.32
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	2	0.32
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB1	3	0.32
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG22	4	0.32
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG23	14	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	2	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	6	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	9	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	11	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	14	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	19	0.32
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	20	0.32
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	16	0.32
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	1	0.32
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG21	2	0.32
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	10	0.32
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD12	14	0.32
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	6	0.31
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	8	0.31
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	11	0.31
(2,180)	1:172:A:ARG:HG2	1:151:A:SER:HB2	8	0.31
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	3	0.31
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	9	0.31
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	15	0.31
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD11	18	0.31
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	15	0.31
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	18	0.31
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	4	0.31
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	7	0.31
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	12	0.31
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD11	16	0.31
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	20	0.31
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB2	1	0.31
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	14	0.31
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	6	0.31
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	14	0.31
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	5	0.31
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	6	0.31
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	9	0.31
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	15	0.31
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	4	0.31
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	14	0.31
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD12	11	0.31
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG21	12	0.31
(1,1590)	1:171:A:ALA:HB3	1:183:A:ILE:HG21	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG11	11	0.31
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	15	0.31
(1,1578)	1:140:A:THR:HG23	1:138:A:LYS:HE3	2	0.31
(1,1578)	1:140:A:THR:HG23	1:138:A:LYS:HE3	17	0.31
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	18	0.31
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	3	0.31
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	1	0.31
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	9	0.31
(1,1540)	1:187:A:GLU:HB3	1:187:A:GLU:HG3	10	0.31
(1,1494)	1:155:A:ILE:HD13	1:155:A:ILE:HB	8	0.31
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	19	0.31
(1,1489)	1:183:A:ILE:HD12	1:183:A:ILE:HG23	6	0.31
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	11	0.31
(1,1441)	1:197:A:LEU:HB3	1:111:A:VAL:HG12	2	0.31
(1,1414)	1:147:A:VAL:HG11	1:145:A:PHE:HZ	5	0.31
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB3	10	0.31
(1,1409)	1:131:A:THR:HG21	1:127:A:LEU:HD21	10	0.31
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD23	18	0.31
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD13	14	0.31
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG22	5	0.31
(1,1366)	1:173:A:LEU:HD13	1:171:A:ALA:HB1	13	0.31
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	10	0.31
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	15	0.31
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	18	0.31
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE3	10	0.31
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	19	0.31
(1,1270)	1:139:A:MET:HG2	1:155:A:ILE:HD12	12	0.31
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	19	0.31
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	6	0.31
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	17	0.31
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	6	0.31
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	10	0.31
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	12	0.31
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG21	12	0.31
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	9	0.31
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	1	0.31
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	11	0.31
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	13	0.31
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	15	0.31
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	18	0.31
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB2	3	0.31
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	4	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	14	0.31
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	17	0.31
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	18	0.31
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	1	0.31
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	8	0.31
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	7	0.31
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	8	0.31
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	4	0.31
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD11	18	0.31
(1,791)	1:123:A:GLU:HA	1:119:A:ILE:HD13	6	0.31
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	14	0.31
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	3	0.31
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	13	0.31
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	17	0.31
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	18	0.31
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	20	0.31
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	5	0.31
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	15	0.31
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	17	0.31
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	7	0.31
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	7	0.31
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	11	0.31
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	10	0.31
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD11	18	0.31
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	8	0.31
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG22	13	0.31
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	6	0.31
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	14	0.31
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	3	0.31
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	4	0.31
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	10	0.31
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	13	0.31
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	10	0.31
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	11	0.31
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	5	0.31
(1,550)	1:164:A:SER:H	1:162:A:PRO:HB3	13	0.31
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	6	0.31
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	13	0.31
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	14	0.31
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	20	0.31
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	17	0.31
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG22	14	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG21	7	0.31
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	6	0.31
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	8	0.31
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	11	0.31
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD13	8	0.31
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB1	5	0.31
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB1	13	0.31
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	19	0.31
(1,425)	1:190:A:ARG:H	1:190:A:ARG:HD2	20	0.31
(1,404)	1:168:A:GLN:H	1:169:A:VAL:HG21	5	0.31
(1,386)	1:133:A:TYR:H	1:128:A:LEU:HD23	2	0.31
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	14	0.31
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	1	0.31
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	9	0.31
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG22	3	0.31
(1,229)	1:200:A:ARG:H	1:200:A:ARG:HG2	6	0.31
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	10	0.31
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	20	0.31
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	15	0.31
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	17	0.31
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	4	0.31
(1,81)	1:186:A:MET:H	1:186:A:MET:HE1	10	0.31
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	12	0.31
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	20	0.31
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	18	0.3
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	11	0.3
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	13	0.3
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	17	0.3
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	9	0.3
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	18	0.3
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	1	0.3
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	4	0.3
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	8	0.3
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	7	0.3
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	14	0.3
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	9	0.3
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	20	0.3
(2,52)	1:134:A:ARG:H	1:136:A:VAL:HG13	19	0.3
(2,38)	1:176:A:ASP:H	1:179:A:HIS:HB3	9	0.3
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD12	9	0.3
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	9	0.3
(1,1680)	1:120:A:SER:HB2	1:121:A:LYS:HG3	15	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	9	0.3
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	15	0.3
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	2	0.3
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	8	0.3
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	15	0.3
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	16	0.3
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG21	5	0.3
(1,1591)	1:183:A:ILE:HG23	1:173:A:LEU:HD13	9	0.3
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD13	16	0.3
(1,1590)	1:171:A:ALA:HB2	1:183:A:ILE:HG22	8	0.3
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG11	17	0.3
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	18	0.3
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	5	0.3
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG11	6	0.3
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG11	8	0.3
(1,1578)	1:140:A:THR:HG21	1:138:A:LYS:HE3	19	0.3
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	14	0.3
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	5	0.3
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	4	0.3
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	15	0.3
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	11	0.3
(1,1474)	1:119:A:ILE:HG23	1:175:A:PHE:HD1	15	0.3
(1,1462)	1:195:A:PHE:HD1	1:183:A:ILE:HG23	20	0.3
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	13	0.3
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG11	14	0.3
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG11	19	0.3
(1,1435)	1:136:A:VAL:HG21	1:139:A:MET:HB2	3	0.3
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	20	0.3
(1,1413)	1:171:A:ALA:HB1	1:195:A:PHE:HZ	3	0.3
(1,1409)	1:131:A:THR:HG21	1:127:A:LEU:HD22	4	0.3
(1,1409)	1:131:A:THR:HG23	1:127:A:LEU:HD22	16	0.3
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	3	0.3
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD12	19	0.3
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	7	0.3
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD21	16	0.3
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	4	0.3
(1,1391)	1:138:A:LYS:HB3	1:138:A:LYS:HG3	11	0.3
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	12	0.3
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB1	11	0.3
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	5	0.3
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	15	0.3
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	13	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	16	0.3
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	6	0.3
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	9	0.3
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	5	0.3
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	6	0.3
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	9	0.3
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	15	0.3
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	16	0.3
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	19	0.3
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	19	0.3
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	15	0.3
(1,1226)	1:165:A:LYS:H	1:165:A:LYS:HB2	5	0.3
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	1	0.3
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	19	0.3
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD23	11	0.3
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	10	0.3
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	6	0.3
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	17	0.3
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD21	11	0.3
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD22	16	0.3
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	1	0.3
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG11	11	0.3
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	10	0.3
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	4	0.3
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	9	0.3
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	17	0.3
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	1	0.3
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	13	0.3
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	16	0.3
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	18	0.3
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	2	0.3
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG21	1	0.3
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG21	4	0.3
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	10	0.3
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG22	11	0.3
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	13	0.3
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG22	19	0.3
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	7	0.3
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	14	0.3
(1,708)	1:131:A:THR:HB	1:127:A:LEU:HD11	1	0.3
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	7	0.3
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	5	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	15	0.3
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	5	0.3
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	14	0.3
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	7	0.3
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	20	0.3
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	5	0.3
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	10	0.3
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	4	0.3
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	18	0.3
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	7	0.3
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	16	0.3
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	18	0.3
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	9	0.3
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	13	0.3
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	15	0.3
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	18	0.3
(1,543)	1:177:A:GLY:H	1:174:A:THR:HA	17	0.3
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	9	0.3
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	10	0.3
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	15	0.3
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	12	0.3
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	18	0.3
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	5	0.3
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	6	0.3
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	16	0.3
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	19	0.3
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	20	0.3
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	10	0.3
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	18	0.3
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	12	0.3
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	16	0.3
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	5	0.3
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	4	0.3
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD12	4	0.3
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD13	13	0.3
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	5	0.3
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	11	0.3
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG12	4	0.3
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	17	0.3
(1,320)	1:129:A:GLU:H	1:127:A:LEU:HD21	6	0.3
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	20	0.3
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG23	12	0.3
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	13	0.3
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	4	0.3
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	11	0.3
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	15	0.3
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	17	0.3
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	18	0.3
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	4	0.3
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	15	0.3
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG22	4	0.3
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	2	0.3
(1,137)	1:157:A:ARG:H	1:197:A:LEU:HD22	8	0.3
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	13	0.3
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	20	0.3
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	7	0.3
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	16	0.3
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	18	0.3
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	7	0.29
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	16	0.29
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	17	0.29
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	18	0.29
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	6	0.29
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	9	0.29
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	10	0.29
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HD3	13	0.29
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	16	0.29
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	8	0.29
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	14	0.29
(2,183)	1:158:A:PRO:HG3	1:158:A:PRO:HA	19	0.29
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	11	0.29
(2,167)	1:109:A:ARG:HB3	1:126:A:LYS:H	11	0.29
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	6	0.29
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	10	0.29
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	6	0.29
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	7	0.29
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	16	0.29
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	8	0.29
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	15	0.29
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	16	0.29
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	16	0.29
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB2	17	0.29
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	12	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	2	0.29
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB2	8	0.29
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	17	0.29
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	20	0.29
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	20	0.29
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	12	0.29
(2,61)	1:133:A:TYR:H	1:129:A:GLU:HB3	2	0.29
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	3	0.29
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	14	0.29
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	6	0.29
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG13	7	0.29
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	3	0.29
(2,5)	1:196:A:ARG:H	1:127:A:LEU:HD13	10	0.29
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG21	12	0.29
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	11	0.29
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	13	0.29
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	8	0.29
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	6	0.29
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	5	0.29
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	4	0.29
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	5	0.29
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG22	19	0.29
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG21	1	0.29
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD13	18	0.29
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG11	12	0.29
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG13	19	0.29
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD11	17	0.29
(1,1494)	1:155:A:ILE:HD13	1:155:A:ILE:HB	6	0.29
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	16	0.29
(1,1485)	1:183:A:ILE:HD11	1:115:A:PRO:HA	10	0.29
(1,1485)	1:183:A:ILE:HD13	1:115:A:PRO:HA	13	0.29
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD21	1	0.29
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD23	16	0.29
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD21	19	0.29
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD23	20	0.29
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	6	0.29
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	20	0.29
(1,1436)	1:136:A:VAL:HG23	1:144:A:GLU:HB2	13	0.29
(1,1413)	1:171:A:ALA:HB1	1:195:A:PHE:HZ	4	0.29
(1,1366)	1:173:A:LEU:HD13	1:171:A:ALA:HB2	12	0.29
(1,1366)	1:173:A:LEU:HD13	1:171:A:ALA:HB2	19	0.29
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	4	0.29
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	10	0.29
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	13	0.29
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	5	0.29
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	1	0.29
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	10	0.29
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	15	0.29
(1,1277)	1:190:A:ARG:HB3	1:190:A:ARG:HD2	20	0.29
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	1	0.29
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	12	0.29
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	13	0.29
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	14	0.29
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	18	0.29
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	14	0.29
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG22	10	0.29
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	10	0.29
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	5	0.29
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	13	0.29
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	20	0.29
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	8	0.29
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	12	0.29
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	16	0.29
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	4	0.29
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	6	0.29
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	10	0.29
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	16	0.29
(1,915)	1:172:A:ARG:HA	1:171:A:ALA:HB1	16	0.29
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	11	0.29
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	10	0.29
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	3	0.29
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	11	0.29
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	10	0.29
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	16	0.29
(1,828)	1:194:A:PHE:HA	1:193:A:GLY:HA2	18	0.29
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	19	0.29
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	15	0.29
(1,804)	1:127:A:LEU:HA	1:127:A:LEU:HD13	1	0.29
(1,797)	1:175:A:PHE:HA	1:175:A:PHE:HD2	20	0.29
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	9	0.29
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	10	0.29
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	15	0.29
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	19	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	16	0.29
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	11	0.29
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	14	0.29
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	7	0.29
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	8	0.29
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG23	6	0.29
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	17	0.29
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	13	0.29
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	17	0.29
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	1	0.29
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	11	0.29
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	14	0.29
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	20	0.29
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	4	0.29
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	11	0.29
(1,678)	1:124:A:MET:H	1:120:A:SER:H	17	0.29
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	18	0.29
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	8	0.29
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	19	0.29
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG23	6	0.29
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	16	0.29
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	6	0.29
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	9	0.29
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	9	0.29
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	12	0.29
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	2	0.29
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	1	0.29
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	3	0.29
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	5	0.29
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	19	0.29
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	4	0.29
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	5	0.29
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	8	0.29
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	12	0.29
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	14	0.29
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	18	0.29
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG21	4	0.29
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	13	0.29
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	5	0.29
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	10	0.29
(1,473)	1:116:A:ASP:H	1:181:A:ALA:HB3	17	0.29
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB1	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	5	0.29
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD12	16	0.29
(1,409)	1:168:A:GLN:H	1:155:A:ILE:HG23	19	0.29
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	3	0.29
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	5	0.29
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	16	0.29
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	7	0.29
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	5	0.29
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	4	0.29
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	1	0.29
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	10	0.29
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	18	0.29
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG23	15	0.29
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	16	0.29
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	18	0.29
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG23	19	0.29
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	8	0.29
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	14	0.29
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	19	0.29
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	18	0.29
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD11	18	0.29
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB1	15	0.29
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	20	0.29
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	11	0.29
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD13	4	0.29
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD12	10	0.29
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	2	0.29
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	5	0.28
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	15	0.28
(2,202)	1:184:A:VAL:HG11	1:172:A:ARG:HG2	1	0.28
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	9	0.28
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	8	0.28
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	18	0.28
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	3	0.28
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	11	0.28
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	1	0.28
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	2	0.28
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	6	0.28
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG21	5	0.28
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	18	0.28
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	4	0.28
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	6	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD12	13	0.28
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	20	0.28
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	4	0.28
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	10	0.28
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	15	0.28
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	10	0.28
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	12	0.28
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	1	0.28
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	9	0.28
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE2	11	0.28
(2,38)	1:176:A:ASP:H	1:179:A:HIS:HB3	7	0.28
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	7	0.28
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	1	0.28
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	2	0.28
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	5	0.28
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD21	18	0.28
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	1	0.28
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	2	0.28
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	4	0.28
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	7	0.28
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	10	0.28
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG22	13	0.28
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	16	0.28
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG23	16	0.28
(1,1585)	1:136:A:VAL:HG22	1:136:A:VAL:HG12	14	0.28
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	4	0.28
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	6	0.28
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	14	0.28
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	20	0.28
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG12	20	0.28
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	7	0.28
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	13	0.28
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	15	0.28
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	9	0.28
(1,1437)	1:147:A:VAL:HG23	1:152:A:ILE:HD11	4	0.28
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	17	0.28
(1,1425)	1:128:A:LEU:HD21	1:131:A:THR:HG22	14	0.28
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	3	0.28
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	3	0.28
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	11	0.28
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD22	18	0.28
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG21	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1382)	1:127:A:LEU:HD22	1:124:A:MET:HB2	9	0.28
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	1	0.28
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	8	0.28
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD12	10	0.28
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	11	0.28
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE2	18	0.28
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	10	0.28
(1,1302)	1:128:A:LEU:H	1:129:A:GLU:HB3	11	0.28
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	5	0.28
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	12	0.28
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	16	0.28
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	18	0.28
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	4	0.28
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	7	0.28
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	8	0.28
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	20	0.28
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	12	0.28
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	4	0.28
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	8	0.28
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG21	7	0.28
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	3	0.28
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	1	0.28
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	9	0.28
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	15	0.28
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	7	0.28
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	16	0.28
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	2	0.28
(1,1010)	1:168:A:GLN:H	1:167:A:GLY:HA3	19	0.28
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD13	5	0.28
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	3	0.28
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	14	0.28
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	1	0.28
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	5	0.28
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	9	0.28
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	18	0.28
(1,875)	1:154:A:MET:HA	1:131:A:THR:HG22	7	0.28
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	15	0.28
(1,825)	1:151:A:SER:HA	1:174:A:THR:HG23	8	0.28
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	7	0.28
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	13	0.28
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	7	0.28
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	3	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	9	0.28
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	10	0.28
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	15	0.28
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	16	0.28
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	1	0.28
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	11	0.28
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	3	0.28
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	9	0.28
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	17	0.28
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	9	0.28
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	10	0.28
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	14	0.28
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	18	0.28
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	6	0.28
(1,687)	1:179:A:HIS:H	1:176:A:ASP:HB3	19	0.28
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	20	0.28
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	18	0.28
(1,678)	1:124:A:MET:H	1:120:A:SER:H	2	0.28
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	1	0.28
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD23	17	0.28
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	8	0.28
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	19	0.28
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	20	0.28
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	12	0.28
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	20	0.28
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	8	0.28
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	15	0.28
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	10	0.28
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	2	0.28
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	7	0.28
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	14	0.28
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	16	0.28
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	17	0.28
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	2	0.28
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	3	0.28
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	7	0.28
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	11	0.28
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	19	0.28
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	2	0.28
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG21	1	0.28
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	2	0.28
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	11	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	6	0.28
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	9	0.28
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	1	0.28
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB1	1	0.28
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB3	4	0.28
(1,452)	1:174:A:THR:H	1:180:A:LEU:HD23	14	0.28
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	12	0.28
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD13	17	0.28
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD12	5	0.28
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	8	0.28
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD12	14	0.28
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD12	19	0.28
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	20	0.28
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	11	0.28
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG21	13	0.28
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	16	0.28
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	2	0.28
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG23	9	0.28
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG23	11	0.28
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	2	0.28
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	3	0.28
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	9	0.28
(1,213)	1:161:A:PHE:H	1:160:A:ASP:HB3	5	0.28
(1,134)	1:180:A:LEU:H	1:180:A:LEU:HD23	2	0.28
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB3	5	0.28
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	3	0.28
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG21	9	0.28
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	14	0.28
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	17	0.28
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	18	0.28
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	15	0.28
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	1	0.28
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD12	7	0.28
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD11	12	0.28
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	5	0.28
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD11	12	0.28
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	14	0.28
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	7	0.27
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	12	0.27
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	9	0.27
(2,179)	1:165:A:LYS:HD3	1:160:A:ASP:HB3	10	0.27
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	4	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	12	0.27
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	10	0.27
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	15	0.27
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	4	0.27
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB3	13	0.27
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG13	8	0.27
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	2	0.27
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	6	0.27
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	16	0.27
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	19	0.27
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	1	0.27
(2,104)	1:162:A:PRO:HA	1:163:A:ASP:HB2	1	0.27
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	10	0.27
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	11	0.27
(2,91)	1:131:A:THR:H	1:197:A:LEU:HD22	8	0.27
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	5	0.27
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	11	0.27
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	13	0.27
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	13	0.27
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	20	0.27
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	1	0.27
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	9	0.27
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	16	0.27
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD12	7	0.27
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG22	1	0.27
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	18	0.27
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	1	0.27
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	11	0.27
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	18	0.27
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	3	0.27
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG22	9	0.27
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	12	0.27
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	15	0.27
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	2	0.27
(1,1631)	1:146:A:THR:HB	1:146:A:THR:HG21	10	0.27
(1,1607)	1:155:A:ILE:HD12	1:170:A:ARG:HG2	12	0.27
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG21	19	0.27
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG11	13	0.27
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG12	8	0.27
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	10	0.27
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG12	16	0.27
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG11	19	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	5	0.27
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	10	0.27
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG13	12	0.27
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG12	15	0.27
(1,1582)	1:136:A:VAL:HB	1:136:A:VAL:HG11	16	0.27
(1,1578)	1:140:A:THR:HG22	1:138:A:LYS:HE3	10	0.27
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD12	13	0.27
(1,1562)	1:173:A:LEU:HD11	1:174:A:THR:H	8	0.27
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG23	14	0.27
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	7	0.27
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	11	0.27
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	11	0.27
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD22	8	0.27
(1,1479)	1:152:A:ILE:HD12	1:175:A:PHE:HE1	3	0.27
(1,1479)	1:152:A:ILE:HD13	1:175:A:PHE:HE1	7	0.27
(1,1479)	1:152:A:ILE:HD13	1:175:A:PHE:HE1	16	0.27
(1,1476)	1:119:A:ILE:HG22	1:117:A:MET:HG3	1	0.27
(1,1476)	1:119:A:ILE:HG22	1:117:A:MET:HG3	18	0.27
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	12	0.27
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	17	0.27
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	20	0.27
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	19	0.27
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG13	15	0.27
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD12	11	0.27
(1,1414)	1:147:A:VAL:HG11	1:145:A:PHE:HZ	1	0.27
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	11	0.27
(1,1413)	1:171:A:ALA:HB1	1:195:A:PHE:HZ	8	0.27
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD13	20	0.27
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	6	0.27
(1,1382)	1:127:A:LEU:HD21	1:124:A:MET:HB2	13	0.27
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	13	0.27
(1,1369)	1:197:A:LEU:HD11	1:197:A:LEU:HG	1	0.27
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	2	0.27
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	16	0.27
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	7	0.27
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	14	0.27
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	17	0.27
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	19	0.27
(1,1279)	1:191:A:GLN:H	1:190:A:ARG:HB3	20	0.27
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	2	0.27
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	11	0.27
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	18	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	10	0.27
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	11	0.27
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	6	0.27
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	16	0.27
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	15	0.27
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG12	15	0.27
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG21	10	0.27
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	15	0.27
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	2	0.27
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	5	0.27
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	3	0.27
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG21	18	0.27
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD22	10	0.27
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD23	14	0.27
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	1	0.27
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	19	0.27
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	5	0.27
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	12	0.27
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	10	0.27
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	11	0.27
(1,829)	1:194:A:PHE:HA	1:183:A:ILE:HD12	14	0.27
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	10	0.27
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG23	2	0.27
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	5	0.27
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	12	0.27
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	17	0.27
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	18	0.27
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	1	0.27
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	2	0.27
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	4	0.27
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	6	0.27
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	11	0.27
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	3	0.27
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	10	0.27
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	12	0.27
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	9	0.27
(1,636)	1:143:A:GLY:H	1:155:A:ILE:HD13	14	0.27
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	7	0.27
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	5	0.27
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	10	0.27
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	1	0.27
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	10	0.27
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	11	0.27
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	14	0.27
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	20	0.27
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	3	0.27
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	6	0.27
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	7	0.27
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	9	0.27
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	14	0.27
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	19	0.27
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	9	0.27
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	15	0.27
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	19	0.27
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	6	0.27
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	19	0.27
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	15	0.27
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	17	0.27
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	20	0.27
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG22	9	0.27
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG21	19	0.27
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	4	0.27
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	19	0.27
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	19	0.27
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	15	0.27
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	17	0.27
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	1	0.27
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	6	0.27
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	1	0.27
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	2	0.27
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	8	0.27
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	17	0.27
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	7	0.27
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	12	0.27
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	16	0.27
(1,202)	1:113:A:LEU:H	1:113:A:LEU:HD12	6	0.27
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	5	0.27
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	19	0.27
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD13	5	0.27
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD11	19	0.27
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB2	4	0.27
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	3	0.27
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	10	0.27
(1,30)	1:196:A:ARG:H	1:196:A:ARG:HB3	18	0.27
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD11	13	0.27
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	15	0.27
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	1	0.26
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	3	0.26
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	2	0.26
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	5	0.26
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	19	0.26
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	5	0.26
(2,156)	1:185:A:ASN:HB3	1:184:A:VAL:HA	8	0.26
(2,155)	1:188:A:ASN:HB3	1:189:A:ASN:HA	15	0.26
(2,132)	1:167:A:GLY:HA3	1:168:A:GLN:HG2	19	0.26
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	1	0.26
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	15	0.26
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	3	0.26
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	10	0.26
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	16	0.26
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	17	0.26
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	1	0.26
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	3	0.26
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	4	0.26
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	3	0.26
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	8	0.26
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	12	0.26
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD13	9	0.26
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	14	0.26
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	15	0.26
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	2	0.26
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG23	1	0.26
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	2	0.26
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	6	0.26
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	7	0.26
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	12	0.26
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	16	0.26
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	19	0.26
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	3	0.26
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	6	0.26
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	11	0.26
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG22	18	0.26
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	19	0.26
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	4	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1634)	1:195:A:PHE:HE2	1:195:A:PHE:HB2	6	0.26
(1,1627)	1:159:A:PHE:HA	1:159:A:PHE:HD1	5	0.26
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	10	0.26
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG21	14	0.26
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	8	0.26
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD12	14	0.26
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB2	6	0.26
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	2	0.26
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	7	0.26
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	9	0.26
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	17	0.26
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG23	18	0.26
(1,1533)	1:139:A:MET:HG2	1:140:A:THR:HG23	2	0.26
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	5	0.26
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	8	0.26
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	12	0.26
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG11	1	0.26
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	2	0.26
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	4	0.26
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	18	0.26
(1,1479)	1:152:A:ILE:HD13	1:175:A:PHE:HE1	9	0.26
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	19	0.26
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD13	14	0.26
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	7	0.26
(1,1414)	1:147:A:VAL:HG11	1:145:A:PHE:HZ	13	0.26
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	7	0.26
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	9	0.26
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	14	0.26
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB1	4	0.26
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD13	11	0.26
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD22	16	0.26
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD12	14	0.26
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	4	0.26
(1,1369)	1:197:A:LEU:HD12	1:197:A:LEU:HG	10	0.26
(1,1369)	1:197:A:LEU:HD12	1:197:A:LEU:HG	14	0.26
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	15	0.26
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	18	0.26
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	3	0.26
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	14	0.26
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	17	0.26
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	20	0.26
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	5	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	3	0.26
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	8	0.26
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	13	0.26
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	20	0.26
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	15	0.26
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	11	0.26
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	20	0.26
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	8	0.26
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	13	0.26
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	18	0.26
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG22	14	0.26
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	4	0.26
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	12	0.26
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	5	0.26
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	20	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	12	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	14	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	15	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	17	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	18	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	19	0.26
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	20	0.26
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG22	10	0.26
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD12	13	0.26
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD12	19	0.26
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	5	0.26
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG12	20	0.26
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	3	0.26
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	19	0.26
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG11	13	0.26
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	9	0.26
(1,783)	1:126:A:LYS:HA	1:125:A:VAL:HG21	19	0.26
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	13	0.26
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	15	0.26
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	19	0.26
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	18	0.26
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	16	0.26
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	1	0.26
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	6	0.26
(1,686)	1:171:A:ALA:H	1:154:A:MET:HG2	18	0.26
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	19	0.26
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	1	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,661)	1:182:A:THR:H	1:182:A:THR:HG22	6	0.26
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	10	0.26
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	9	0.26
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	9	0.26
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	13	0.26
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	17	0.26
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	10	0.26
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	17	0.26
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	11	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	1	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	2	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	3	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	5	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	6	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	11	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	16	0.26
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	18	0.26
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	4	0.26
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	2	0.26
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	6	0.26
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	17	0.26
(1,511)	1:189:A:ASN:H	1:187:A:GLU:HB3	16	0.26
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	18	0.26
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	2	0.26
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	11	0.26
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	13	0.26
(1,463)	1:154:A:MET:H	1:146:A:THR:HA	6	0.26
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	2	0.26
(1,461)	1:154:A:MET:H	1:171:A:ALA:HB2	10	0.26
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG23	9	0.26
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	3	0.26
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	10	0.26
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD11	4	0.26
(1,333)	1:124:A:MET:H	1:110:A:MET:H	6	0.26
(1,333)	1:124:A:MET:H	1:110:A:MET:H	20	0.26
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	3	0.26
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG21	18	0.26
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	4	0.26
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB1	15	0.26
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	5	0.26
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	7	0.26
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG22	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	20	0.26
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	1	0.26
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	6	0.26
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	13	0.26
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	13	0.26
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD13	15	0.26
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB2	2	0.26
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	20	0.26
(1,41)	1:153:A:GLU:H	1:186:A:MET:HE2	14	0.26
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	14	0.26
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	9	0.26
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD3	9	0.25
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD3	11	0.25
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	4	0.25
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	3	0.25
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	5	0.25
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	18	0.25
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	7	0.25
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	14	0.25
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	18	0.25
(2,145)	1:194:A:PHE:HB3	1:114:A:GLU:HG3	13	0.25
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	20	0.25
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	19	0.25
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	20	0.25
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	6	0.25
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	9	0.25
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	2	0.25
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG13	5	0.25
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	10	0.25
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	2	0.25
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	5	0.25
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	19	0.25
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	2	0.25
(2,54)	1:129:A:GLU:H	1:126:A:LYS:HE3	12	0.25
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	5	0.25
(2,7)	1:135:A:GLN:H	1:136:A:VAL:HG13	17	0.25
(1,1695)	1:111:A:VAL:HA	1:197:A:LEU:HD13	1	0.25
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	7	0.25
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	8	0.25
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	3	0.25
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	9	0.25
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	13	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	15	0.25
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	17	0.25
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG22	5	0.25
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	14	0.25
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG23	20	0.25
(1,1647)	1:195:A:PHE:HE2	1:171:A:ALA:HB1	8	0.25
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	7	0.25
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	17	0.25
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	7	0.25
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD11	15	0.25
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD13	20	0.25
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD13	3	0.25
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD11	8	0.25
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD11	17	0.25
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	2	0.25
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG22	5	0.25
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	8	0.25
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	7	0.25
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	11	0.25
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	13	0.25
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	12	0.25
(1,1490)	1:119:A:ILE:HD12	1:119:A:ILE:HA	9	0.25
(1,1481)	1:152:A:ILE:HD13	1:128:A:LEU:HD22	13	0.25
(1,1437)	1:147:A:VAL:HG21	1:152:A:ILE:HD11	20	0.25
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	14	0.25
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	10	0.25
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	16	0.25
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	18	0.25
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	10	0.25
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD22	8	0.25
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	9	0.25
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	16	0.25
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	19	0.25
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD11	13	0.25
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	9	0.25
(1,1369)	1:197:A:LEU:HD11	1:197:A:LEU:HG	13	0.25
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	19	0.25
(1,1366)	1:173:A:LEU:HD12	1:171:A:ALA:HB1	6	0.25
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	4	0.25
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	8	0.25
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	10	0.25
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	13	0.25
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	6	0.25
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	8	0.25
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	12	0.25
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	4	0.25
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	13	0.25
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	4	0.25
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	11	0.25
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	7	0.25
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	13	0.25
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	2	0.25
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	3	0.25
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	5	0.25
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	1	0.25
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	12	0.25
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	20	0.25
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	1	0.25
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	3	0.25
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	4	0.25
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	7	0.25
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	8	0.25
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	11	0.25
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	16	0.25
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	20	0.25
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	11	0.25
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	9	0.25
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	6	0.25
(1,1011)	1:167:A:GLY:HA3	1:168:A:GLN:HB2	17	0.25
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD11	19	0.25
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	1	0.25
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	17	0.25
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG12	19	0.25
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	7	0.25
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE2	20	0.25
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	6	0.25
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	7	0.25
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	8	0.25
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	15	0.25
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	18	0.25
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG23	20	0.25
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	4	0.25
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	2	0.25
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	9	0.25
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	10	0.25
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	6	0.25
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	4	0.25
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	9	0.25
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	5	0.25
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	1	0.25
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	18	0.25
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	2	0.25
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	4	0.25
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	14	0.25
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	1	0.25
(1,678)	1:124:A:MET:H	1:120:A:SER:H	6	0.25
(1,678)	1:124:A:MET:H	1:120:A:SER:H	16	0.25
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	7	0.25
(1,661)	1:182:A:THR:H	1:182:A:THR:HG21	8	0.25
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	7	0.25
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	11	0.25
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	20	0.25
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	15	0.25
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	16	0.25
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	17	0.25
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	18	0.25
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	2	0.25
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	3	0.25
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	4	0.25
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	5	0.25
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	15	0.25
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	16	0.25
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	4	0.25
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	19	0.25
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	5	0.25
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	6	0.25
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	7	0.25
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	8	0.25
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	20	0.25
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	3	0.25
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	13	0.25
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	15	0.25
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	1	0.25
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	12	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	19	0.25
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	16	0.25
(1,497)	1:126:A:LYS:H	1:111:A:VAL:HG23	12	0.25
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	14	0.25
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	3	0.25
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	20	0.25
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	16	0.25
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	18	0.25
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	4	0.25
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	13	0.25
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	10	0.25
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	16	0.25
(1,227)	1:200:A:ARG:H	1:199:A:PRO:HB2	2	0.25
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB2	20	0.25
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	6	0.25
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG22	11	0.25
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	4	0.25
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	15	0.25
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	13	0.25
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD13	18	0.25
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	4	0.24
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	20	0.24
(2,161)	1:186:A:MET:HG3	1:170:A:ARG:HD3	14	0.24
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	15	0.24
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	4	0.24
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	17	0.24
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	4	0.24
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	8	0.24
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	15	0.24
(2,130)	1:171:A:ALA:HA	1:172:A:ARG:HB2	1	0.24
(2,126)	1:112:A:ASN:HA	1:196:A:ARG:HG3	12	0.24
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	13	0.24
(2,110)	1:126:A:LYS:HA	1:200:A:ARG:HA	15	0.24
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	11	0.24
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	1	0.24
(2,66)	1:168:A:GLN:H	1:142:A:PRO:HA	19	0.24
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	16	0.24
(2,55)	1:123:A:GLU:H	1:109:A:ARG:HA	11	0.24
(2,7)	1:135:A:GLN:H	1:136:A:VAL:HG11	20	0.24
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	12	0.24
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	15	0.24
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	19	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	20	0.24
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	4	0.24
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG23	4	0.24
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	5	0.24
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	10	0.24
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	14	0.24
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG22	20	0.24
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	15	0.24
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG22	17	0.24
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	6	0.24
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	3	0.24
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	16	0.24
(1,1626)	1:159:A:PHE:HD2	1:161:A:PHE:HD2	7	0.24
(1,1597)	1:180:A:LEU:HD12	1:152:A:ILE:HD13	16	0.24
(1,1593)	1:119:A:ILE:H	1:119:A:ILE:HG23	14	0.24
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	4	0.24
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG21	11	0.24
(1,1578)	1:140:A:THR:HG21	1:138:A:LYS:HE3	1	0.24
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	1	0.24
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	4	0.24
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	8	0.24
(1,1571)	1:197:A:LEU:HD22	1:197:A:LEU:HG	12	0.24
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	13	0.24
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	20	0.24
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	3	0.24
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	10	0.24
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	10	0.24
(1,1479)	1:152:A:ILE:HD12	1:175:A:PHE:HE1	14	0.24
(1,1476)	1:119:A:ILE:HG22	1:117:A:MET:HG3	13	0.24
(1,1435)	1:136:A:VAL:HG21	1:139:A:MET:HB2	8	0.24
(1,1413)	1:171:A:ALA:HB3	1:195:A:PHE:HZ	2	0.24
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	20	0.24
(1,1377)	1:132:A:GLN:HB3	1:132:A:GLN:H	9	0.24
(1,1358)	1:197:A:LEU:HG	1:197:A:LEU:H	15	0.24
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	6	0.24
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	7	0.24
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	16	0.24
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	17	0.24
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	18	0.24
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	10	0.24
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	7	0.24
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	8	0.24
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	14	0.24
(1,1243)	1:117:A:MET:HA	1:117:A:MET:HG3	3	0.24
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	18	0.24
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	14	0.24
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	15	0.24
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	12	0.24
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	17	0.24
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	7	0.24
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	18	0.24
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	20	0.24
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	1	0.24
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	19	0.24
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	6	0.24
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	9	0.24
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	10	0.24
(1,1104)	1:128:A:LEU:H	1:128:A:LEU:HB3	13	0.24
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD21	13	0.24
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD21	13	0.24
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD23	16	0.24
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	4	0.24
(1,1041)	1:180:A:LEU:HB3	1:117:A:MET:HG3	10	0.24
(1,1017)	1:197:A:LEU:HB2	1:197:A:LEU:HD21	2	0.24
(1,1007)	1:167:A:GLY:HA2	1:168:A:GLN:HB2	2	0.24
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	18	0.24
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	12	0.24
(1,992)	1:193:A:GLY:HA3	1:115:A:PRO:HG3	20	0.24
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	10	0.24
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	4	0.24
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	9	0.24
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	12	0.24
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	13	0.24
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	2	0.24
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	4	0.24
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	11	0.24
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	13	0.24
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	12	0.24
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	2	0.24
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	6	0.24
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	1	0.24
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	7	0.24
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG22	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	16	0.24
(1,773)	1:136:A:VAL:HA	1:138:A:LYS:H	4	0.24
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	1	0.24
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	8	0.24
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	10	0.24
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	12	0.24
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	16	0.24
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	17	0.24
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	20	0.24
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	10	0.24
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	8	0.24
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	16	0.24
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	15	0.24
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	8	0.24
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	18	0.24
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	19	0.24
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	20	0.24
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	5	0.24
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	12	0.24
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD22	7	0.24
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD23	18	0.24
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	2	0.24
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	2	0.24
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	7	0.24
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	11	0.24
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	20	0.24
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	7	0.24
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	13	0.24
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	14	0.24
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	17	0.24
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	12	0.24
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	20	0.24
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	12	0.24
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	5	0.24
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	1	0.24
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	4	0.24
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	16	0.24
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	7	0.24
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	9	0.24
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	4	0.24
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	13	0.24
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	8	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	8	0.24
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	4	0.24
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	14	0.24
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	11	0.24
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	7	0.24
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	8	0.24
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	9	0.24
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	6	0.24
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	7	0.24
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	18	0.24
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	20	0.24
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	14	0.24
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	12	0.24
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	5	0.24
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD11	12	0.24
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	3	0.24
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	4	0.24
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	12	0.24
(1,120)	1:175:A:PHE:H	1:174:A:THR:HG23	20	0.24
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	2	0.24
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	17	0.24
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	12	0.24
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	16	0.24
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	4	0.24
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD3	2	0.23
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD3	19	0.23
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	1	0.23
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	13	0.23
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	16	0.23
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	11	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	2	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	5	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	6	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	8	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	11	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	12	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	13	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	15	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	19	0.23
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	20	0.23
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	13	0.23
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	14	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	14	0.23
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	5	0.23
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	19	0.23
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	2	0.23
(2,102)	1:195:A:PHE:H	1:115:A:PRO:HD3	13	0.23
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	6	0.23
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	11	0.23
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	2	0.23
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	16	0.23
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG3	19	0.23
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	4	0.23
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	16	0.23
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG22	17	0.23
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	18	0.23
(2,37)	1:191:A:GLN:H	1:184:A:VAL:HG12	4	0.23
(2,34)	1:166:A:GLU:H	1:159:A:PHE:HB2	2	0.23
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD23	8	0.23
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	8	0.23
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	5	0.23
(1,1678)	1:121:A:LYS:H	1:120:A:SER:HB2	10	0.23
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG23	8	0.23
(1,1664)	1:118:A:THR:HB	1:118:A:THR:HG21	11	0.23
(1,1655)	1:195:A:PHE:HZ	1:156:A:ARG:HD2	12	0.23
(1,1653)	1:174:A:THR:HB	1:174:A:THR:HG21	8	0.23
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	20	0.23
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	20	0.23
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	20	0.23
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	8	0.23
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	15	0.23
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	20	0.23
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	1	0.23
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	2	0.23
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	7	0.23
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG21	12	0.23
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG21	19	0.23
(1,1597)	1:180:A:LEU:HD11	1:152:A:ILE:HD13	9	0.23
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG22	1	0.23
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG21	10	0.23
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	15	0.23
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	9	0.23
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG12	6	0.23
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	17	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	12	0.23
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	6	0.23
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	5	0.23
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	16	0.23
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	19	0.23
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	13	0.23
(1,1494)	1:155:A:ILE:HD11	1:155:A:ILE:HB	1	0.23
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	9	0.23
(1,1465)	1:146:A:THR:H	1:152:A:ILE:HG21	14	0.23
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG11	19	0.23
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	4	0.23
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	13	0.23
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	17	0.23
(1,1389)	1:138:A:LYS:HG3	1:139:A:MET:H	7	0.23
(1,1369)	1:197:A:LEU:HD12	1:197:A:LEU:HG	16	0.23
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	1	0.23
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	3	0.23
(1,1352)	1:190:A:ARG:HD2	1:190:A:ARG:HG3	5	0.23
(1,1325)	1:171:A:ALA:H	1:170:A:ARG:HG3	4	0.23
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	14	0.23
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	2	0.23
(1,1284)	1:187:A:GLU:H	1:187:A:GLU:HB2	11	0.23
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	7	0.23
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	1	0.23
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	7	0.23
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	16	0.23
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	17	0.23
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	15	0.23
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	2	0.23
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	4	0.23
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	5	0.23
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	11	0.23
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	6	0.23
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	8	0.23
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	8	0.23
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	6	0.23
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	7	0.23
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	17	0.23
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	17	0.23
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD22	9	0.23
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	5	0.23
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	8	0.23
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	15	0.23
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	20	0.23
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	9	0.23
(1,949)	1:133:A:TYR:HD1	1:146:A:THR:H	14	0.23
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	11	0.23
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD1	3	0.23
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	11	0.23
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	12	0.23
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	15	0.23
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	13	0.23
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	6	0.23
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	6	0.23
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	8	0.23
(1,745)	1:131:A:THR:HA	1:132:A:GLN:HG3	12	0.23
(1,720)	1:137:A:SER:HB2	1:138:A:LYS:HB3	19	0.23
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	2	0.23
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	13	0.23
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	14	0.23
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	18	0.23
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	14	0.23
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	13	0.23
(1,688)	1:192:A:PHE:H	1:183:A:ILE:H	11	0.23
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	6	0.23
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	13	0.23
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	3	0.23
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	8	0.23
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	19	0.23
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	20	0.23
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	3	0.23
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	9	0.23
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	11	0.23
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	6	0.23
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	15	0.23
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	16	0.23
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	5	0.23
(1,573)	1:179:A:HIS:H	1:179:A:HIS:HB2	20	0.23
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	4	0.23
(1,568)	1:180:A:LEU:H	1:179:A:HIS:H	8	0.23
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	15	0.23
(1,496)	1:126:A:LYS:H	1:125:A:VAL:HG23	10	0.23
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	8	0.23
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	17	0.23
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	18	0.23
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	7	0.23
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	12	0.23
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	20	0.23
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG22	17	0.23
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	1	0.23
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	12	0.23
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	15	0.23
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	11	0.23
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	15	0.23
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG23	19	0.23
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	14	0.23
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD13	6	0.23
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD12	9	0.23
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	11	0.23
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	1	0.23
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG21	2	0.23
(1,229)	1:200:A:ARG:H	1:200:A:ARG:HG2	15	0.23
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG22	10	0.23
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	3	0.23
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	6	0.23
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	7	0.23
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	12	0.23
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	20	0.23
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD11	9	0.23
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	7	0.23
(1,113)	1:185:A:ASN:H	1:190:A:ARG:HB3	20	0.23
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	5	0.23
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	6	0.23
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	18	0.23
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	17	0.23
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD11	17	0.23
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	6	0.23
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	14	0.22
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	17	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	1	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	3	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	4	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	7	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	10	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	14	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	16	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	17	0.22
(2,174)	1:124:A:MET:HB2	1:124:A:MET:HB3	18	0.22
(2,161)	1:186:A:MET:HG3	1:170:A:ARG:HD3	5	0.22
(2,146)	1:163:A:ASP:HB2	1:161:A:PHE:HB3	5	0.22
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	14	0.22
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB3	5	0.22
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	12	0.22
(2,114)	1:194:A:PHE:HA	1:114:A:GLU:HB2	6	0.22
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	10	0.22
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	17	0.22
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	12	0.22
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	14	0.22
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	18	0.22
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	8	0.22
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	18	0.22
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	19	0.22
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	3	0.22
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	13	0.22
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG13	19	0.22
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	10	0.22
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	18	0.22
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	15	0.22
(1,1646)	1:195:A:PHE:HE1	1:169:A:VAL:HG11	5	0.22
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	13	0.22
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD13	6	0.22
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD13	8	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG23	3	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG23	4	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	5	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG23	8	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG23	9	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	10	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG21	11	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	13	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG23	14	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	15	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	16	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG23	17	0.22
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1591)	1:183:A:ILE:HG23	1:173:A:LEU:HD13	14	0.22
(1,1589)	1:192:A:PHE:HB3	1:183:A:ILE:HG23	6	0.22
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	2	0.22
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	3	0.22
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	8	0.22
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	13	0.22
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG21	20	0.22
(1,1585)	1:136:A:VAL:HG23	1:136:A:VAL:HG13	1	0.22
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD13	16	0.22
(1,1571)	1:197:A:LEU:HD22	1:197:A:LEU:HG	6	0.22
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	7	0.22
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	14	0.22
(1,1571)	1:197:A:LEU:HD22	1:197:A:LEU:HG	16	0.22
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	19	0.22
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	1	0.22
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	9	0.22
(1,1562)	1:173:A:LEU:HD13	1:174:A:THR:H	11	0.22
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	15	0.22
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	18	0.22
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	20	0.22
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	6	0.22
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	8	0.22
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	16	0.22
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	18	0.22
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	20	0.22
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	4	0.22
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	13	0.22
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	20	0.22
(1,1483)	1:183:A:ILE:HD13	1:195:A:PHE:HD1	4	0.22
(1,1481)	1:152:A:ILE:HD11	1:128:A:LEU:HD21	6	0.22
(1,1479)	1:152:A:ILE:HD12	1:175:A:PHE:HE2	6	0.22
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	3	0.22
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	5	0.22
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	19	0.22
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	12	0.22
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD22	7	0.22
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD21	15	0.22
(1,1403)	1:180:A:LEU:HD13	1:183:A:ILE:HD12	8	0.22
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG22	19	0.22
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD23	5	0.22
(1,1369)	1:197:A:LEU:HD11	1:197:A:LEU:HG	6	0.22
(1,1369)	1:197:A:LEU:HD12	1:197:A:LEU:HG	11	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	7	0.22
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	3	0.22
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	8	0.22
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	16	0.22
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	18	0.22
(1,1335)	1:162:A:PRO:HG2	1:161:A:PHE:HA	1	0.22
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	3	0.22
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	12	0.22
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	18	0.22
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	7	0.22
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	4	0.22
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	13	0.22
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	20	0.22
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	5	0.22
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	7	0.22
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	12	0.22
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	15	0.22
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	11	0.22
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	18	0.22
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	4	0.22
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	11	0.22
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	19	0.22
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	9	0.22
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	1	0.22
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD22	4	0.22
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	5	0.22
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	12	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	1	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	2	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	3	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	6	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	11	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	16	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	17	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	18	0.22
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	20	0.22
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	1	0.22
(1,973)	1:158:A:PRO:HD2	1:157:A:ARG:H	2	0.22
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	10	0.22
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	1	0.22
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE2	8	0.22
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	2	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	9	0.22
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG23	16	0.22
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG12	6	0.22
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG12	8	0.22
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	3	0.22
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	9	0.22
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	19	0.22
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	5	0.22
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	1	0.22
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	14	0.22
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	12	0.22
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	2	0.22
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	5	0.22
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	17	0.22
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG22	7	0.22
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG21	15	0.22
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	9	0.22
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	5	0.22
(1,716)	1:162:A:PRO:HA	1:163:A:ASP:HA	7	0.22
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	7	0.22
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	2	0.22
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	4	0.22
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	12	0.22
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	15	0.22
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD13	10	0.22
(1,636)	1:143:A:GLY:H	1:155:A:ILE:HD12	17	0.22
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	8	0.22
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	3	0.22
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	12	0.22
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	17	0.22
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	2	0.22
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	6	0.22
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	7	0.22
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	8	0.22
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	11	0.22
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	17	0.22
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	18	0.22
(1,597)	1:185:A:ASN:H	1:188:A:ASN:H	19	0.22
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	2	0.22
(1,589)	1:131:A:THR:H	1:132:A:GLN:HA	8	0.22
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	7	0.22
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB1	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,540)	1:122:A:ASN:H	1:121:A:LYS:HG3	5	0.22
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	10	0.22
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG22	9	0.22
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	1	0.22
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	9	0.22
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	15	0.22
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	3	0.22
(1,473)	1:116:A:ASP:H	1:181:A:ALA:HB1	10	0.22
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	10	0.22
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	19	0.22
(1,415)	1:159:A:PHE:H	1:159:A:PHE:HE2	12	0.22
(1,407)	1:168:A:GLN:H	1:158:A:PRO:HD2	5	0.22
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD13	8	0.22
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	17	0.22
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	12	0.22
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD13	11	0.22
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD12	13	0.22
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	9	0.22
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	1	0.22
(1,216)	1:161:A:PHE:H	1:162:A:PRO:HD2	5	0.22
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	6	0.22
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	7	0.22
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	19	0.22
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	20	0.22
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	6	0.22
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	16	0.22
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	7	0.22
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	12	0.22
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	17	0.22
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	13	0.22
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	16	0.22
(1,99)	1:165:A:LYS:H	1:163:A:ASP:HA	5	0.22
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	8	0.22
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	19	0.22
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	19	0.22
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	20	0.22
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	2	0.22
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD3	15	0.21
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	11	0.21
(2,202)	1:184:A:VAL:HG11	1:172:A:ARG:HG2	19	0.21
(2,202)	1:184:A:VAL:HG12	1:172:A:ARG:HG2	20	0.21
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	6	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	3	0.21
(2,178)	1:165:A:LYS:HD2	1:165:A:LYS:HG3	5	0.21
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	1	0.21
(2,141)	1:126:A:LYS:HE3	1:109:A:ARG:HA	16	0.21
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	1	0.21
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	2	0.21
(2,117)	1:124:A:MET:HA	1:119:A:ILE:HD13	10	0.21
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	19	0.21
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG2	11	0.21
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	9	0.21
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	1	0.21
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	4	0.21
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	15	0.21
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	4	0.21
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	11	0.21
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	15	0.21
(2,7)	1:135:A:GLN:H	1:136:A:VAL:HG13	4	0.21
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	11	0.21
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	9	0.21
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	19	0.21
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	20	0.21
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	12	0.21
(1,1705)	1:127:A:LEU:HB2	1:124:A:MET:HA	8	0.21
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	17	0.21
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	17	0.21
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	7	0.21
(1,1669)	1:125:A:VAL:HA	1:128:A:LEU:HD23	7	0.21
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG23	10	0.21
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	3	0.21
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	5	0.21
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	8	0.21
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	9	0.21
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	10	0.21
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	14	0.21
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	18	0.21
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	19	0.21
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	20	0.21
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	12	0.21
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	10	0.21
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	13	0.21
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG21	6	0.21
(1,1603)	1:182:A:THR:HB	1:182:A:THR:HG22	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG21	14	0.21
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	17	0.21
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG13	20	0.21
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	3	0.21
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	15	0.21
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	19	0.21
(1,1562)	1:173:A:LEU:HD12	1:174:A:THR:H	20	0.21
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	4	0.21
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	6	0.21
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	8	0.21
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	3	0.21
(1,1479)	1:152:A:ILE:HD13	1:175:A:PHE:HE1	8	0.21
(1,1476)	1:119:A:ILE:HG21	1:117:A:MET:HG3	6	0.21
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	2	0.21
(1,1461)	1:183:A:ILE:HG21	1:183:A:ILE:HG13	6	0.21
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	12	0.21
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	6	0.21
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB1	19	0.21
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD22	10	0.21
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG22	1	0.21
(1,1399)	1:121:A:LYS:HG3	1:147:A:VAL:HG23	2	0.21
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD12	6	0.21
(1,1369)	1:197:A:LEU:HD11	1:197:A:LEU:HG	2	0.21
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	9	0.21
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	3	0.21
(1,1315)	1:173:A:LEU:HG	1:183:A:ILE:HA	7	0.21
(1,1312)	1:126:A:LYS:HD3	1:109:A:ARG:HB3	20	0.21
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	20	0.21
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	1	0.21
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	9	0.21
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	15	0.21
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	17	0.21
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	15	0.21
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	4	0.21
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	3	0.21
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	13	0.21
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	14	0.21
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	4	0.21
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	16	0.21
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	15	0.21
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	8	0.21
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	3	0.21
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	10	0.21
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	11	0.21
(1,1076)	1:127:A:LEU:HB2	1:127:A:LEU:HD21	18	0.21
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	6	0.21
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	13	0.21
(1,1010)	1:168:A:GLN:H	1:167:A:GLY:HA3	12	0.21
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD12	14	0.21
(1,990)	1:177:A:GLY:HA2	1:176:A:ASP:HB3	8	0.21
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	14	0.21
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	19	0.21
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	7	0.21
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD12	12	0.21
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	15	0.21
(1,958)	1:159:A:PHE:HD2	1:161:A:PHE:H	16	0.21
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD22	20	0.21
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	2	0.21
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	10	0.21
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	18	0.21
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	19	0.21
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	16	0.21
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	20	0.21
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG11	19	0.21
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	14	0.21
(1,844)	1:145:A:PHE:HA	1:154:A:MET:HB2	16	0.21
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	20	0.21
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	1	0.21
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	2	0.21
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	3	0.21
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	4	0.21
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	10	0.21
(1,751)	1:184:A:VAL:HA	1:192:A:PHE:HD2	8	0.21
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	13	0.21
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	2	0.21
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	10	0.21
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	19	0.21
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	8	0.21
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	9	0.21
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	5	0.21
(1,678)	1:124:A:MET:H	1:120:A:SER:H	15	0.21
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	1	0.21
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	2	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,671)	1:156:A:ARG:H	1:156:A:ARG:HG2	5	0.21
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	3	0.21
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	4	0.21
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	13	0.21
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB2	6	0.21
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	13	0.21
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	14	0.21
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	20	0.21
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	15	0.21
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	18	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	1	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	3	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	9	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	12	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	13	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	18	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	19	0.21
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	20	0.21
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	20	0.21
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	2	0.21
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	19	0.21
(1,498)	1:194:A:PHE:H	1:183:A:ILE:HG23	8	0.21
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	7	0.21
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	12	0.21
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	19	0.21
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	20	0.21
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	13	0.21
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	17	0.21
(1,475)	1:116:A:ASP:H	1:182:A:THR:HG21	15	0.21
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	13	0.21
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	15	0.21
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	5	0.21
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	10	0.21
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD13	1	0.21
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	18	0.21
(1,333)	1:124:A:MET:H	1:110:A:MET:H	12	0.21
(1,333)	1:124:A:MET:H	1:110:A:MET:H	18	0.21
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	2	0.21
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	8	0.21
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG22	12	0.21
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	12	0.21
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD13	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	6	0.21
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	16	0.21
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	7	0.21
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	8	0.21
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	17	0.21
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	19	0.21
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	18	0.21
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	20	0.21
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	15	0.21
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	1	0.21
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	17	0.21
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB3	7	0.21
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG22	13	0.21
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	5	0.21
(1,99)	1:165:A:LYS:H	1:163:A:ASP:HA	19	0.21
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG21	14	0.21
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG21	16	0.21
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG22	18	0.21
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	13	0.21
(1,66)	1:153:A:GLU:H	1:128:A:LEU:HD21	6	0.21
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	6	0.21
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	11	0.21
(2,222)	1:172:A:ARG:HD3	1:172:A:ARG:HB3	3	0.2
(2,180)	1:172:A:ARG:HG3	1:151:A:SER:HB2	14	0.2
(2,178)	1:165:A:LYS:HD2	1:165:A:LYS:HG3	9	0.2
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	20	0.2
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD3	4	0.2
(2,153)	1:133:A:TYR:HB2	1:128:A:LEU:HB3	2	0.2
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	19	0.2
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	9	0.2
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG22	12	0.2
(2,121)	1:171:A:ALA:H	1:153:A:GLU:HA	20	0.2
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	11	0.2
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	17	0.2
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD2	10	0.2
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	16	0.2
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	12	0.2
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	11	0.2
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	9	0.2
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	20	0.2
(2,55)	1:123:A:GLU:H	1:109:A:ARG:HA	17	0.2
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG23	6	0.2
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	9	0.2
(2,34)	1:166:A:GLU:H	1:159:A:PHE:HB2	12	0.2
(2,32)	1:166:A:GLU:H	1:164:A:SER:HB3	10	0.2
(2,31)	1:166:A:GLU:H	1:159:A:PHE:H	5	0.2
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	4	0.2
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	10	0.2
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	19	0.2
(2,10)	1:195:A:PHE:H	1:194:A:PHE:HB2	15	0.2
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	1	0.2
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	7	0.2
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	8	0.2
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	12	0.2
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	17	0.2
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	14	0.2
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	7	0.2
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	15	0.2
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	5	0.2
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	11	0.2
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	18	0.2
(1,1644)	1:173:A:LEU:HB3	1:175:A:PHE:HE1	14	0.2
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	1	0.2
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	2	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	4	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	6	0.2
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	7	0.2
(1,1642)	1:175:A:PHE:HD2	1:175:A:PHE:HE2	11	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	12	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	13	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	15	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	16	0.2
(1,1642)	1:175:A:PHE:HD1	1:175:A:PHE:HE1	17	0.2
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	12	0.2
(1,1626)	1:159:A:PHE:HD2	1:161:A:PHE:HD2	17	0.2
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG21	9	0.2
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG23	13	0.2
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD13	1	0.2
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB3	16	0.2
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	11	0.2
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	17	0.2
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG21	1	0.2
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	17	0.2
(1,1494)	1:155:A:ILE:HD13	1:155:A:ILE:HB	7	0.2
(1,1494)	1:155:A:ILE:HD13	1:155:A:ILE:HB	14	0.2
(1,1485)	1:183:A:ILE:HD12	1:115:A:PRO:HA	17	0.2
(1,1480)	1:152:A:ILE:HD13	1:152:A:ILE:HA	18	0.2
(1,1471)	1:119:A:ILE:HG23	1:175:A:PHE:HE2	19	0.2
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG22	7	0.2
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG23	13	0.2
(1,1459)	1:183:A:ILE:HG21	1:172:A:ARG:HB3	1	0.2
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG13	7	0.2
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	13	0.2
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	15	0.2
(1,1414)	1:147:A:VAL:HG13	1:145:A:PHE:HZ	16	0.2
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	1	0.2
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	13	0.2
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD13	8	0.2
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD13	13	0.2
(1,1369)	1:197:A:LEU:HD12	1:197:A:LEU:HG	17	0.2
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB3	3	0.2
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	17	0.2
(1,1342)	1:183:A:ILE:HG13	1:183:A:ILE:HA	14	0.2
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	6	0.2
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	14	0.2
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG21	9	0.2
(1,1239)	1:151:A:SER:HB3	1:172:A:ARG:HB2	7	0.2
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	17	0.2
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	12	0.2
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	20	0.2
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE3	7	0.2
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG12	14	0.2
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	16	0.2
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	17	0.2
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	20	0.2
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	7	0.2
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	6	0.2
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	10	0.2
(1,1084)	1:150:A:ASN:HB3	1:174:A:THR:HG22	10	0.2
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	15	0.2
(1,988)	1:177:A:GLY:H	1:177:A:GLY:HA3	10	0.2
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD13	10	0.2
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	18	0.2
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD2	8	0.2
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	4	0.2
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	2	0.2
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	2	0.2
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	7	0.2
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	12	0.2
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	16	0.2
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	1	0.2
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	14	0.2
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG21	3	0.2
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	19	0.2
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	8	0.2
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	17	0.2
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	19	0.2
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	1	0.2
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	11	0.2
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	16	0.2
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	18	0.2
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	4	0.2
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	6	0.2
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	20	0.2
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	9	0.2
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	3	0.2
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	17	0.2
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	3	0.2
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	5	0.2
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	9	0.2
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	12	0.2
(1,661)	1:182:A:THR:H	1:182:A:THR:HG21	4	0.2
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	13	0.2
(1,652)	1:181:A:ALA:H	1:180:A:LEU:HD12	8	0.2
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	15	0.2
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD21	11	0.2
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD21	15	0.2
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	18	0.2
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	7	0.2
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	14	0.2
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	16	0.2
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	5	0.2
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	10	0.2
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	14	0.2
(1,571)	1:179:A:HIS:H	1:178:A:ASP:HA	12	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	14	0.2
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	1	0.2
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	4	0.2
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	6	0.2
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	8	0.2
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	9	0.2
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	16	0.2
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB1	7	0.2
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB3	20	0.2
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	10	0.2
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	11	0.2
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	10	0.2
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	2	0.2
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	5	0.2
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	3	0.2
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	5	0.2
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	1	0.2
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	3	0.2
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	12	0.2
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG11	3	0.2
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	13	0.2
(1,333)	1:124:A:MET:H	1:110:A:MET:H	4	0.2
(1,333)	1:124:A:MET:H	1:110:A:MET:H	8	0.2
(1,333)	1:124:A:MET:H	1:110:A:MET:H	14	0.2
(1,333)	1:124:A:MET:H	1:110:A:MET:H	17	0.2
(1,315)	1:147:A:VAL:H	1:152:A:ILE:HG23	15	0.2
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB1	9	0.2
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD11	4	0.2
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	9	0.2
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	13	0.2
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	8	0.2
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	11	0.2
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	15	0.2
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	16	0.2
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD1	4	0.2
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	16	0.2
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	19	0.2
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	18	0.2
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	8	0.2
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG23	9	0.2
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG22	10	0.2
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	9	0.2
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	8	0.2
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	10	0.2
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	17	0.2
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	12	0.19
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	18	0.19
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	15	0.19
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	18	0.19
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	16	0.19
(2,188)	1:132:A:GLN:HB2	1:144:A:GLU:H	18	0.19
(2,179)	1:165:A:LYS:HD2	1:160:A:ASP:HB3	14	0.19
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	13	0.19
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	17	0.19
(2,173)	1:124:A:MET:HB3	1:123:A:GLU:HB3	2	0.19
(2,147)	1:112:A:ASN:HB3	1:114:A:GLU:HB2	13	0.19
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	15	0.19
(2,141)	1:126:A:LYS:HE3	1:109:A:ARG:HA	4	0.19
(2,138)	1:151:A:SER:HB2	1:172:A:ARG:HD3	6	0.19
(2,127)	1:112:A:ASN:HA	1:111:A:VAL:HG21	10	0.19
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG12	3	0.19
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD23	9	0.19
(2,117)	1:124:A:MET:HA	1:111:A:VAL:HG23	3	0.19
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	11	0.19
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	9	0.19
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	13	0.19
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	6	0.19
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	2	0.19
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	20	0.19
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	8	0.19
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	6	0.19
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	17	0.19
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	8	0.19
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	2	0.19
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	15	0.19
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG22	7	0.19
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG23	8	0.19
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	10	0.19
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	14	0.19
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	4	0.19
(1,1746)	1:128:A:LEU:HD23	1:127:A:LEU:HD22	11	0.19
(1,1729)	1:150:A:ASN:HA	1:174:A:THR:HG23	20	0.19
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	1	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	3	0.19
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	20	0.19
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	16	0.19
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	4	0.19
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD22	5	0.19
(1,1633)	1:195:A:PHE:HE2	1:195:A:PHE:HA	19	0.19
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	13	0.19
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG23	7	0.19
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	17	0.19
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	7	0.19
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD12	12	0.19
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG22	5	0.19
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	6	0.19
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	16	0.19
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG22	19	0.19
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	3	0.19
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	5	0.19
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	2	0.19
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	1	0.19
(1,1535)	1:154:A:MET:HG3	1:173:A:LEU:HD12	16	0.19
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	1	0.19
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	3	0.19
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	10	0.19
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	12	0.19
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	13	0.19
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	19	0.19
(1,1494)	1:155:A:ILE:HD12	1:155:A:ILE:HB	17	0.19
(1,1481)	1:152:A:ILE:HD12	1:128:A:LEU:HD21	9	0.19
(1,1479)	1:152:A:ILE:HD13	1:175:A:PHE:HE1	1	0.19
(1,1474)	1:119:A:ILE:HG22	1:175:A:PHE:HD1	12	0.19
(1,1471)	1:119:A:ILE:HG22	1:175:A:PHE:HE2	11	0.19
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG21	18	0.19
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG22	14	0.19
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	12	0.19
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	6	0.19
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	8	0.19
(1,1414)	1:147:A:VAL:HG11	1:145:A:PHE:HZ	20	0.19
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD21	5	0.19
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD22	12	0.19
(1,1389)	1:138:A:LYS:HG3	1:139:A:MET:H	17	0.19
(1,1370)	1:197:A:LEU:HD11	1:127:A:LEU:HD13	4	0.19
(1,1369)	1:197:A:LEU:HD12	1:197:A:LEU:HG	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	18	0.19
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	5	0.19
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	10	0.19
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	16	0.19
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	4	0.19
(1,1220)	1:186:A:MET:HG2	1:172:A:ARG:HB3	14	0.19
(1,1214)	1:144:A:GLU:HB2	1:136:A:VAL:HG11	13	0.19
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	17	0.19
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	9	0.19
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	10	0.19
(1,1195)	1:118:A:THR:H	1:117:A:MET:HB3	10	0.19
(1,1195)	1:118:A:THR:H	1:117:A:MET:HB3	14	0.19
(1,1189)	1:191:A:GLN:HG3	1:182:A:THR:HG23	8	0.19
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	16	0.19
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	2	0.19
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	4	0.19
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	10	0.19
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	14	0.19
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	14	0.19
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	11	0.19
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	13	0.19
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	14	0.19
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	15	0.19
(1,963)	1:192:A:PHE:HE1	1:192:A:PHE:HA	5	0.19
(1,916)	1:172:A:ARG:HA	1:173:A:LEU:HD11	17	0.19
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD1	11	0.19
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	1	0.19
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	9	0.19
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	5	0.19
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	3	0.19
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	9	0.19
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	11	0.19
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	3	0.19
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	8	0.19
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	12	0.19
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	15	0.19
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	18	0.19
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	5	0.19
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	6	0.19
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	12	0.19
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	14	0.19
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	16	0.19
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	18	0.19
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	20	0.19
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	4	0.19
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG21	16	0.19
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	5	0.19
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	12	0.19
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	12	0.19
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	16	0.19
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	1	0.19
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	20	0.19
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	2	0.19
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	7	0.19
(1,661)	1:182:A:THR:H	1:182:A:THR:HG21	17	0.19
(1,636)	1:143:A:GLY:H	1:155:A:ILE:HD13	7	0.19
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG22	7	0.19
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD22	20	0.19
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	4	0.19
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	6	0.19
(1,606)	1:188:A:ASN:H	1:187:A:GLU:HB3	10	0.19
(1,599)	1:188:A:ASN:H	1:187:A:GLU:HA	4	0.19
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	18	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	3	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	10	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	11	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	12	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	14	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	15	0.19
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	18	0.19
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB3	6	0.19
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	8	0.19
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	12	0.19
(1,510)	1:189:A:ASN:H	1:185:A:ASN:HB2	9	0.19
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	10	0.19
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	14	0.19
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	16	0.19
(1,490)	1:126:A:LYS:H	1:122:A:ASN:HA	17	0.19
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD11	20	0.19
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	6	0.19
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	11	0.19
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	12	0.19
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	14	0.19
(1,399)	1:117:A:MET:H	1:180:A:LEU:HD11	13	0.19
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	10	0.19
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	10	0.19
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD11	5	0.19
(1,333)	1:124:A:MET:H	1:110:A:MET:H	2	0.19
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	7	0.19
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	8	0.19
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	11	0.19
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB3	12	0.19
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	2	0.19
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD13	7	0.19
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG22	4	0.19
(1,249)	1:183:A:ILE:H	1:182:A:THR:HG23	6	0.19
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	3	0.19
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG23	14	0.19
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	11	0.19
(1,229)	1:200:A:ARG:H	1:200:A:ARG:HG2	12	0.19
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	2	0.19
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	4	0.19
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	5	0.19
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	17	0.19
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG22	5	0.19
(1,168)	1:130:A:ALA:H	1:129:A:GLU:HB2	11	0.19
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	9	0.19
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	2	0.19
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	5	0.19
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	4	0.19
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	8	0.19
(1,139)	1:157:A:ARG:H	1:159:A:PHE:HZ	12	0.19
(1,135)	1:180:A:LEU:H	1:180:A:LEU:HD12	4	0.19
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	14	0.19
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB1	17	0.19
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	3	0.19
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	17	0.19
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG21	3	0.19
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG21	13	0.19
(1,73)	1:139:A:MET:H	1:138:A:LYS:HB3	7	0.19
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD13	15	0.19
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	7	0.19
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	15	0.19
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:171:A:ALA:H	1:186:A:MET:HE3	18	0.19
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	9	0.18
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	15	0.18
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	10	0.18
(2,202)	1:184:A:VAL:HG11	1:172:A:ARG:HG2	17	0.18
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HD3	1	0.18
(2,179)	1:165:A:LYS:HD2	1:160:A:ASP:HB3	1	0.18
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	6	0.18
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	18	0.18
(2,178)	1:165:A:LYS:HD2	1:165:A:LYS:HG3	19	0.18
(2,157)	1:122:A:ASN:HB2	1:121:A:LYS:HB2	8	0.18
(2,147)	1:112:A:ASN:HB2	1:114:A:GLU:HB2	20	0.18
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	11	0.18
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG13	5	0.18
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	4	0.18
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB3	7	0.18
(2,97)	1:173:A:LEU:H	1:172:A:ARG:HG2	8	0.18
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	8	0.18
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	15	0.18
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	3	0.18
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	15	0.18
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	2	0.18
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	3	0.18
(2,56)	1:110:A:MET:H	1:123:A:GLU:HB3	5	0.18
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	9	0.18
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	4	0.18
(2,34)	1:166:A:GLU:H	1:159:A:PHE:HB2	18	0.18
(2,29)	1:124:A:MET:H	1:173:A:LEU:HD22	13	0.18
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG13	12	0.18
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	9	0.18
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	4	0.18
(1,1718)	1:138:A:LYS:HA	1:136:A:VAL:HG12	16	0.18
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	11	0.18
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	2	0.18
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	3	0.18
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	20	0.18
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	16	0.18
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	20	0.18
(1,1674)	1:152:A:ILE:H	1:151:A:SER:HB3	8	0.18
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	5	0.18
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	12	0.18
(1,1638)	1:113:A:LEU:HB3	1:195:A:PHE:HD1	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD11	19	0.18
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	6	0.18
(1,1588)	1:142:A:PRO:HA	1:155:A:ILE:HG21	13	0.18
(1,1577)	1:115:A:PRO:HB3	1:182:A:THR:HG21	5	0.18
(1,1571)	1:197:A:LEU:HD22	1:197:A:LEU:HG	10	0.18
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	7	0.18
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	15	0.18
(1,1527)	1:117:A:MET:HG3	1:180:A:LEU:HD22	14	0.18
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	7	0.18
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	9	0.18
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	11	0.18
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	17	0.18
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	11	0.18
(1,1496)	1:183:A:ILE:HB	1:192:A:PHE:HD2	2	0.18
(1,1491)	1:119:A:ILE:HD13	1:119:A:ILE:HB	11	0.18
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD1	7	0.18
(1,1483)	1:183:A:ILE:HD12	1:195:A:PHE:HD1	12	0.18
(1,1474)	1:119:A:ILE:HG21	1:175:A:PHE:HD1	13	0.18
(1,1461)	1:183:A:ILE:HG23	1:183:A:ILE:HG13	5	0.18
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	2	0.18
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG12	17	0.18
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	18	0.18
(1,1413)	1:171:A:ALA:HB2	1:195:A:PHE:HZ	17	0.18
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB2	10	0.18
(1,1406)	1:180:A:LEU:HD13	1:175:A:PHE:HD1	3	0.18
(1,1406)	1:180:A:LEU:HD13	1:175:A:PHE:HD1	11	0.18
(1,1406)	1:180:A:LEU:HD12	1:175:A:PHE:HD1	13	0.18
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD13	16	0.18
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD21	14	0.18
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	20	0.18
(1,1392)	1:197:A:LEU:HD23	1:195:A:PHE:HE1	4	0.18
(1,1370)	1:197:A:LEU:HD12	1:127:A:LEU:HD11	9	0.18
(1,1369)	1:197:A:LEU:HD11	1:197:A:LEU:HG	20	0.18
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	11	0.18
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	17	0.18
(1,1315)	1:173:A:LEU:HG	1:183:A:ILE:HA	20	0.18
(1,1312)	1:126:A:LYS:HD3	1:109:A:ARG:HB3	19	0.18
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	11	0.18
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	13	0.18
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	20	0.18
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	2	0.18
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD12	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD11	10	0.18
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD11	13	0.18
(1,1216)	1:111:A:VAL:HB	1:197:A:LEU:HD13	18	0.18
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	10	0.18
(1,1195)	1:118:A:THR:H	1:117:A:MET:HB3	17	0.18
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	20	0.18
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE3	8	0.18
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE2	10	0.18
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	6	0.18
(1,1166)	1:153:A:GLU:HG3	1:172:A:ARG:HB2	3	0.18
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	6	0.18
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	9	0.18
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	11	0.18
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	13	0.18
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	2	0.18
(1,1141)	1:185:A:ASN:HB3	1:186:A:MET:HA	19	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	3	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	5	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	6	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	7	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	9	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	12	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	13	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	15	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	17	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	18	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	19	0.18
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	20	0.18
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	5	0.18
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	12	0.18
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	19	0.18
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	17	0.18
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	2	0.18
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	17	0.18
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	18	0.18
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG22	1	0.18
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	18	0.18
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	10	0.18
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	5	0.18
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	19	0.18
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG11	13	0.18
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	5	0.18
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	8	0.18
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	12	0.18
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	19	0.18
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	20	0.18
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	9	0.18
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	3	0.18
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	20	0.18
(1,860)	1:168:A:GLN:HA	1:168:A:GLN:HB2	5	0.18
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	15	0.18
(1,824)	1:151:A:SER:HA	1:175:A:PHE:HB3	6	0.18
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	8	0.18
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	20	0.18
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	4	0.18
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	17	0.18
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	10	0.18
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	8	0.18
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	19	0.18
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG22	8	0.18
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG21	15	0.18
(1,775)	1:136:A:VAL:HA	1:136:A:VAL:HG23	19	0.18
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	7	0.18
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	11	0.18
(1,746)	1:119:A:ILE:HA	1:117:A:MET:HG3	10	0.18
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	2	0.18
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	9	0.18
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	11	0.18
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	3	0.18
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	6	0.18
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	9	0.18
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	16	0.18
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	17	0.18
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	16	0.18
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	6	0.18
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	10	0.18
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	18	0.18
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	19	0.18
(1,678)	1:124:A:MET:H	1:120:A:SER:H	1	0.18
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	11	0.18
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	20	0.18
(1,661)	1:182:A:THR:H	1:182:A:THR:HG22	11	0.18
(1,626)	1:151:A:SER:H	1:150:A:ASN:HB3	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,626)	1:151:A:SER:H	1:150:A:ASN:HB3	19	0.18
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	15	0.18
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG23	10	0.18
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	10	0.18
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	16	0.18
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	17	0.18
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	17	0.18
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	3	0.18
(1,494)	1:126:A:LYS:H	1:125:A:VAL:HB	5	0.18
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	15	0.18
(1,476)	1:116:A:ASP:H	1:180:A:LEU:HD11	16	0.18
(1,475)	1:116:A:ASP:H	1:182:A:THR:HG23	10	0.18
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	9	0.18
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	9	0.18
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	14	0.18
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	20	0.18
(1,333)	1:124:A:MET:H	1:110:A:MET:H	5	0.18
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	1	0.18
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	5	0.18
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	3	0.18
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	4	0.18
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	6	0.18
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	15	0.18
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	15	0.18
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	18	0.18
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	4	0.18
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	8	0.18
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	1	0.18
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	9	0.18
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	12	0.18
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	13	0.18
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	14	0.18
(1,168)	1:130:A:ALA:H	1:129:A:GLU:HB2	5	0.18
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	3	0.18
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	8	0.18
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG22	7	0.18
(1,94)	1:184:A:VAL:H	1:184:A:VAL:HG22	17	0.18
(1,65)	1:153:A:GLU:H	1:173:A:LEU:HD11	13	0.18
(1,36)	1:135:A:GLN:H	1:136:A:VAL:HB	3	0.18
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	3	0.18
(1,11)	1:119:A:ILE:H	1:179:A:HIS:HB3	12	0.18
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,202)	1:184:A:VAL:HG12	1:172:A:ARG:HG2	7	0.17
(2,199)	1:140:A:THR:HG23	1:138:A:LYS:HD3	17	0.17
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	7	0.17
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	8	0.17
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	12	0.17
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	15	0.17
(2,175)	1:119:A:ILE:HA	1:123:A:GLU:HB3	14	0.17
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	8	0.17
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	9	0.17
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	5	0.17
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	1	0.17
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	6	0.17
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	9	0.17
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	14	0.17
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	14	0.17
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD2	4	0.17
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	20	0.17
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	19	0.17
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	5	0.17
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	7	0.17
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	16	0.17
(2,79)	1:189:A:ASN:H	1:190:A:ARG:HB3	17	0.17
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	10	0.17
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	7	0.17
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	12	0.17
(2,44)	1:200:A:ARG:H	1:200:A:ARG:HD3	20	0.17
(2,42)	1:128:A:LEU:H	1:129:A:GLU:HG2	2	0.17
(2,33)	1:166:A:GLU:H	1:165:A:LYS:HE2	3	0.17
(2,33)	1:166:A:GLU:H	1:165:A:LYS:HE2	17	0.17
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD12	14	0.17
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	10	0.17
(2,7)	1:135:A:GLN:H	1:128:A:LEU:HB3	11	0.17
(1,1734)	1:195:A:PHE:HD2	1:195:A:PHE:HB2	2	0.17
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	5	0.17
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	15	0.17
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	16	0.17
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	17	0.17
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	19	0.17
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG21	5	0.17
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG23	10	0.17
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG22	11	0.17
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	9	0.17
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	13	0.17
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG22	20	0.17
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	17	0.17
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	12	0.17
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	19	0.17
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	20	0.17
(1,1636)	1:195:A:PHE:HA	1:195:A:PHE:HD2	6	0.17
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	1	0.17
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	4	0.17
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	12	0.17
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	17	0.17
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD11	15	0.17
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG22	18	0.17
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG12	13	0.17
(1,1571)	1:197:A:LEU:HD23	1:197:A:LEU:HG	9	0.17
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	10	0.17
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	16	0.17
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	12	0.17
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG21	7	0.17
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG22	12	0.17
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	4	0.17
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	14	0.17
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	15	0.17
(1,1507)	1:185:A:ASN:HB2	1:169:A:VAL:HG12	5	0.17
(1,1503)	1:122:A:ASN:HB3	1:123:A:GLU:HB2	14	0.17
(1,1480)	1:152:A:ILE:HD12	1:152:A:ILE:HA	2	0.17
(1,1474)	1:119:A:ILE:HG21	1:175:A:PHE:HD2	16	0.17
(1,1453)	1:138:A:LYS:H	1:136:A:VAL:HG13	3	0.17
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	6	0.17
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	8	0.17
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB3	10	0.17
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	2	0.17
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	16	0.17
(1,1435)	1:136:A:VAL:HG23	1:139:A:MET:HB2	5	0.17
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	12	0.17
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB3	12	0.17
(1,1406)	1:180:A:LEU:HD11	1:175:A:PHE:HD1	17	0.17
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD21	1	0.17
(1,1404)	1:181:A:ALA:H	1:180:A:LEU:HD23	19	0.17
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	5	0.17
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	12	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	16	0.17
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE2	16	0.17
(1,1315)	1:173:A:LEU:HG	1:183:A:ILE:HA	11	0.17
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	9	0.17
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	2	0.17
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	4	0.17
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	6	0.17
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	13	0.17
(1,1227)	1:166:A:GLU:H	1:165:A:LYS:HB2	19	0.17
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	7	0.17
(1,1187)	1:117:A:MET:HB2	1:119:A:ILE:HG23	5	0.17
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	10	0.17
(1,1182)	1:132:A:GLN:HG3	1:132:A:GLN:HA	19	0.17
(1,1178)	1:184:A:VAL:HB	1:172:A:ARG:HB3	11	0.17
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	7	0.17
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	13	0.17
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	10	0.17
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	17	0.17
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	18	0.17
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	1	0.17
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	2	0.17
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	4	0.17
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	8	0.17
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	10	0.17
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	14	0.17
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	16	0.17
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	1	0.17
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	3	0.17
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	13	0.17
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	7	0.17
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	10	0.17
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	13	0.17
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	16	0.17
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	1	0.17
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG21	2	0.17
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	16	0.17
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	17	0.17
(1,1041)	1:180:A:LEU:HB3	1:117:A:MET:HG3	17	0.17
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	19	0.17
(1,963)	1:192:A:PHE:HE1	1:192:A:PHE:HA	11	0.17
(1,940)	1:185:A:ASN:HA	1:169:A:VAL:HG13	5	0.17
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	9	0.17
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	10	0.17
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	3	0.17
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	7	0.17
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	17	0.17
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	16	0.17
(1,879)	1:170:A:ARG:HA	1:170:A:ARG:HD2	17	0.17
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG23	14	0.17
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	15	0.17
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	4	0.17
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	12	0.17
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	17	0.17
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	2	0.17
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	3	0.17
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	4	0.17
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	11	0.17
(1,770)	1:146:A:THR:HA	1:135:A:GLN:HG3	16	0.17
(1,758)	1:137:A:SER:HA	1:138:A:LYS:H	13	0.17
(1,725)	1:158:A:PRO:HA	1:158:A:PRO:HB2	5	0.17
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	20	0.17
(1,708)	1:131:A:THR:HB	1:127:A:LEU:HD12	13	0.17
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	10	0.17
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	14	0.17
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	15	0.17
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	16	0.17
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	1	0.17
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	2	0.17
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	7	0.17
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	11	0.17
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	15	0.17
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	18	0.17
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	15	0.17
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	18	0.17
(1,681)	1:139:A:MET:H	1:139:A:MET:HB3	10	0.17
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	19	0.17
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	1	0.17
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	9	0.17
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB1	18	0.17
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	1	0.17
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	13	0.17
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	19	0.17
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	9	0.17
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	11	0.17
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	12	0.17
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	5	0.17
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	13	0.17
(1,563)	1:163:A:ASP:H	1:162:A:PRO:HA	20	0.17
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB1	5	0.17
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	2	0.17
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	9	0.17
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	7	0.17
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	18	0.17
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	2	0.17
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	18	0.17
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	1	0.17
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	8	0.17
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG12	18	0.17
(1,333)	1:124:A:MET:H	1:110:A:MET:H	9	0.17
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	13	0.17
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	19	0.17
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG23	1	0.17
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	12	0.17
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	16	0.17
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	3	0.17
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	8	0.17
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	16	0.17
(1,258)	1:192:A:PHE:H	1:183:A:ILE:HG22	15	0.17
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	15	0.17
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	3	0.17
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	3	0.17
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	17	0.17
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	18	0.17
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	20	0.17
(1,120)	1:175:A:PHE:H	1:174:A:THR:HG23	7	0.17
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB1	13	0.17
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB3	14	0.17
(1,113)	1:185:A:ASN:H	1:190:A:ARG:HB3	2	0.17
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	1	0.17
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	9	0.17
(1,44)	1:195:A:PHE:H	1:194:A:PHE:HD2	5	0.17
(1,19)	1:171:A:ALA:H	1:173:A:LEU:HD12	11	0.17
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	8	0.17
(1,11)	1:119:A:ILE:H	1:179:A:HIS:HB3	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	6	0.16
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	19	0.16
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	1	0.16
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	2	0.16
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	16	0.16
(2,176)	1:187:A:GLU:HB2	1:169:A:VAL:HG12	15	0.16
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	2	0.16
(2,170)	1:109:A:ARG:HB3	1:109:A:ARG:H	13	0.16
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	3	0.16
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	10	0.16
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	12	0.16
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	2	0.16
(2,140)	1:165:A:LYS:HE2	1:160:A:ASP:HB3	5	0.16
(2,139)	1:172:A:ARG:HD2	1:174:A:THR:HG21	1	0.16
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	2	0.16
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	8	0.16
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD21	18	0.16
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD2	8	0.16
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	1	0.16
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	9	0.16
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	14	0.16
(2,61)	1:133:A:TYR:H	1:129:A:GLU:HB3	8	0.16
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	16	0.16
(2,32)	1:166:A:GLU:H	1:164:A:SER:HB3	1	0.16
(2,32)	1:166:A:GLU:H	1:164:A:SER:HB3	13	0.16
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD11	20	0.16
(2,7)	1:135:A:GLN:H	1:136:A:VAL:HG11	2	0.16
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	10	0.16
(1,1722)	1:170:A:ARG:HA	1:155:A:ILE:HG13	7	0.16
(1,1697)	1:131:A:THR:HA	1:131:A:THR:HG23	4	0.16
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	1	0.16
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	19	0.16
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	2	0.16
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	4	0.16
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	11	0.16
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	19	0.16
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	20	0.16
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	2	0.16
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	3	0.16
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	7	0.16
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	8	0.16
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	10	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	15	0.16
(1,1661)	1:195:A:PHE:HZ	1:169:A:VAL:HG12	11	0.16
(1,1648)	1:195:A:PHE:HE2	1:183:A:ILE:HG22	9	0.16
(1,1640)	1:159:A:PHE:HE2	1:198:A:ASP:HB3	5	0.16
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	5	0.16
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	6	0.16
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	19	0.16
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	19	0.16
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD13	7	0.16
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG21	16	0.16
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	10	0.16
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	19	0.16
(1,1599)	1:182:A:THR:HB	1:180:A:LEU:HD22	17	0.16
(1,1593)	1:119:A:ILE:H	1:119:A:ILE:HG23	4	0.16
(1,1571)	1:197:A:LEU:HD21	1:197:A:LEU:HG	18	0.16
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	3	0.16
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	4	0.16
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	11	0.16
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	13	0.16
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	20	0.16
(1,1555)	1:136:A:VAL:H	1:135:A:GLN:HB2	2	0.16
(1,1527)	1:117:A:MET:HG3	1:180:A:LEU:HD21	17	0.16
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	2	0.16
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	14	0.16
(1,1477)	1:186:A:MET:HE2	1:170:A:ARG:HD2	13	0.16
(1,1471)	1:119:A:ILE:HG23	1:175:A:PHE:HE2	1	0.16
(1,1459)	1:183:A:ILE:HG22	1:172:A:ARG:HB3	15	0.16
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	3	0.16
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	7	0.16
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	11	0.16
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB3	3	0.16
(1,1442)	1:184:A:VAL:HG11	1:172:A:ARG:HB3	8	0.16
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	6	0.16
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	1	0.16
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB2	9	0.16
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD12	12	0.16
(1,1389)	1:138:A:LYS:HG3	1:139:A:MET:H	19	0.16
(1,1369)	1:197:A:LEU:HD11	1:197:A:LEU:HG	3	0.16
(1,1369)	1:197:A:LEU:HD13	1:197:A:LEU:HG	7	0.16
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	3	0.16
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	8	0.16
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	16	0.16
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	20	0.16
(1,1312)	1:126:A:LYS:HD3	1:109:A:ARG:HB3	1	0.16
(1,1269)	1:126:A:LYS:HB2	1:126:A:LYS:HG3	19	0.16
(1,1254)	1:196:A:ARG:HB3	1:196:A:ARG:HD3	2	0.16
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	1	0.16
(1,1220)	1:186:A:MET:HG2	1:172:A:ARG:HB3	13	0.16
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	6	0.16
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	2	0.16
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	14	0.16
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	15	0.16
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	16	0.16
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	11	0.16
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	19	0.16
(1,1139)	1:189:A:ASN:HA	1:189:A:ASN:HB3	11	0.16
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	9	0.16
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	17	0.16
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	6	0.16
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	8	0.16
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	9	0.16
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	11	0.16
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	15	0.16
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	18	0.16
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	10	0.16
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	14	0.16
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	15	0.16
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD23	5	0.16
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD21	12	0.16
(1,1084)	1:150:A:ASN:HB3	1:174:A:THR:HG23	8	0.16
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG22	8	0.16
(1,1056)	1:126:A:LYS:HE3	1:109:A:ARG:HB3	9	0.16
(1,969)	1:162:A:PRO:HD3	1:161:A:PHE:HB2	9	0.16
(1,956)	1:112:A:ASN:HA	1:196:A:ARG:HA	4	0.16
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	10	0.16
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD23	1	0.16
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD22	4	0.16
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	11	0.16
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	14	0.16
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	13	0.16
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	15	0.16
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	3	0.16
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	6	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	17	0.16
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD1	10	0.16
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	7	0.16
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	14	0.16
(1,862)	1:191:A:GLN:H	1:190:A:ARG:HA	2	0.16
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	1	0.16
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	9	0.16
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	13	0.16
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG23	2	0.16
(1,730)	1:147:A:VAL:HA	1:147:A:VAL:HG22	14	0.16
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	18	0.16
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	2	0.16
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG21	6	0.16
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	15	0.16
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	17	0.16
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG21	19	0.16
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	8	0.16
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	13	0.16
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	20	0.16
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	13	0.16
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	16	0.16
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	17	0.16
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	1	0.16
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	7	0.16
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	15	0.16
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	19	0.16
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	14	0.16
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	16	0.16
(1,675)	1:120:A:SER:H	1:119:A:ILE:HG13	14	0.16
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	11	0.16
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	5	0.16
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	10	0.16
(1,661)	1:182:A:THR:H	1:182:A:THR:HG22	14	0.16
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	18	0.16
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	10	0.16
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB2	5	0.16
(1,612)	1:132:A:GLN:H	1:159:A:PHE:HZ	1	0.16
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	1	0.16
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	8	0.16
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG21	7	0.16
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG23	17	0.16
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG21	19	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	1	0.16
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	2	0.16
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	15	0.16
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	4	0.16
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	8	0.16
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	20	0.16
(1,475)	1:116:A:ASP:H	1:182:A:THR:HG23	2	0.16
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	3	0.16
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	4	0.16
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	14	0.16
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	19	0.16
(1,439)	1:114:A:GLU:H	1:119:A:ILE:HD11	7	0.16
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	6	0.16
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	10	0.16
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	12	0.16
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	6	0.16
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	11	0.16
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	18	0.16
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD13	2	0.16
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	5	0.16
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	6	0.16
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	9	0.16
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	20	0.16
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD12	6	0.16
(1,333)	1:124:A:MET:H	1:110:A:MET:H	1	0.16
(1,333)	1:124:A:MET:H	1:110:A:MET:H	3	0.16
(1,333)	1:124:A:MET:H	1:110:A:MET:H	10	0.16
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	17	0.16
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	1	0.16
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	5	0.16
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	12	0.16
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	17	0.16
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	19	0.16
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	20	0.16
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	11	0.16
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	10	0.16
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG23	13	0.16
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	12	0.16
(1,229)	1:200:A:ARG:H	1:200:A:ARG:HG2	10	0.16
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	6	0.16
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	9	0.16
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,202)	1:113:A:LEU:H	1:113:A:LEU:HD12	2	0.16
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	3	0.16
(1,142)	1:157:A:ARG:H	1:156:A:ARG:HG2	5	0.16
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	9	0.16
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	11	0.16
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	19	0.16
(1,50)	1:195:A:PHE:H	1:195:A:PHE:HD2	11	0.16
(1,49)	1:195:A:PHE:H	1:183:A:ILE:HG22	5	0.16
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	19	0.16
(1,11)	1:119:A:ILE:H	1:179:A:HIS:HB3	10	0.16
(2,224)	1:190:A:ARG:HG2	1:190:A:ARG:HD2	20	0.15
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	5	0.15
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	7	0.15
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	10	0.15
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD2	13	0.15
(2,209)	1:194:A:PHE:HD1	1:194:A:PHE:HB3	11	0.15
(2,161)	1:186:A:MET:HG2	1:172:A:ARG:HD3	18	0.15
(2,157)	1:122:A:ASN:HB2	1:121:A:LYS:HB2	20	0.15
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	4	0.15
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	20	0.15
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	3	0.15
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	20	0.15
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	9	0.15
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	7	0.15
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	11	0.15
(2,132)	1:167:A:GLY:HA3	1:166:A:GLU:HG3	9	0.15
(2,129)	1:115:A:PRO:HD3	1:117:A:MET:HE2	1	0.15
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	7	0.15
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	18	0.15
(2,120)	1:170:A:ARG:HA	1:155:A:ILE:HG12	7	0.15
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	18	0.15
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	12	0.15
(2,94)	1:188:A:ASN:H	1:169:A:VAL:HG11	1	0.15
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	6	0.15
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	18	0.15
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	4	0.15
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	4	0.15
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	10	0.15
(2,66)	1:168:A:GLN:H	1:158:A:PRO:HA	15	0.15
(2,61)	1:133:A:TYR:H	1:129:A:GLU:HB3	12	0.15
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG23	16	0.15
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	18	0.15
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	6	0.15
(2,22)	1:121:A:LYS:H	1:152:A:ILE:HG13	14	0.15
(2,12)	1:195:A:PHE:H	1:197:A:LEU:HD22	15	0.15
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	14	0.15
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	2	0.15
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	12	0.15
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	3	0.15
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	12	0.15
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	17	0.15
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	20	0.15
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG21	9	0.15
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG21	11	0.15
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG23	19	0.15
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	3	0.15
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	2	0.15
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	12	0.15
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	15	0.15
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	1	0.15
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	6	0.15
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	16	0.15
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD21	2	0.15
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	11	0.15
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	17	0.15
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	18	0.15
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG21	3	0.15
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	17	0.15
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	18	0.15
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	5	0.15
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	6	0.15
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	14	0.15
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	15	0.15
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	20	0.15
(1,1591)	1:183:A:ILE:HG23	1:173:A:LEU:HD11	5	0.15
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD11	6	0.15
(1,1588)	1:142:A:PRO:HA	1:155:A:ILE:HG21	16	0.15
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB3	2	0.15
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB1	18	0.15
(1,1583)	1:139:A:MET:HB3	1:136:A:VAL:HG11	11	0.15
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG13	17	0.15
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG12	18	0.15
(1,1573)	1:180:A:LEU:HB3	1:180:A:LEU:HD13	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	17	0.15
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	20	0.15
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	10	0.15
(1,1551)	1:126:A:LYS:H	1:126:A:LYS:HD3	4	0.15
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG21	8	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	1	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	3	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	7	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	8	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	9	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	12	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	14	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	15	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	17	0.15
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	18	0.15
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	9	0.15
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	6	0.15
(1,1476)	1:119:A:ILE:HG23	1:117:A:MET:HG3	5	0.15
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	14	0.15
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB3	5	0.15
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB3	7	0.15
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB1	13	0.15
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB3	14	0.15
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB1	15	0.15
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG13	5	0.15
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	18	0.15
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	10	0.15
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB2	2	0.15
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB2	15	0.15
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB2	19	0.15
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB1	20	0.15
(1,1406)	1:180:A:LEU:HD11	1:175:A:PHE:HD1	9	0.15
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD22	13	0.15
(1,1389)	1:138:A:LYS:HG3	1:139:A:MET:H	8	0.15
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	8	0.15
(1,1370)	1:197:A:LEU:HD13	1:127:A:LEU:HD11	18	0.15
(1,1328)	1:115:A:PRO:HG3	1:114:A:GLU:HA	15	0.15
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	11	0.15
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	9	0.15
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	3	0.15
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	12	0.15
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	20	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	10	0.15
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	12	0.15
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE1	13	0.15
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	18	0.15
(1,1159)	1:144:A:GLU:HG2	1:136:A:VAL:HG22	6	0.15
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	19	0.15
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	10	0.15
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	2	0.15
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	6	0.15
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	7	0.15
(1,1138)	1:189:A:ASN:H	1:189:A:ASN:HB3	15	0.15
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	2	0.15
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	3	0.15
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	4	0.15
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	5	0.15
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	19	0.15
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	12	0.15
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	16	0.15
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG22	10	0.15
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	8	0.15
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	8	0.15
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	18	0.15
(1,1016)	1:197:A:LEU:HB2	1:111:A:VAL:HG12	15	0.15
(1,1007)	1:167:A:GLY:HA2	1:168:A:GLN:HB2	11	0.15
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	8	0.15
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	12	0.15
(1,956)	1:112:A:ASN:HA	1:196:A:ARG:HA	16	0.15
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	8	0.15
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	1	0.15
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	18	0.15
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	6	0.15
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	15	0.15
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	12	0.15
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD2	20	0.15
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	6	0.15
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	8	0.15
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	10	0.15
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	11	0.15
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	15	0.15
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	19	0.15
(1,875)	1:154:A:MET:HA	1:131:A:THR:HG22	12	0.15
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG21	5	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	11	0.15
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	2	0.15
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	15	0.15
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	8	0.15
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	6	0.15
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	20	0.15
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	7	0.15
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	16	0.15
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	11	0.15
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	18	0.15
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	20	0.15
(1,708)	1:131:A:THR:HB	1:127:A:LEU:HD13	14	0.15
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	9	0.15
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	16	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG21	1	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG21	3	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG21	7	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	8	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	9	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	12	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	13	0.15
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	14	0.15
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	20	0.15
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	3	0.15
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	5	0.15
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	20	0.15
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	8	0.15
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	12	0.15
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	13	0.15
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	1	0.15
(1,678)	1:124:A:MET:H	1:120:A:SER:H	13	0.15
(1,661)	1:182:A:THR:H	1:182:A:THR:HG21	3	0.15
(1,661)	1:182:A:THR:H	1:182:A:THR:HG22	9	0.15
(1,661)	1:182:A:THR:H	1:182:A:THR:HG22	19	0.15
(1,633)	1:167:A:GLY:H	1:166:A:GLU:HG3	5	0.15
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	13	0.15
(1,623)	1:151:A:SER:H	1:147:A:VAL:HG22	3	0.15
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	12	0.15
(1,607)	1:188:A:ASN:H	1:187:A:GLU:HB2	5	0.15
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	3	0.15
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	8	0.15
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	3	0.15
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	1	0.15
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	13	0.15
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	8	0.15
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	16	0.15
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	18	0.15
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	8	0.15
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	12	0.15
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	12	0.15
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	14	0.15
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	4	0.15
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	14	0.15
(1,404)	1:168:A:GLN:H	1:169:A:VAL:HG22	7	0.15
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	6	0.15
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG13	12	0.15
(1,333)	1:124:A:MET:H	1:110:A:MET:H	15	0.15
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	18	0.15
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	18	0.15
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	7	0.15
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	12	0.15
(1,289)	1:134:A:ARG:H	1:144:A:GLU:HA	3	0.15
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	1	0.15
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	20	0.15
(1,257)	1:192:A:PHE:H	1:183:A:ILE:HD11	17	0.15
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	8	0.15
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG22	17	0.15
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	20	0.15
(1,192)	1:176:A:ASP:H	1:175:A:PHE:HB2	10	0.15
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	6	0.15
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	10	0.15
(1,113)	1:185:A:ASN:H	1:190:A:ARG:HB3	19	0.15
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	4	0.15
(1,81)	1:186:A:MET:H	1:186:A:MET:HE2	17	0.15
(1,74)	1:139:A:MET:H	1:146:A:THR:HG22	13	0.15
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	9	0.15
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	20	0.14
(2,209)	1:194:A:PHE:HD2	1:194:A:PHE:HB2	12	0.14
(2,209)	1:194:A:PHE:HD2	1:194:A:PHE:HB2	14	0.14
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG21	11	0.14
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	11	0.14
(2,145)	1:194:A:PHE:HB3	1:114:A:GLU:HG3	1	0.14
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	18	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,139)	1:172:A:ARG:HD2	1:174:A:THR:HG22	19	0.14
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	10	0.14
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	10	0.14
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	16	0.14
(2,111)	1:195:A:PHE:HA	1:171:A:ALA:HB1	18	0.14
(2,109)	1:129:A:GLU:HA	1:200:A:ARG:HG3	18	0.14
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD3	9	0.14
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	3	0.14
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	9	0.14
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	19	0.14
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	19	0.14
(2,33)	1:166:A:GLU:H	1:165:A:LYS:HE2	2	0.14
(2,30)	1:111:A:VAL:H	1:197:A:LEU:HD13	12	0.14
(2,17)	1:165:A:LYS:H	1:164:A:SER:HB3	17	0.14
(2,12)	1:195:A:PHE:H	1:183:A:ILE:HG13	20	0.14
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD21	10	0.14
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	4	0.14
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	4	0.14
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	11	0.14
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	10	0.14
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	14	0.14
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG22	2	0.14
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG21	5	0.14
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG23	1	0.14
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG22	10	0.14
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG22	13	0.14
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	3	0.14
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	7	0.14
(1,1667)	1:151:A:SER:HB2	1:175:A:PHE:HD1	16	0.14
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	9	0.14
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	13	0.14
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	14	0.14
(1,1655)	1:195:A:PHE:HZ	1:156:A:ARG:HD2	4	0.14
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	15	0.14
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	17	0.14
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	14	0.14
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG22	4	0.14
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD12	12	0.14
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG23	9	0.14
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	3	0.14
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	4	0.14
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	11	0.14
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	13	0.14
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	16	0.14
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	18	0.14
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD11	4	0.14
(1,1591)	1:183:A:ILE:HG23	1:173:A:LEU:HD13	11	0.14
(1,1587)	1:155:A:ILE:HA	1:155:A:ILE:HG23	9	0.14
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB3	11	0.14
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG13	11	0.14
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG12	12	0.14
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	15	0.14
(1,1573)	1:180:A:LEU:HB3	1:180:A:LEU:HD11	4	0.14
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	11	0.14
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	15	0.14
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	5	0.14
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	7	0.14
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG22	17	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	2	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	4	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	5	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	6	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	10	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	11	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	13	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	16	0.14
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	20	0.14
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	2	0.14
(1,1519)	1:168:A:GLN:HG2	1:168:A:GLN:HB2	5	0.14
(1,1471)	1:119:A:ILE:HG23	1:175:A:PHE:HE1	2	0.14
(1,1460)	1:173:A:LEU:HG	1:183:A:ILE:HG21	8	0.14
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB3	4	0.14
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB3	16	0.14
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB2	17	0.14
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	4	0.14
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	9	0.14
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB3	12	0.14
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	20	0.14
(1,1435)	1:136:A:VAL:HG22	1:139:A:MET:HB2	16	0.14
(1,1414)	1:147:A:VAL:HG12	1:145:A:PHE:HZ	14	0.14
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB1	5	0.14
(1,1408)	1:131:A:THR:HG22	1:145:A:PHE:HB2	2	0.14
(1,1406)	1:180:A:LEU:HD13	1:175:A:PHE:HD1	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:156:A:ARG:HD3	1:197:A:LEU:HD21	2	0.14
(1,1390)	1:138:A:LYS:HG3	1:138:A:LYS:HA	7	0.14
(1,1389)	1:138:A:LYS:HG3	1:139:A:MET:H	1	0.14
(1,1389)	1:138:A:LYS:HG3	1:139:A:MET:H	9	0.14
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	15	0.14
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	2	0.14
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	12	0.14
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	16	0.14
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	8	0.14
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	10	0.14
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	17	0.14
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	6	0.14
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	19	0.14
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE3	11	0.14
(1,1172)	1:187:A:GLU:HG2	1:189:A:ASN:H	20	0.14
(1,1166)	1:153:A:GLU:HG3	1:172:A:ARG:HB2	17	0.14
(1,1166)	1:153:A:GLU:HG3	1:172:A:ARG:HB2	20	0.14
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG13	19	0.14
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	14	0.14
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	9	0.14
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	16	0.14
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG23	14	0.14
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	7	0.14
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	6	0.14
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	12	0.14
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	20	0.14
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	14	0.14
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	17	0.14
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	18	0.14
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	20	0.14
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	4	0.14
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	1	0.14
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	18	0.14
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	19	0.14
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	5	0.14
(1,982)	1:171:A:ALA:HA	1:173:A:LEU:HD12	20	0.14
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	3	0.14
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	6	0.14
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	7	0.14
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	13	0.14
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	15	0.14
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	16	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	17	0.14
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	18	0.14
(1,956)	1:112:A:ASN:HA	1:196:A:ARG:HA	19	0.14
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	15	0.14
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	18	0.14
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	9	0.14
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	10	0.14
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	14	0.14
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	19	0.14
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD1	7	0.14
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	17	0.14
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	18	0.14
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	17	0.14
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	5	0.14
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	10	0.14
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	13	0.14
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	14	0.14
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	16	0.14
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	18	0.14
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	2	0.14
(1,790)	1:123:A:GLU:HA	1:123:A:GLU:HB2	11	0.14
(1,786)	1:126:A:LYS:HA	1:129:A:GLU:HA	17	0.14
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	12	0.14
(1,781)	1:126:A:LYS:HA	1:128:A:LEU:HA	10	0.14
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	13	0.14
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	4	0.14
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG22	5	0.14
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	11	0.14
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	18	0.14
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	12	0.14
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	2	0.14
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	12	0.14
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	6	0.14
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	2	0.14
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	4	0.14
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	11	0.14
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	16	0.14
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	16	0.14
(1,678)	1:124:A:MET:H	1:120:A:SER:H	18	0.14
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	15	0.14
(1,661)	1:182:A:THR:H	1:182:A:THR:HG22	12	0.14
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB2	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,580)	1:131:A:THR:H	1:129:A:GLU:HA	15	0.14
(1,580)	1:131:A:THR:H	1:129:A:GLU:HA	16	0.14
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	4	0.14
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	5	0.14
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	17	0.14
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	1	0.14
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	10	0.14
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	17	0.14
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	19	0.14
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	7	0.14
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	4	0.14
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	8	0.14
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	20	0.14
(1,395)	1:117:A:MET:H	1:115:A:PRO:HA	3	0.14
(1,395)	1:117:A:MET:H	1:115:A:PRO:HA	8	0.14
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD11	16	0.14
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	17	0.14
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD13	4	0.14
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG11	10	0.14
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG11	16	0.14
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG22	6	0.14
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	9	0.14
(1,307)	1:129:A:GLU:H	1:128:A:LEU:HD13	6	0.14
(1,307)	1:129:A:GLU:H	1:128:A:LEU:HD12	13	0.14
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	10	0.14
(1,289)	1:134:A:ARG:H	1:144:A:GLU:HA	20	0.14
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	5	0.14
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	4	0.14
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	20	0.14
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	15	0.14
(1,225)	1:128:A:LEU:H	1:127:A:LEU:HD21	5	0.14
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	2	0.14
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	7	0.14
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	20	0.14
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG22	12	0.14
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	2	0.14
(1,142)	1:157:A:ARG:H	1:156:A:ARG:HG2	4	0.14
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	2	0.14
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	15	0.14
(1,120)	1:175:A:PHE:H	1:174:A:THR:HG21	12	0.14
(1,114)	1:185:A:ASN:H	1:184:A:VAL:HG23	11	0.14
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:165:A:LYS:H	1:163:A:ASP:HA	11	0.14
(1,81)	1:186:A:MET:H	1:186:A:MET:HE2	12	0.14
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	16	0.13
(2,209)	1:194:A:PHE:HD2	1:194:A:PHE:HB2	15	0.13
(2,200)	1:156:A:ARG:HB3	1:169:A:VAL:HG22	7	0.13
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HD3	19	0.13
(2,178)	1:165:A:LYS:HD3	1:165:A:LYS:HG2	14	0.13
(2,164)	1:199:A:PRO:HB3	1:200:A:ARG:HD2	19	0.13
(2,152)	1:161:A:PHE:H	1:159:A:PHE:HB2	19	0.13
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	17	0.13
(2,144)	1:127:A:LEU:HB2	1:124:A:MET:HB3	19	0.13
(2,142)	1:165:A:LYS:HE3	1:160:A:ASP:HB2	17	0.13
(2,139)	1:172:A:ARG:HD2	1:174:A:THR:HG22	4	0.13
(2,139)	1:172:A:ARG:HD2	1:174:A:THR:HG22	16	0.13
(2,136)	1:172:A:ARG:HD3	1:172:A:ARG:HB2	18	0.13
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	17	0.13
(2,118)	1:124:A:MET:HA	1:173:A:LEU:HD23	16	0.13
(2,116)	1:124:A:MET:HA	1:111:A:VAL:HA	16	0.13
(2,112)	1:151:A:SER:HA	1:175:A:PHE:HB2	14	0.13
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	14	0.13
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD2	1	0.13
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD2	5	0.13
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD3	14	0.13
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	13	0.13
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	20	0.13
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	13	0.13
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	10	0.13
(2,61)	1:133:A:TYR:H	1:129:A:GLU:HB3	15	0.13
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	12	0.13
(2,33)	1:166:A:GLU:H	1:165:A:LYS:HE3	8	0.13
(2,29)	1:124:A:MET:H	1:173:A:LEU:HD22	6	0.13
(1,1746)	1:128:A:LEU:HD23	1:127:A:LEU:HD23	15	0.13
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	6	0.13
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	18	0.13
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	2	0.13
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	3	0.13
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	9	0.13
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	10	0.13
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	13	0.13
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	1	0.13
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	18	0.13
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG22	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG22	2	0.13
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG22	14	0.13
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG21	15	0.13
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	4	0.13
(1,1649)	1:195:A:PHE:HD1	1:197:A:LEU:HD22	16	0.13
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	13	0.13
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	9	0.13
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	3	0.13
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	8	0.13
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	15	0.13
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD11	2	0.13
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	10	0.13
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	1	0.13
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	7	0.13
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	8	0.13
(1,1591)	1:183:A:ILE:HG21	1:173:A:LEU:HD11	2	0.13
(1,1591)	1:183:A:ILE:HG22	1:173:A:LEU:HD13	7	0.13
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	5	0.13
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	14	0.13
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	13	0.13
(1,1564)	1:126:A:LYS:HG3	1:126:A:LYS:H	16	0.13
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	9	0.13
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG22	20	0.13
(1,1548)	1:126:A:LYS:HD2	1:126:A:LYS:HD3	19	0.13
(1,1536)	1:123:A:GLU:HB3	1:119:A:ILE:HG13	2	0.13
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	3	0.13
(1,1491)	1:119:A:ILE:HD11	1:119:A:ILE:HB	3	0.13
(1,1491)	1:119:A:ILE:HD12	1:119:A:ILE:HB	8	0.13
(1,1491)	1:119:A:ILE:HD12	1:119:A:ILE:HB	20	0.13
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB1	5	0.13
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB3	9	0.13
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB1	12	0.13
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB2	13	0.13
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB1	18	0.13
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	9	0.13
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB3	17	0.13
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	6	0.13
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	19	0.13
(1,1437)	1:147:A:VAL:HG22	1:152:A:ILE:HD12	5	0.13
(1,1412)	1:192:A:PHE:HE2	1:171:A:ALA:HB2	11	0.13
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB3	8	0.13
(1,1406)	1:180:A:LEU:HD11	1:175:A:PHE:HD1	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1405)	1:174:A:THR:H	1:180:A:LEU:HD11	15	0.13
(1,1390)	1:138:A:LYS:HG3	1:138:A:LYS:HA	13	0.13
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	5	0.13
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	11	0.13
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	3	0.13
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	1	0.13
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	4	0.13
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	6	0.13
(1,1254)	1:196:A:ARG:HB3	1:196:A:ARG:HD3	8	0.13
(1,1232)	1:171:A:ALA:HA	1:186:A:MET:HB3	20	0.13
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	8	0.13
(1,1198)	1:146:A:THR:HA	1:147:A:VAL:HB	19	0.13
(1,1195)	1:118:A:THR:H	1:117:A:MET:HB3	3	0.13
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	1	0.13
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	6	0.13
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	19	0.13
(1,1178)	1:184:A:VAL:HB	1:172:A:ARG:HB3	7	0.13
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE3	1	0.13
(1,1166)	1:153:A:GLU:HG3	1:172:A:ARG:HB2	11	0.13
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	17	0.13
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	4	0.13
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	20	0.13
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	13	0.13
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	18	0.13
(1,1116)	1:117:A:MET:H	1:116:A:ASP:HB2	1	0.13
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	7	0.13
(1,1092)	1:150:A:ASN:HB2	1:174:A:THR:HG23	4	0.13
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	2	0.13
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	3	0.13
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	6	0.13
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	8	0.13
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	9	0.13
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	14	0.13
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	15	0.13
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG23	9	0.13
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG21	14	0.13
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG22	18	0.13
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	2	0.13
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	9	0.13
(1,1056)	1:126:A:LYS:HE3	1:109:A:ARG:HB3	10	0.13
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	6	0.13
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	9	0.13
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	10	0.13
(1,1010)	1:168:A:GLN:H	1:167:A:GLY:HA3	11	0.13
(1,956)	1:112:A:ASN:HA	1:196:A:ARG:HA	13	0.13
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	2	0.13
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	6	0.13
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	9	0.13
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD23	5	0.13
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	13	0.13
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	18	0.13
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	4	0.13
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	8	0.13
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	11	0.13
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	4	0.13
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	13	0.13
(1,912)	1:154:A:MET:H	1:172:A:ARG:HA	15	0.13
(1,907)	1:180:A:LEU:HA	1:180:A:LEU:HD22	10	0.13
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	5	0.13
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	12	0.13
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	16	0.13
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG23	12	0.13
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	10	0.13
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG11	12	0.13
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	2	0.13
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	13	0.13
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	3	0.13
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	4	0.13
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	11	0.13
(1,815)	1:132:A:GLN:HA	1:129:A:GLU:HG3	15	0.13
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	6	0.13
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	15	0.13
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	5	0.13
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	17	0.13
(1,774)	1:136:A:VAL:HA	1:136:A:VAL:HB	4	0.13
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG22	20	0.13
(1,770)	1:146:A:THR:HA	1:135:A:GLN:HG3	6	0.13
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	3	0.13
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	13	0.13
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	15	0.13
(1,751)	1:184:A:VAL:HA	1:192:A:PHE:HD2	4	0.13
(1,747)	1:119:A:ILE:HA	1:123:A:GLU:HB3	3	0.13
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	15	0.13
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	12	0.13
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	19	0.13
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	14	0.13
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	7	0.13
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	2	0.13
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	5	0.13
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	6	0.13
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	5	0.13
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	10	0.13
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	4	0.13
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	14	0.13
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	17	0.13
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	3	0.13
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	5	0.13
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	17	0.13
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	20	0.13
(1,679)	1:122:A:ASN:H	1:120:A:SER:HB3	12	0.13
(1,678)	1:124:A:MET:H	1:120:A:SER:H	9	0.13
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	9	0.13
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	13	0.13
(1,675)	1:120:A:SER:H	1:119:A:ILE:HG13	7	0.13
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	16	0.13
(1,671)	1:156:A:ARG:H	1:156:A:ARG:HG2	19	0.13
(1,661)	1:182:A:THR:H	1:182:A:THR:HG21	15	0.13
(1,661)	1:182:A:THR:H	1:182:A:THR:HG23	16	0.13
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	4	0.13
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	12	0.13
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	20	0.13
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB2	4	0.13
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB3	16	0.13
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	20	0.13
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	17	0.13
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	18	0.13
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	9	0.13
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	13	0.13
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	14	0.13
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	11	0.13
(1,487)	1:110:A:MET:H	1:126:A:LYS:H	15	0.13
(1,451)	1:174:A:THR:H	1:184:A:VAL:HG21	16	0.13
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	17	0.13
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	16	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	16	0.13
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	18	0.13
(1,335)	1:110:A:MET:H	1:125:A:VAL:HG12	6	0.13
(1,332)	1:110:A:MET:H	1:109:A:ARG:HB2	10	0.13
(1,326)	1:123:A:GLU:H	1:119:A:ILE:HG23	9	0.13
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	2	0.13
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	10	0.13
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	14	0.13
(1,302)	1:129:A:GLU:H	1:130:A:ALA:HB2	13	0.13
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	4	0.13
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	19	0.13
(1,264)	1:197:A:LEU:H	1:197:A:LEU:HB3	15	0.13
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG23	2	0.13
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG22	4	0.13
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG23	7	0.13
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	11	0.13
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	14	0.13
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	18	0.13
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	16	0.13
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	10	0.13
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	13	0.13
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	12	0.13
(1,164)	1:130:A:ALA:H	1:126:A:LYS:HA	13	0.13
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	11	0.13
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	16	0.13
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	19	0.13
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	5	0.13
(1,33)	1:178:A:ASP:H	1:175:A:PHE:HB2	13	0.13
(1,13)	1:119:A:ILE:H	1:119:A:ILE:HD12	5	0.13
(1,1)	1:170:A:ARG:H	1:156:A:ARG:H	19	0.13
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	2	0.12
(2,209)	1:194:A:PHE:HD1	1:194:A:PHE:HB2	13	0.12
(2,202)	1:184:A:VAL:HG12	1:172:A:ARG:HG2	2	0.12
(2,197)	1:184:A:VAL:HG23	1:172:A:ARG:HG2	14	0.12
(2,178)	1:165:A:LYS:HD2	1:165:A:LYS:HG3	10	0.12
(2,175)	1:119:A:ILE:HA	1:123:A:GLU:HB3	5	0.12
(2,157)	1:122:A:ASN:HB2	1:121:A:LYS:HB2	3	0.12
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	16	0.12
(2,141)	1:126:A:LYS:HE3	1:109:A:ARG:HA	9	0.12
(2,141)	1:126:A:LYS:HE3	1:109:A:ARG:HA	19	0.12
(2,139)	1:172:A:ARG:HD2	1:174:A:THR:HG22	3	0.12
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	20	0.12
(2,119)	1:122:A:ASN:HA	1:125:A:VAL:HG11	20	0.12
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	19	0.12
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD3	15	0.12
(2,92)	1:188:A:ASN:H	1:190:A:ARG:HD2	20	0.12
(2,88)	1:163:A:ASP:H	1:164:A:SER:HB3	9	0.12
(2,59)	1:172:A:ARG:H	1:172:A:ARG:HD3	8	0.12
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG23	3	0.12
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG21	11	0.12
(2,45)	1:169:A:VAL:H	1:169:A:VAL:HG23	13	0.12
(2,42)	1:128:A:LEU:H	1:126:A:LYS:HE3	20	0.12
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	9	0.12
(2,41)	1:161:A:PHE:H	1:164:A:SER:HB2	20	0.12
(2,38)	1:113:A:LEU:H	1:196:A:ARG:HD2	3	0.12
(2,24)	1:121:A:LYS:H	1:123:A:GLU:HB2	2	0.12
(2,20)	1:112:A:ASN:H	1:119:A:ILE:HD13	12	0.12
(2,1)	1:170:A:ARG:H	1:187:A:GLU:HG3	1	0.12
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	11	0.12
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	13	0.12
(1,1722)	1:170:A:ARG:HA	1:155:A:ILE:HG13	1	0.12
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	5	0.12
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	3	0.12
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	5	0.12
(1,1684)	1:199:A:PRO:HA	1:199:A:PRO:HD3	8	0.12
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG22	19	0.12
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG23	7	0.12
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG23	8	0.12
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG21	16	0.12
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG21	20	0.12
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	19	0.12
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	11	0.12
(1,1663)	1:118:A:THR:H	1:118:A:THR:HB	17	0.12
(1,1647)	1:195:A:PHE:HE2	1:171:A:ALA:HB2	1	0.12
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	14	0.12
(1,1628)	1:146:A:THR:H	1:146:A:THR:HB	4	0.12
(1,1618)	1:192:A:PHE:HD2	1:183:A:ILE:HG21	11	0.12
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	18	0.12
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	20	0.12
(1,1609)	1:145:A:PHE:HD1	1:128:A:LEU:HD13	17	0.12
(1,1604)	1:182:A:THR:HB	1:184:A:VAL:HG22	11	0.12
(1,1602)	1:182:A:THR:HB	1:182:A:THR:HA	8	0.12
(1,1601)	1:182:A:THR:HB	1:182:A:THR:H	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1588)	1:142:A:PRO:HA	1:155:A:ILE:HG23	18	0.12
(1,1581)	1:136:A:VAL:H	1:136:A:VAL:HG11	10	0.12
(1,1574)	1:173:A:LEU:HB2	1:180:A:LEU:HD11	10	0.12
(1,1571)	1:197:A:LEU:HD22	1:197:A:LEU:HG	5	0.12
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	8	0.12
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	12	0.12
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	14	0.12
(1,1527)	1:117:A:MET:HG3	1:180:A:LEU:HD23	10	0.12
(1,1491)	1:119:A:ILE:HD12	1:119:A:ILE:HB	6	0.12
(1,1491)	1:119:A:ILE:HD11	1:119:A:ILE:HB	7	0.12
(1,1477)	1:186:A:MET:HE1	1:170:A:ARG:HD2	1	0.12
(1,1471)	1:119:A:ILE:HG22	1:175:A:PHE:HE2	17	0.12
(1,1463)	1:183:A:ILE:HG23	1:195:A:PHE:HB3	15	0.12
(1,1462)	1:195:A:PHE:HD2	1:183:A:ILE:HG22	11	0.12
(1,1460)	1:173:A:LEU:HG	1:183:A:ILE:HG23	14	0.12
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB1	3	0.12
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	1	0.12
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	20	0.12
(1,1443)	1:184:A:VAL:HA	1:184:A:VAL:HG11	11	0.12
(1,1432)	1:146:A:THR:H	1:146:A:THR:HG23	13	0.12
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB1	11	0.12
(1,1408)	1:131:A:THR:HG22	1:145:A:PHE:HB2	17	0.12
(1,1381)	1:165:A:LYS:HG3	1:165:A:LYS:HA	5	0.12
(1,1356)	1:127:A:LEU:HG	1:127:A:LEU:HA	6	0.12
(1,1355)	1:200:A:ARG:HG3	1:200:A:ARG:HB3	19	0.12
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	8	0.12
(1,1328)	1:115:A:PRO:HG3	1:114:A:GLU:HA	20	0.12
(1,1327)	1:170:A:ARG:HG3	1:186:A:MET:HE2	5	0.12
(1,1315)	1:173:A:LEU:HG	1:183:A:ILE:HA	8	0.12
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	7	0.12
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	10	0.12
(1,1254)	1:196:A:ARG:HB3	1:196:A:ARG:HD3	13	0.12
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	1	0.12
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	17	0.12
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	3	0.12
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	14	0.12
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	13	0.12
(1,1202)	1:134:A:ARG:HB2	1:133:A:TYR:H	14	0.12
(1,1190)	1:192:A:PHE:H	1:191:A:GLN:HG3	5	0.12
(1,1173)	1:153:A:GLU:HG2	1:186:A:MET:HE1	9	0.12
(1,1160)	1:144:A:GLU:HG2	1:136:A:VAL:HG13	9	0.12
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	8	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1156)	1:144:A:GLU:HG2	1:144:A:GLU:H	11	0.12
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	7	0.12
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	14	0.12
(1,1129)	1:154:A:MET:HB3	1:131:A:THR:HG23	11	0.12
(1,1123)	1:188:A:ASN:HB3	1:190:A:ARG:HG3	2	0.12
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	8	0.12
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	14	0.12
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	17	0.12
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	13	0.12
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	14	0.12
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	16	0.12
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	9	0.12
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	10	0.12
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	16	0.12
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	17	0.12
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	18	0.12
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	19	0.12
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	7	0.12
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	12	0.12
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	15	0.12
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	1	0.12
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	20	0.12
(1,1056)	1:126:A:LYS:HE3	1:109:A:ARG:HB3	14	0.12
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	16	0.12
(1,1021)	1:195:A:PHE:HB3	1:113:A:LEU:HB2	12	0.12
(1,963)	1:192:A:PHE:HE1	1:192:A:PHE:HA	19	0.12
(1,956)	1:112:A:ASN:HA	1:196:A:ARG:HA	12	0.12
(1,951)	1:151:A:SER:H	1:150:A:ASN:HA	14	0.12
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD23	10	0.12
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	17	0.12
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	11	0.12
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	16	0.12
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	6	0.12
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	9	0.12
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	20	0.12
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB2	9	0.12
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB3	10	0.12
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB1	14	0.12
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE2	14	0.12
(1,888)	1:135:A:GLN:HA	1:136:A:VAL:HA	13	0.12
(1,869)	1:138:A:LYS:HA	1:146:A:THR:HG22	4	0.12
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	18	0.12
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	18	0.12
(1,819)	1:151:A:SER:HA	1:153:A:GLU:H	19	0.12
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	1	0.12
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	6	0.12
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	17	0.12
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	20	0.12
(1,797)	1:175:A:PHE:HA	1:175:A:PHE:HD1	3	0.12
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	7	0.12
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	9	0.12
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	14	0.12
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	19	0.12
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG22	12	0.12
(1,770)	1:146:A:THR:HA	1:135:A:GLN:HG3	18	0.12
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	5	0.12
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	12	0.12
(1,763)	1:129:A:GLU:HA	1:129:A:GLU:HB3	18	0.12
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	5	0.12
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	8	0.12
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	9	0.12
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	19	0.12
(1,725)	1:158:A:PRO:HA	1:158:A:PRO:HB2	2	0.12
(1,725)	1:158:A:PRO:HA	1:158:A:PRO:HB2	19	0.12
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	12	0.12
(1,700)	1:140:A:THR:HB	1:140:A:THR:HG23	20	0.12
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	1	0.12
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	8	0.12
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	9	0.12
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	11	0.12
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	13	0.12
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	8	0.12
(1,689)	1:189:A:ASN:H	1:188:A:ASN:HB2	14	0.12
(1,685)	1:169:A:VAL:H	1:168:A:GLN:HG3	10	0.12
(1,682)	1:141:A:ARG:H	1:140:A:THR:HA	3	0.12
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	6	0.12
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	9	0.12
(1,680)	1:178:A:ASP:H	1:178:A:ASP:HB2	14	0.12
(1,678)	1:124:A:MET:H	1:120:A:SER:H	10	0.12
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	4	0.12
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	18	0.12
(1,674)	1:114:A:GLU:H	1:117:A:MET:HE2	15	0.12
(1,674)	1:114:A:GLU:H	1:117:A:MET:HE1	17	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	4	0.12
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	7	0.12
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	13	0.12
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	6	0.12
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	9	0.12
(1,630)	1:167:A:GLY:H	1:168:A:GLN:HA	7	0.12
(1,630)	1:167:A:GLY:H	1:168:A:GLN:HA	8	0.12
(1,630)	1:167:A:GLY:H	1:168:A:GLN:HA	16	0.12
(1,630)	1:167:A:GLY:H	1:168:A:GLN:HA	20	0.12
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	7	0.12
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	17	0.12
(1,626)	1:151:A:SER:H	1:150:A:ASN:HB3	16	0.12
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB3	14	0.12
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	13	0.12
(1,580)	1:131:A:THR:H	1:129:A:GLU:HA	4	0.12
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	7	0.12
(1,527)	1:145:A:PHE:H	1:139:A:MET:HB3	13	0.12
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	12	0.12
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	15	0.12
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	16	0.12
(1,501)	1:192:A:PHE:H	1:194:A:PHE:H	4	0.12
(1,462)	1:154:A:MET:H	1:173:A:LEU:HD13	6	0.12
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	5	0.12
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	3	0.12
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	13	0.12
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	15	0.12
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	13	0.12
(1,395)	1:117:A:MET:H	1:115:A:PRO:HA	9	0.12
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	15	0.12
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD11	12	0.12
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	1	0.12
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	19	0.12
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	8	0.12
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	12	0.12
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	1	0.12
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	3	0.12
(1,199)	1:191:A:GLN:H	1:190:A:ARG:HG2	19	0.12
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG23	2	0.12
(1,179)	1:124:A:MET:H	1:119:A:ILE:HG23	20	0.12
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	17	0.12
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	15	0.12
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB2	16	0.12
(1,99)	1:165:A:LYS:H	1:163:A:ASP:HA	20	0.12
(1,81)	1:186:A:MET:H	1:186:A:MET:HE3	2	0.12
(1,78)	1:186:A:MET:H	1:192:A:PHE:HE2	14	0.12
(1,50)	1:195:A:PHE:H	1:195:A:PHE:HD2	15	0.12
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG21	16	0.12
(1,11)	1:119:A:ILE:H	1:179:A:HIS:HB3	18	0.12
(1,9)	1:119:A:ILE:H	1:179:A:HIS:H	2	0.12
(1,1)	1:170:A:ARG:H	1:156:A:ARG:H	2	0.12
(1,1)	1:170:A:ARG:H	1:156:A:ARG:H	10	0.12
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	3	0.11
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	4	0.11
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	17	0.11
(2,215)	1:151:A:SER:HA	1:172:A:ARG:HD3	8	0.11
(2,209)	1:194:A:PHE:HD1	1:194:A:PHE:HB3	8	0.11
(2,209)	1:194:A:PHE:HD2	1:194:A:PHE:HB2	9	0.11
(2,209)	1:194:A:PHE:HD1	1:194:A:PHE:HB3	10	0.11
(2,209)	1:194:A:PHE:HD2	1:194:A:PHE:HB2	16	0.11
(2,199)	1:140:A:THR:HG21	1:138:A:LYS:HD3	7	0.11
(2,179)	1:165:A:LYS:HD3	1:160:A:ASP:HB3	5	0.11
(2,175)	1:123:A:GLU:HB3	1:124:A:MET:HA	7	0.11
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	6	0.11
(2,142)	1:165:A:LYS:HE2	1:160:A:ASP:HB2	19	0.11
(2,141)	1:126:A:LYS:HE3	1:109:A:ARG:HA	11	0.11
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	12	0.11
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	19	0.11
(2,101)	1:171:A:ALA:H	1:154:A:MET:HG3	7	0.11
(2,82)	1:134:A:ARG:H	1:145:A:PHE:H	17	0.11
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	7	0.11
(2,77)	1:194:A:PHE:H	1:194:A:PHE:HB3	8	0.11
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	8	0.11
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	15	0.11
(2,68)	1:159:A:PHE:H	1:158:A:PRO:HG2	20	0.11
(2,67)	1:159:A:PHE:H	1:165:A:LYS:HA	19	0.11
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	10	0.11
(2,16)	1:184:A:VAL:H	1:172:A:ARG:HG3	8	0.11
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD21	1	0.11
(1,1746)	1:128:A:LEU:HD21	1:127:A:LEU:HD22	4	0.11
(1,1725)	1:134:A:ARG:HA	1:133:A:TYR:H	16	0.11
(1,1722)	1:170:A:ARG:HA	1:155:A:ILE:HG13	9	0.11
(1,1710)	1:139:A:MET:HB3	1:139:A:MET:HA	4	0.11
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1706)	1:124:A:MET:HA	1:127:A:LEU:HB3	15	0.11
(1,1683)	1:164:A:SER:H	1:162:A:PRO:HA	16	0.11
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG22	16	0.11
(1,1676)	1:151:A:SER:HB2	1:174:A:THR:HG21	17	0.11
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG23	4	0.11
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG22	18	0.11
(1,1651)	1:145:A:PHE:HE2	1:133:A:TYR:HA	7	0.11
(1,1647)	1:195:A:PHE:HE2	1:171:A:ALA:HB2	6	0.11
(1,1646)	1:195:A:PHE:HE2	1:169:A:VAL:HG11	19	0.11
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	12	0.11
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	4	0.11
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	12	0.11
(1,1602)	1:182:A:THR:HB	1:182:A:THR:HA	2	0.11
(1,1602)	1:182:A:THR:HB	1:182:A:THR:HA	6	0.11
(1,1600)	1:184:A:VAL:H	1:182:A:THR:HB	13	0.11
(1,1600)	1:184:A:VAL:H	1:182:A:THR:HB	17	0.11
(1,1591)	1:183:A:ILE:HG23	1:173:A:LEU:HD13	1	0.11
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB3	1	0.11
(1,1586)	1:127:A:LEU:HA	1:130:A:ALA:HB2	5	0.11
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	12	0.11
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	1	0.11
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	2	0.11
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	5	0.11
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	6	0.11
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	13	0.11
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	18	0.11
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	19	0.11
(1,1518)	1:191:A:GLN:HG2	1:190:A:ARG:HA	15	0.11
(1,1503)	1:122:A:ASN:HB3	1:123:A:GLU:HB2	19	0.11
(1,1491)	1:119:A:ILE:HD11	1:119:A:ILE:HB	14	0.11
(1,1477)	1:186:A:MET:HE3	1:170:A:ARG:HD2	10	0.11
(1,1471)	1:119:A:ILE:HG21	1:175:A:PHE:HE1	13	0.11
(1,1471)	1:119:A:ILE:HG21	1:175:A:PHE:HE1	18	0.11
(1,1466)	1:153:A:GLU:H	1:152:A:ILE:HG23	10	0.11
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB1	1	0.11
(1,1450)	1:176:A:ASP:HB3	1:181:A:ALA:HB2	15	0.11
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	2	0.11
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	4	0.11
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	5	0.11
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	16	0.11
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB2	18	0.11
(1,1449)	1:181:A:ALA:HA	1:181:A:ALA:HB1	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB2	11	0.11
(1,1439)	1:111:A:VAL:H	1:111:A:VAL:HG12	9	0.11
(1,1438)	1:147:A:VAL:HB	1:147:A:VAL:HG21	2	0.11
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB1	6	0.11
(1,1410)	1:171:A:ALA:HB1	1:154:A:MET:HG3	13	0.11
(1,1390)	1:138:A:LYS:HG3	1:138:A:LYS:HA	9	0.11
(1,1370)	1:197:A:LEU:HD13	1:127:A:LEU:HD13	1	0.11
(1,1366)	1:173:A:LEU:HD11	1:171:A:ALA:HB1	1	0.11
(1,1354)	1:113:A:LEU:HG	1:112:A:ASN:HA	20	0.11
(1,1328)	1:115:A:PRO:HG3	1:114:A:GLU:HA	14	0.11
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	19	0.11
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	20	0.11
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	2	0.11
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	19	0.11
(1,1312)	1:126:A:LYS:HD3	1:109:A:ARG:HB3	7	0.11
(1,1312)	1:126:A:LYS:HD3	1:109:A:ARG:HB3	11	0.11
(1,1311)	1:126:A:LYS:HE3	1:126:A:LYS:HD3	18	0.11
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	5	0.11
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	7	0.11
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	9	0.11
(1,1288)	1:168:A:GLN:HB2	1:155:A:ILE:HG21	17	0.11
(1,1270)	1:139:A:MET:HG2	1:155:A:ILE:HD11	7	0.11
(1,1254)	1:196:A:ARG:HB3	1:196:A:ARG:HD3	6	0.11
(1,1254)	1:196:A:ARG:HB3	1:196:A:ARG:HD3	17	0.11
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	7	0.11
(1,1234)	1:171:A:ALA:HA	1:186:A:MET:HG2	16	0.11
(1,1212)	1:135:A:GLN:HG3	1:145:A:PHE:HE1	12	0.11
(1,1208)	1:135:A:GLN:HG2	1:145:A:PHE:HE1	5	0.11
(1,1178)	1:184:A:VAL:HB	1:172:A:ARG:HB3	18	0.11
(1,1158)	1:144:A:GLU:HG2	1:141:A:ARG:HG3	3	0.11
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	3	0.11
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	8	0.11
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	12	0.11
(1,1142)	1:185:A:ASN:H	1:185:A:ASN:HB3	2	0.11
(1,1122)	1:161:A:PHE:HB3	1:162:A:PRO:HG3	3	0.11
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	7	0.11
(1,1114)	1:116:A:ASP:HB3	1:115:A:PRO:HB3	16	0.11
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	9	0.11
(1,1113)	1:116:A:ASP:HB2	1:115:A:PRO:HA	11	0.11
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	4	0.11
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	7	0.11
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	20	0.11
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG22	4	0.11
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	17	0.11
(1,1073)	1:128:A:LEU:H	1:127:A:LEU:HB2	19	0.11
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	3	0.11
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	7	0.11
(1,1070)	1:175:A:PHE:HE2	1:175:A:PHE:HB3	18	0.11
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	10	0.11
(1,1006)	1:152:A:ILE:HB	1:173:A:LEU:HD13	15	0.11
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	1	0.11
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	9	0.11
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	11	0.11
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	14	0.11
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	20	0.11
(1,943)	1:133:A:TYR:HD1	1:128:A:LEU:HD21	8	0.11
(1,932)	1:197:A:LEU:HA	1:197:A:LEU:HB2	4	0.11
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	2	0.11
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB3	5	0.11
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB3	13	0.11
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB3	17	0.11
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB2	18	0.11
(1,907)	1:180:A:LEU:HA	1:180:A:LEU:HD22	8	0.11
(1,907)	1:180:A:LEU:HA	1:180:A:LEU:HD22	18	0.11
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	2	0.11
(1,903)	1:180:A:LEU:HA	1:175:A:PHE:HE1	6	0.11
(1,866)	1:196:A:ARG:HA	1:196:A:ARG:HD3	14	0.11
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG13	5	0.11
(1,859)	1:139:A:MET:HA	1:136:A:VAL:HG12	16	0.11
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	3	0.11
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	8	0.11
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	11	0.11
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	14	0.11
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	18	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	4	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	5	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	6	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	7	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	8	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	11	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	14	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	15	0.11
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	7	0.11
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	13	0.11
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	19	0.11
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	11	0.11
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	15	0.11
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	16	0.11
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG23	11	0.11
(1,770)	1:146:A:THR:HA	1:135:A:GLN:HG3	19	0.11
(1,768)	1:146:A:THR:HA	1:145:A:PHE:HE1	10	0.11
(1,763)	1:129:A:GLU:HA	1:129:A:GLU:HB3	11	0.11
(1,751)	1:184:A:VAL:HA	1:192:A:PHE:HD2	3	0.11
(1,747)	1:119:A:ILE:HA	1:123:A:GLU:HB3	20	0.11
(1,738)	1:111:A:VAL:HA	1:112:A:ASN:HA	6	0.11
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	1	0.11
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	4	0.11
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	17	0.11
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	18	0.11
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	20	0.11
(1,709)	1:125:A:VAL:HA	1:126:A:LYS:HE3	6	0.11
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	15	0.11
(1,698)	1:161:A:PHE:H	1:165:A:LYS:HB2	9	0.11
(1,698)	1:161:A:PHE:H	1:165:A:LYS:HB2	19	0.11
(1,696)	1:147:A:VAL:H	1:135:A:GLN:HA	3	0.11
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	15	0.11
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	16	0.11
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	18	0.11
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	20	0.11
(1,692)	1:196:A:ARG:H	1:196:A:ARG:HD2	8	0.11
(1,684)	1:169:A:VAL:H	1:168:A:GLN:HG2	8	0.11
(1,682)	1:141:A:ARG:H	1:140:A:THR:HA	7	0.11
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	12	0.11
(1,675)	1:120:A:SER:H	1:119:A:ILE:HG13	3	0.11
(1,675)	1:120:A:SER:H	1:119:A:ILE:HG13	8	0.11
(1,675)	1:120:A:SER:H	1:119:A:ILE:HG13	20	0.11
(1,674)	1:114:A:GLU:H	1:117:A:MET:HE2	12	0.11
(1,673)	1:114:A:GLU:H	1:117:A:MET:HG2	8	0.11
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	13	0.11
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	18	0.11
(1,617)	1:146:A:THR:H	1:128:A:LEU:HD22	16	0.11
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB3	2	0.11
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB3	11	0.11
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB2	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB1	15	0.11
(1,615)	1:132:A:GLN:H	1:130:A:ALA:HB2	20	0.11
(1,613)	1:132:A:GLN:H	1:133:A:TYR:HB3	8	0.11
(1,611)	1:132:A:GLN:H	1:144:A:GLU:H	19	0.11
(1,565)	1:163:A:ASP:H	1:162:A:PRO:HB3	7	0.11
(1,536)	1:122:A:ASN:H	1:122:A:ASN:HB3	4	0.11
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	3	0.11
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	7	0.11
(1,508)	1:189:A:ASN:H	1:190:A:ARG:HA	14	0.11
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	2	0.11
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	4	0.11
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	10	0.11
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	15	0.11
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	16	0.11
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	15	0.11
(1,415)	1:159:A:PHE:H	1:159:A:PHE:HE1	9	0.11
(1,415)	1:159:A:PHE:H	1:159:A:PHE:HE2	17	0.11
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	9	0.11
(1,413)	1:159:A:PHE:H	1:158:A:PRO:HB3	10	0.11
(1,408)	1:168:A:GLN:H	1:168:A:GLN:HG2	15	0.11
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	4	0.11
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	8	0.11
(1,401)	1:168:A:GLN:H	1:166:A:GLU:H	16	0.11
(1,392)	1:117:A:MET:H	1:183:A:ILE:HD12	4	0.11
(1,367)	1:133:A:TYR:H	1:130:A:ALA:H	19	0.11
(1,364)	1:152:A:ILE:H	1:152:A:ILE:HD12	3	0.11
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	6	0.11
(1,330)	1:110:A:MET:H	1:110:A:MET:HB2	9	0.11
(1,325)	1:123:A:GLU:H	1:119:A:ILE:HG12	2	0.11
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	11	0.11
(1,312)	1:147:A:VAL:H	1:146:A:THR:HB	13	0.11
(1,307)	1:129:A:GLU:H	1:128:A:LEU:HD12	10	0.11
(1,307)	1:129:A:GLU:H	1:128:A:LEU:HD11	17	0.11
(1,294)	1:129:A:GLU:H	1:145:A:PHE:HZ	15	0.11
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	17	0.11
(1,268)	1:144:A:GLU:H	1:155:A:ILE:HD11	5	0.11
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG21	5	0.11
(1,246)	1:183:A:ILE:H	1:183:A:ILE:HG22	15	0.11
(1,238)	1:138:A:LYS:H	1:138:A:LYS:HG3	5	0.11
(1,228)	1:200:A:ARG:H	1:200:A:ARG:HB3	10	0.11
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	5	0.11
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	14	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	17	0.11
(1,208)	1:160:A:ASP:H	1:161:A:PHE:HD2	5	0.11
(1,190)	1:176:A:ASP:H	1:175:A:PHE:HD2	14	0.11
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	1	0.11
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	8	0.11
(1,167)	1:130:A:ALA:H	1:129:A:GLU:HG3	7	0.11
(1,164)	1:130:A:ALA:H	1:126:A:LYS:HA	10	0.11
(1,164)	1:130:A:ALA:H	1:126:A:LYS:HA	15	0.11
(1,152)	1:127:A:LEU:H	1:127:A:LEU:HG	6	0.11
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	14	0.11
(1,142)	1:157:A:ARG:H	1:156:A:ARG:HG2	6	0.11
(1,125)	1:180:A:LEU:H	1:179:A:HIS:HB3	19	0.11
(1,119)	1:175:A:PHE:H	1:181:A:ALA:HB3	1	0.11
(1,113)	1:185:A:ASN:H	1:190:A:ARG:HB3	11	0.11
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	13	0.11
(1,12)	1:119:A:ILE:H	1:118:A:THR:HG22	3	0.11
(1,11)	1:119:A:ILE:H	1:179:A:HIS:HB3	2	0.11
(1,1)	1:170:A:ARG:H	1:156:A:ARG:H	20	0.11
(2,223)	1:172:A:ARG:HG3	1:172:A:ARG:HD2	1	0.1
(2,209)	1:194:A:PHE:HD2	1:194:A:PHE:HB2	18	0.1
(2,172)	1:170:A:ARG:HB3	1:155:A:ILE:HG12	20	0.1
(2,146)	1:163:A:ASP:HB3	1:161:A:PHE:HB3	12	0.1
(2,146)	1:163:A:ASP:HB2	1:161:A:PHE:HB3	13	0.1
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	4	0.1
(2,123)	1:163:A:ASP:HA	1:163:A:ASP:HB2	9	0.1
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	4	0.1
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	7	0.1
(2,105)	1:115:A:PRO:HA	1:182:A:THR:HA	10	0.1
(2,90)	1:179:A:HIS:H	1:175:A:PHE:HA	3	0.1
(2,62)	1:109:A:ARG:H	1:123:A:GLU:HA	8	0.1
(2,61)	1:133:A:TYR:H	1:129:A:GLU:HB3	4	0.1
(2,61)	1:133:A:TYR:H	1:129:A:GLU:HB3	16	0.1
(2,55)	1:123:A:GLU:H	1:119:A:ILE:HA	6	0.1
(1,1746)	1:128:A:LEU:HD22	1:127:A:LEU:HD23	18	0.1
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG22	3	0.1
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG23	5	0.1
(1,1672)	1:125:A:VAL:HA	1:125:A:VAL:HG21	12	0.1
(1,1671)	1:128:A:LEU:HB3	1:125:A:VAL:HA	1	0.1
(1,1659)	1:156:A:ARG:HG2	1:195:A:PHE:HZ	5	0.1
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	4	0.1
(1,1635)	1:195:A:PHE:HE1	1:195:A:PHE:HB3	20	0.1
(1,1630)	1:146:A:THR:HB	1:146:A:THR:HA	11	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1628)	1:146:A:THR:H	1:146:A:THR:HB	2	0.1
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	2	0.1
(1,1610)	1:145:A:PHE:HD1	1:147:A:VAL:H	5	0.1
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD12	3	0.1
(1,1605)	1:141:A:ARG:HA	1:155:A:ILE:HD11	11	0.1
(1,1602)	1:182:A:THR:HB	1:182:A:THR:HA	4	0.1
(1,1563)	1:126:A:LYS:HG3	1:126:A:LYS:HA	1	0.1
(1,1551)	1:126:A:LYS:H	1:126:A:LYS:HD3	19	0.1
(1,1549)	1:126:A:LYS:HD2	1:125:A:VAL:HG22	9	0.1
(1,1534)	1:154:A:MET:HB3	1:154:A:MET:HG3	3	0.1
(1,1524)	1:166:A:GLU:H	1:166:A:GLU:HB3	16	0.1
(1,1503)	1:122:A:ASN:HB3	1:123:A:GLU:HB2	7	0.1
(1,1503)	1:122:A:ASN:HB3	1:123:A:GLU:HB2	13	0.1
(1,1477)	1:186:A:MET:HE1	1:170:A:ARG:HD2	7	0.1
(1,1474)	1:119:A:ILE:HG22	1:175:A:PHE:HD2	5	0.1
(1,1471)	1:119:A:ILE:HG22	1:175:A:PHE:HE1	12	0.1
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB3	1	0.1
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB1	8	0.1
(1,1448)	1:182:A:THR:H	1:181:A:ALA:HB1	17	0.1
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB3	4	0.1
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB1	14	0.1
(1,1411)	1:171:A:ALA:H	1:171:A:ALA:HB1	17	0.1
(1,1382)	1:127:A:LEU:HD23	1:124:A:MET:HB2	14	0.1
(1,1326)	1:170:A:ARG:HG3	1:170:A:ARG:HD2	20	0.1
(1,1320)	1:170:A:ARG:H	1:170:A:ARG:HG2	7	0.1
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	1	0.1
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	4	0.1
(1,1313)	1:173:A:LEU:HG	1:173:A:LEU:H	15	0.1
(1,1306)	1:152:A:ILE:HG13	1:153:A:GLU:H	13	0.1
(1,1249)	1:199:A:PRO:HB3	1:199:A:PRO:HG2	1	0.1
(1,1195)	1:118:A:THR:H	1:117:A:MET:HB3	2	0.1
(1,1178)	1:184:A:VAL:HB	1:172:A:ARG:HB3	4	0.1
(1,1178)	1:184:A:VAL:HB	1:172:A:ARG:HB3	10	0.1
(1,1166)	1:153:A:GLU:HG3	1:172:A:ARG:HB2	14	0.1
(1,1146)	1:122:A:ASN:HA	1:122:A:ASN:HB3	12	0.1
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	3	0.1
(1,1145)	1:123:A:GLU:H	1:122:A:ASN:HB3	17	0.1
(1,1109)	1:183:A:ILE:HB	1:172:A:ARG:HB3	8	0.1
(1,1096)	1:178:A:ASP:HB2	1:118:A:THR:HG23	6	0.1
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	5	0.1
(1,1090)	1:150:A:ASN:HA	1:150:A:ASN:HB2	12	0.1
(1,1089)	1:133:A:TYR:HB3	1:128:A:LEU:HD22	3	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1083)	1:192:A:PHE:HB3	1:184:A:VAL:HG21	3	0.1
(1,1069)	1:175:A:PHE:H	1:175:A:PHE:HB3	10	0.1
(1,1056)	1:126:A:LYS:HE3	1:109:A:ARG:HB3	12	0.1
(1,1030)	1:190:A:ARG:HD2	1:185:A:ASN:HB3	3	0.1
(1,1007)	1:167:A:GLY:HA2	1:168:A:GLN:HB2	7	0.1
(1,963)	1:192:A:PHE:HE1	1:192:A:PHE:HA	20	0.1
(1,961)	1:188:A:ASN:HA	1:188:A:ASN:HB3	5	0.1
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	12	0.1
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	15	0.1
(1,937)	1:145:A:PHE:HD2	1:131:A:THR:HB	20	0.1
(1,931)	1:164:A:SER:H	1:163:A:ASP:HA	12	0.1
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB1	1	0.1
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB2	3	0.1
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB1	11	0.1
(1,924)	1:130:A:ALA:HA	1:130:A:ALA:HB1	12	0.1
(1,902)	1:180:A:LEU:HA	1:175:A:PHE:HD1	18	0.1
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	2	0.1
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	4	0.1
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	7	0.1
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	10	0.1
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	13	0.1
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	16	0.1
(1,836)	1:117:A:MET:H	1:117:A:MET:HA	20	0.1
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	1	0.1
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	12	0.1
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	19	0.1
(1,835)	1:118:A:THR:H	1:117:A:MET:HA	20	0.1
(1,832)	1:156:A:ARG:HA	1:159:A:PHE:HZ	16	0.1
(1,816)	1:132:A:GLN:HA	1:132:A:GLN:HB3	8	0.1
(1,787)	1:109:A:ARG:H	1:123:A:GLU:HA	14	0.1
(1,784)	1:126:A:LYS:HA	1:128:A:LEU:H	4	0.1
(1,774)	1:136:A:VAL:HA	1:136:A:VAL:HB	1	0.1
(1,774)	1:136:A:VAL:HA	1:136:A:VAL:HB	2	0.1
(1,771)	1:146:A:THR:HA	1:146:A:THR:HG21	4	0.1
(1,770)	1:146:A:THR:HA	1:135:A:GLN:HG3	12	0.1
(1,763)	1:129:A:GLU:HA	1:129:A:GLU:HB3	5	0.1
(1,751)	1:184:A:VAL:HA	1:192:A:PHE:HD2	16	0.1
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	11	0.1
(1,736)	1:140:A:THR:HB	1:140:A:THR:HA	14	0.1
(1,706)	1:131:A:THR:HB	1:159:A:PHE:HZ	6	0.1
(1,705)	1:174:A:THR:H	1:174:A:THR:HB	1	0.1
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	4	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:118:A:THR:H	1:117:A:MET:HB2	19	0.1
(1,682)	1:141:A:ARG:H	1:140:A:THR:HA	1	0.1
(1,682)	1:141:A:ARG:H	1:140:A:THR:HA	11	0.1
(1,682)	1:141:A:ARG:H	1:140:A:THR:HA	15	0.1
(1,677)	1:123:A:GLU:H	1:120:A:SER:H	15	0.1
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	5	0.1
(1,660)	1:182:A:THR:H	1:175:A:PHE:HA	19	0.1
(1,638)	1:143:A:GLY:H	1:159:A:PHE:HZ	5	0.1
(1,630)	1:167:A:GLY:H	1:168:A:GLN:HA	18	0.1
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	3	0.1
(1,629)	1:167:A:GLY:H	1:165:A:LYS:H	6	0.1
(1,583)	1:131:A:THR:H	1:132:A:GLN:HG3	9	0.1
(1,580)	1:131:A:THR:H	1:129:A:GLU:HA	18	0.1
(1,578)	1:179:A:HIS:H	1:119:A:ILE:HG21	8	0.1
(1,545)	1:177:A:GLY:H	1:181:A:ALA:HB2	8	0.1
(1,491)	1:126:A:LYS:H	1:123:A:GLU:HA	8	0.1
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	1	0.1
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	6	0.1
(1,486)	1:126:A:LYS:H	1:124:A:MET:H	9	0.1
(1,448)	1:174:A:THR:H	1:175:A:PHE:H	20	0.1
(1,435)	1:114:A:GLU:H	1:113:A:LEU:HB2	2	0.1
(1,430)	1:114:A:GLU:H	1:115:A:PRO:HA	10	0.1
(1,374)	1:155:A:ILE:H	1:155:A:ILE:HG12	11	0.1
(1,333)	1:124:A:MET:H	1:110:A:MET:H	13	0.1
(1,322)	1:123:A:GLU:H	1:123:A:GLU:HB3	4	0.1
(1,282)	1:136:A:VAL:H	1:145:A:PHE:HE1	4	0.1
(1,260)	1:197:A:LEU:H	1:111:A:VAL:HG22	11	0.1
(1,258)	1:192:A:PHE:H	1:183:A:ILE:HG22	12	0.1
(1,224)	1:128:A:LEU:H	1:124:A:MET:HA	19	0.1
(1,182)	1:166:A:GLU:H	1:166:A:GLU:HG3	19	0.1
(1,170)	1:130:A:ALA:H	1:131:A:THR:HG21	12	0.1
(1,164)	1:130:A:ALA:H	1:126:A:LYS:HA	2	0.1
(1,164)	1:130:A:ALA:H	1:126:A:LYS:HA	14	0.1
(1,145)	1:121:A:LYS:H	1:122:A:ASN:HB3	10	0.1
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	2	0.1
(1,103)	1:112:A:ASN:H	1:114:A:GLU:HB2	15	0.1
(1,81)	1:186:A:MET:H	1:186:A:MET:HE2	7	0.1
(1,81)	1:186:A:MET:H	1:186:A:MET:HE3	16	0.1
(1,81)	1:186:A:MET:H	1:186:A:MET:HE1	19	0.1
(1,78)	1:186:A:MET:H	1:192:A:PHE:HE2	3	0.1

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

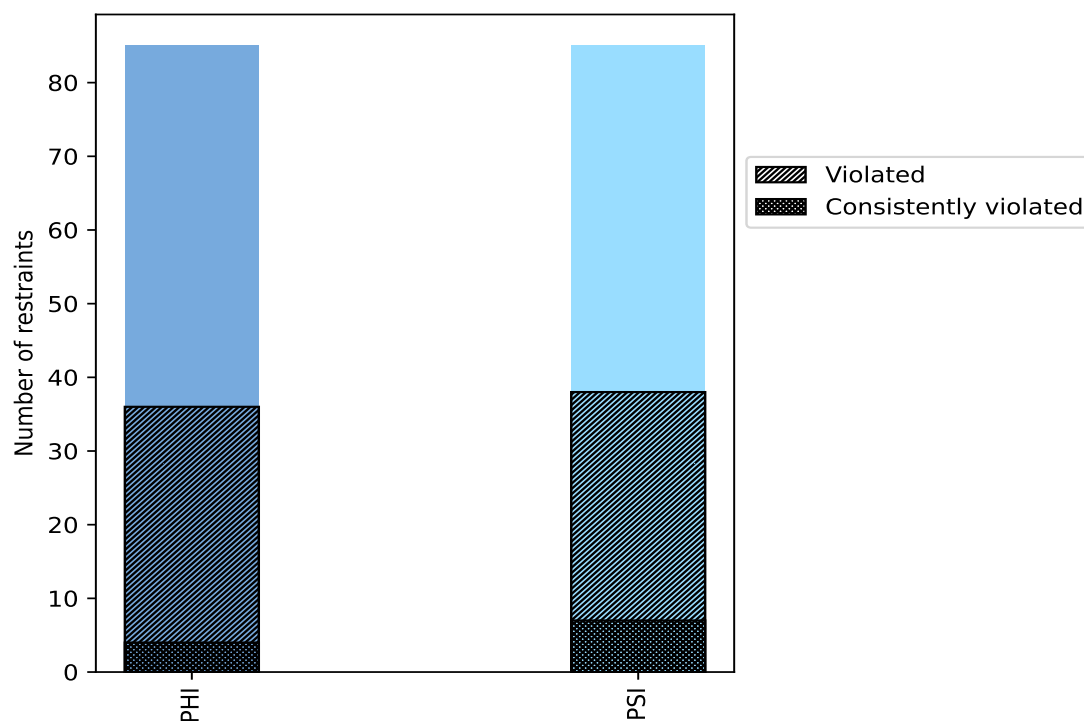
10.1 Summary of dihedral-angle violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	85	50.0	36	42.4	21.2	4	4.7	2.4
PSI	85	50.0	38	44.7	22.4	7	8.2	4.1
Total	170	100.0	74	43.5	43.5	11	6.5	6.5

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

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



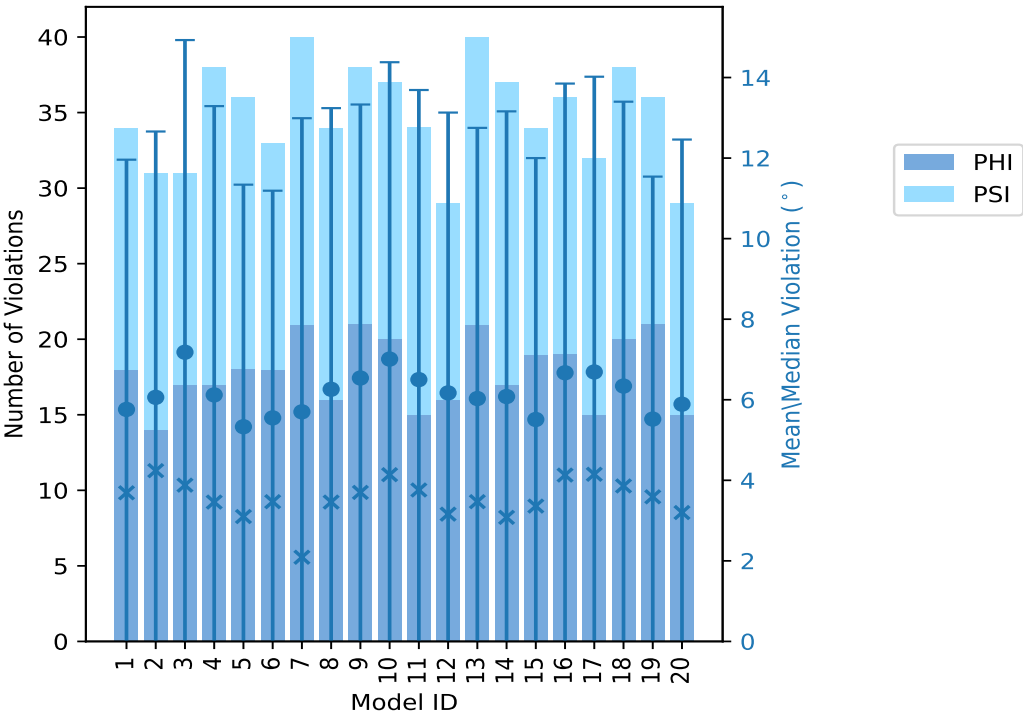
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	18	16	34	5.76	26.11	6.2	3.69
2	14	17	31	6.06	27.97	6.6	4.24
3	17	14	31	7.18	27.56	7.75	3.88
4	17	21	38	6.12	27.58	7.17	3.46
5	18	18	36	5.33	25.61	6.01	3.1
6	18	15	33	5.55	27.83	5.64	3.47
7	21	19	40	5.7	27.46	7.29	2.09
8	16	18	34	6.26	26.13	6.98	3.46
9	21	17	38	6.54	28.73	6.79	3.7
10	20	17	37	7.01	28.41	7.37	4.14
11	15	19	34	6.5	27.54	7.19	3.76
12	16	13	29	6.17	26.08	6.96	3.16
13	21	19	40	6.03	27.58	6.72	3.47
14	17	20	37	6.08	27.02	7.08	3.08
15	19	15	34	5.51	28.77	6.49	3.36
16	19	17	36	6.67	27.48	7.18	4.13
17	15	17	32	6.69	27.73	7.33	4.15
18	20	18	38	6.34	27.92	7.06	3.86
19	21	15	36	5.52	24.21	6.02	3.59
20	15	14	29	5.89	24.85	6.57	3.2

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 ¹	%
3	5	8	1	5.0
4	9	13	2	10.0
3	2	5	3	15.0
1	0	1	4	20.0
1	1	2	5	25.0
1	1	2	6	30.0
3	0	3	7	35.0
2	2	4	8	40.0
1	1	2	9	45.0
0	2	2	10	50.0
2	1	3	11	55.0

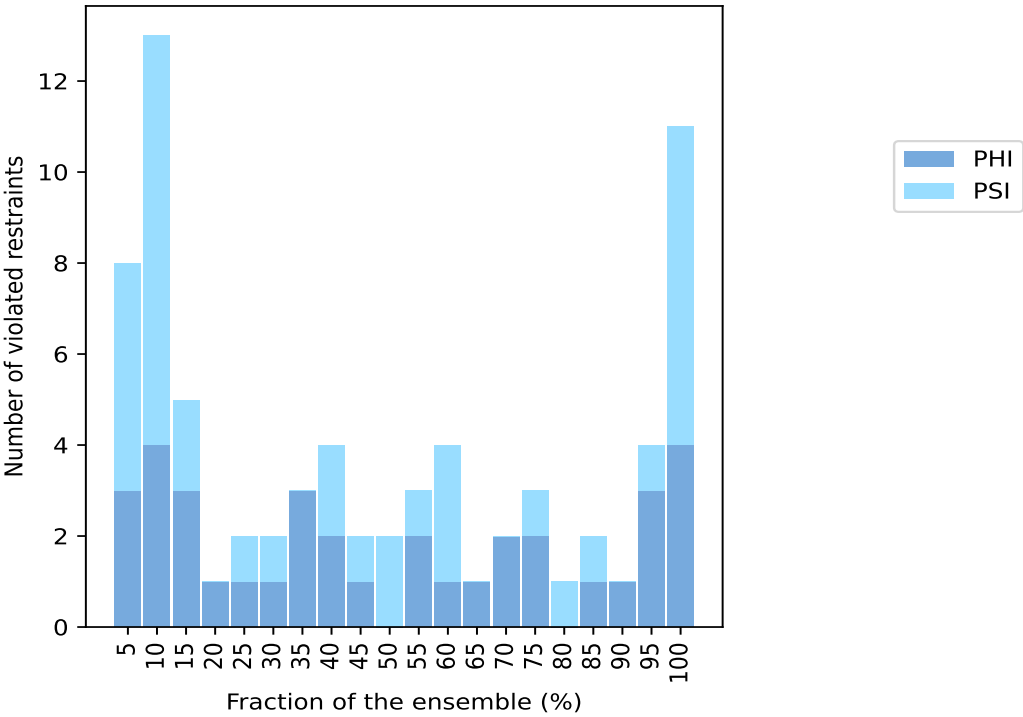
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
1	3	4	12	60.0
1	0	1	13	65.0
2	0	2	14	70.0
2	1	3	15	75.0
0	1	1	16	80.0
1	1	2	17	85.0
1	0	1	18	90.0
3	1	4	19	95.0
4	7	11	20	100.0

¹ Number of models with violations

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

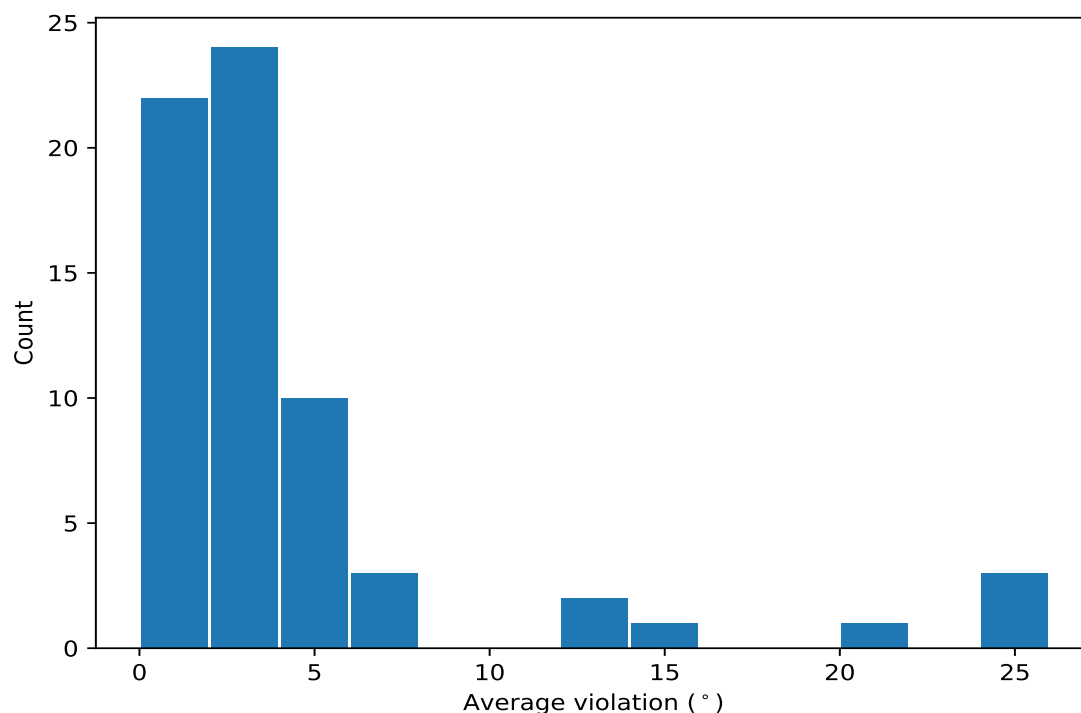


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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 ¹	Mean	SD ²	Median
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	20	25.94	1.55	25.96
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	20	24.91	3.59	27.1
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	20	20.08	2.58	19.26
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	20	14.58	1.59	14.68
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	20	6.96	0.92	6.96
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	20	5.99	2.27	5.4
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	20	5.14	1.48	5.39
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	20	5.08	0.56	5.12
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	20	4.59	0.73	4.66
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	20	3.35	1.24	3.58
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	20	2.55	1.01	2.54
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	19	12.98	4.91	15.99
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	19	5.11	2.09	5.09
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	19	4.96	1.54	5.3
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	19	4.53	1.72	4.01
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	18	2.37	0.76	2.45
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	17	3.39	1.45	3.36
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	17	3.3	0.98	3.26
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	16	1.94	0.64	1.72
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	15	6.37	1.36	6.64

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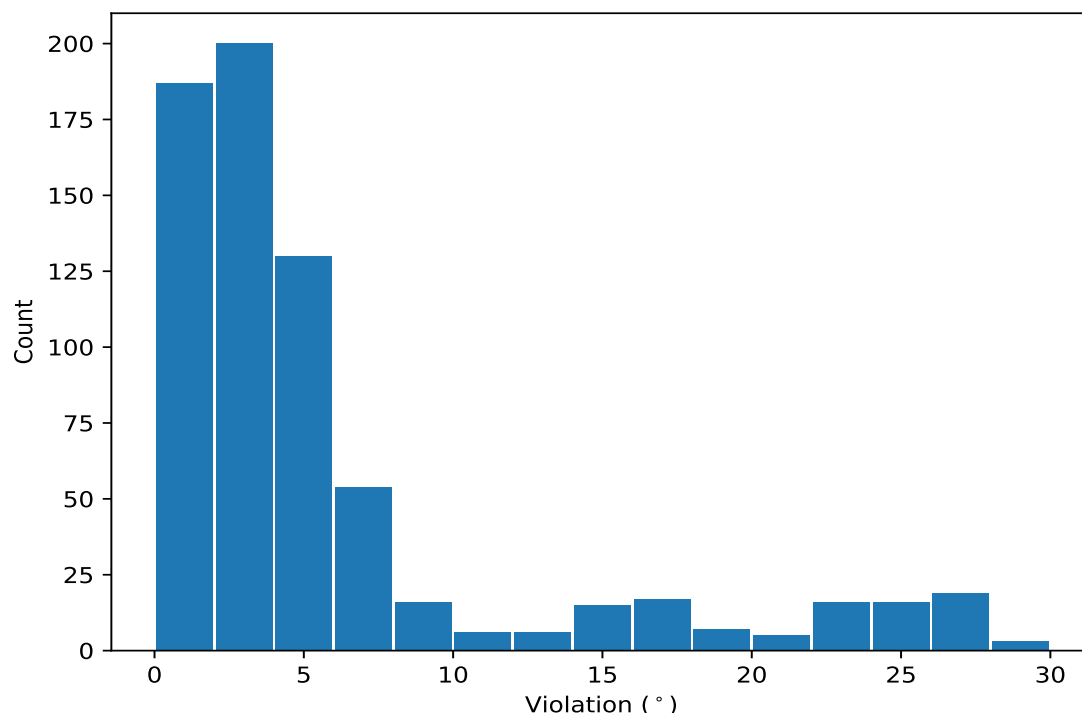
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	15	2.85	0.78	2.59
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	15	2.34	1.19	1.69
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	14	3.31	1.67	3.6
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	14	2.53	0.97	2.28
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	13	2.74	0.8	2.76
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	12	24.23	0.57	24.16
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	12	3.55	1.65	3.75
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	12	1.82	0.52	1.62
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	12	1.57	0.3	1.6
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	11	7.47	3.67	8.31
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	11	3.08	1.06	3.28
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	11	1.38	0.35	1.26
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	10	2.54	1.19	2.39
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	10	2.51	1.16	2.06
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	9	2.84	0.86	2.66
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	9	2.55	1.92	1.58
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	8	2.34	0.8	2.17
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	8	1.58	0.33	1.52
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	8	1.44	0.27	1.4
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	8	1.39	0.16	1.38
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	7	4.51	1.17	4.69
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	7	2.05	0.64	2.0
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	7	1.36	0.17	1.37
(1,133)	1:179:A:HIS:C	1:180:A:LEU:N	1:180:A:LEU:CA	1:180:A:LEU:C	6	1.64	0.62	1.38
(1,76)	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1:148:A:GLN:N	6	1.64	0.55	1.58
(1,84)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:MET:N	5	3.37	1.27	3.78
(1,103)	1:164:A:SER:C	1:165:A:LYS:N	1:165:A:LYS:CA	1:165:A:LYS:C	5	1.58	0.37	1.63
(1,1)	1:107:A:MET:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	4	2.94	1.11	3.13
(1,165)	1:195:A:PHE:C	1:196:A:ARG:N	1:196:A:ARG:CA	1:196:A:ARG:C	3	2.91	0.59	3.23
(1,17)	1:116:A:ASP:C	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	3	1.56	0.21	1.47
(1,77)	1:149:A:ALA:C	1:150:A:ASN:N	1:150:A:ASN:CA	1:150:A:ASN:C	3	1.49	0.38	1.33
(1,106)	1:166:A:GLU:N	1:166:A:GLU:CA	1:166:A:GLU:C	1:167:A:GLY:N	3	1.47	0.16	1.38
(1,30)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	3	1.4	0.16	1.3
(1,91)	1:156:A:ARG:C	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	2	12.6	3.95	12.6
(1,94)	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	1:160:A:ASP:N	2	4.58	0.88	4.58
(1,108)	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	1:168:A:GLN:N	2	4.32	1.51	4.32
(1,12)	1:113:A:LEU:N	1:113:A:LEU:CA	1:113:A:LEU:C	1:114:A:GLU:N	2	2.84	0.78	2.84
(1,118)	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	1:173:A:LEU:N	2	2.3	0.96	2.3
(1,70)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:PHE:N	2	2.12	0.02	2.12
(1,144)	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	1:186:A:MET:N	2	1.83	0.17	1.83
(1,99)	1:162:A:PRO:C	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	2	1.67	0.17	1.67
(1,102)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:LYS:N	2	1.5	0.21	1.5
(1,26)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:ASN:N	2	1.44	0.26	1.44
(1,46)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	2	1.37	0.2	1.37
(1,101)	1:163:A:ASP:C	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	2	1.36	0.34	1.36
(1,33)	1:124:A:MET:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	2	1.2	0.09	1.2

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

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

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

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	15	28.77
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	9	28.73
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	10	28.41
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	2	27.97
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	18	27.92
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	6	27.83
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	17	27.73
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	10	27.67
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	4	27.58
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	13	27.58
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	3	27.56
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	11	27.54
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	16	27.48
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	7	27.46

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	16	27.18
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	14	27.02
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	3	26.84
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	4	26.39
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	8	26.13
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	18	26.12
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	1	26.11
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	12	26.08
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	14	25.85
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	5	25.61
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	11	25.44
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	7	25.42
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	3	25.2
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	10	25.09
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	20	24.85
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	7	24.69
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	8	24.67
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	18	24.63
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	9	24.5
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	15	24.27
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	8	24.23
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	19	24.21
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	13	24.1
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	16	24.03
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	1	23.98
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	17	23.79
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	17	23.75
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	4	23.74
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	13	23.64
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	12	23.55
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	11	23.47
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	19	23.44
(1,64)	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1:141:A:ARG:N	9	23.41
(1,160)	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1:194:A:PHE:N	14	23.39
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	20	23.33
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	12	23.22
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	2	23.21
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	1	22.99
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	19	22.55
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	15	22.14
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	2	21.19
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	20	21.09
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	5	20.66
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	4	20.47
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	7	20.08
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	5	19.94
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	17	19.5
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	3	19.01
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	14	18.89
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	11	18.86
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	13	18.71

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	10	18.09
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	3	17.86
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	10	17.75
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	16	17.72
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	18	17.69
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	10	17.31
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	9	17.19
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	17	17.08
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	7	17.07
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	8	16.99
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	4	16.88
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	14	16.73
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	16	16.62
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	7	16.62
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	2	16.61
(1,91)	1:156:A:ARG:C	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	5	16.56
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	18	16.42
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	9	16.32
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	8	15.99
(1,158)	1:192:A:PHE:N	1:192:A:PHE:CA	1:192:A:PHE:C	1:193:A:GLY:N	6	15.96
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	6	15.69
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	11	15.66
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	3	15.65
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	11	15.52
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	16	15.39
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	12	15.23
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	4	15.12
(1,159)	1:192:A:PHE:C	1:193:A:GLY:N	1:193:A:GLY:CA	1:193:A:GLY:C	6	14.9
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	19	14.73
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	18	14.64
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	13	14.61
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	20	14.18
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	8	14.14
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	14	13.93
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	17	13.51
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	5	13.42
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	13	13.34
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	9	12.62
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	7	12.13
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	20	11.59
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	10	11.49
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	15	11.39
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	12	11.28
(1,65)	1:140:A:THR:C	1:141:A:ARG:N	1:141:A:ARG:CA	1:141:A:ARG:C	1	11.07
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	9	10.43
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	16	9.91
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	20	9.81
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	12	8.9
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	9	8.85
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	19	8.76
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	13	8.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:156:A:ARG:C	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	19	8.65
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	9	8.53
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	10	8.47
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	13	8.45
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	14	8.44
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	9	8.4
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	14	8.31
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	16	8.24
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	13	8.23
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	6	8.22
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	6	7.99
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	18	7.96
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	6	7.89
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	13	7.88
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	4	7.73
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	10	7.72
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1	7.71
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	1	7.67
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	3	7.62
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	6	7.56
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	1	7.5
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	16	7.5
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	2	7.38
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	18	7.37
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	14	7.35
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	12	7.34
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	6	7.31
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	10	7.23
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	11	7.23
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	18	7.19
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	13	7.08
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	4	7.06
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	8	7.04
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	10	7.02
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	18	6.96
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	17	6.89
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	3	6.83
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	15	6.79
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	18	6.79
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	14	6.78
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	3	6.74
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	6	6.69
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	15	6.67
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	15	6.64
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	2	6.63
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	5	6.6
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	3	6.58
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	6	6.55
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	9	6.53
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	9	6.51
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	18	6.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	5	6.4
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	5	6.3
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	16	6.29
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	10	6.26
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	12	6.22
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	4	6.19
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	19	6.17
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	12	6.15
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	11	6.09
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	13	6.04
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	3	6.03
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	8	6.03
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	2	6.01
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	2	5.95
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	10	5.94
(1,92)	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	1:158:A:PRO:N	5	5.94
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	17	5.94
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	11	5.93
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	17	5.92
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	12	5.91
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	20	5.88
(1,108)	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	1:168:A:GLN:N	17	5.83
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	1	5.8
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	17	5.78
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	17	5.78
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	5	5.76
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	9	5.75
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	13	5.73
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	19	5.71
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	1	5.64
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	1	5.63
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	17	5.63
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	16	5.61
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	11	5.6
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	3	5.57
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	1	5.51
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	13	5.5
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	16	5.49
(1,50)	1:133:A:TYR:N	1:133:A:TYR:CA	1:133:A:TYR:C	1:134:A:ARG:N	7	5.49
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	19	5.48
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	7	5.46
(1,94)	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	1:160:A:ASP:N	19	5.46
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	19	5.45
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	7	5.45
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	13	5.44
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	18	5.44
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	1	5.42
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	2	5.39
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	2	5.37
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	16	5.36
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	7	5.31

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	15	5.31
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	7	5.31
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	8	5.3
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	4	5.27
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	8	5.26
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	18	5.25
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	5	5.24
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	15	5.24
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	17	5.22
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	10	5.18
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	6	5.17
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	2	5.16
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	6	5.11
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	14	5.1
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	7	5.09
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	15	5.07
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	19	5.06
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	9	5.03
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	13	5.02
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	8	5.01
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	18	5.01
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	19	5.01
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	10	4.99
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	10	4.97
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	15	4.97
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	11	4.96
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	18	4.93
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	11	4.9
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	9	4.87
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	19	4.87
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	11	4.84
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	14	4.83
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	4	4.82
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	15	4.81
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	2	4.8
(1,84)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:MET:N	17	4.8
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	4	4.74
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	12	4.74
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	8	4.73
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	4	4.73
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	19	4.7
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	15	4.69
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	3	4.68
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	20	4.68
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	11	4.68
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	18	4.67
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	9	4.65
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	7	4.62
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	11	4.57
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	1	4.57
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	12	4.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	16	4.56
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	2	4.53
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	16	4.51
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	19	4.5
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	16	4.49
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	18	4.45
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	8	4.45
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	4	4.43
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	14	4.41
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	2	4.41
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	5	4.37
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	19	4.37
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	2	4.36
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	1	4.34
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	3	4.33
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	10	4.32
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	16	4.32
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	6	4.3
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	1	4.3
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	8	4.3
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	16	4.25
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	4	4.24
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	2	4.24
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	13	4.22
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	10	4.22
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	15	4.22
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	4	4.15
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	17	4.15
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	17	4.15
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	5	4.14
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	10	4.14
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	20	4.1
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	4	4.1
(1,1)	1:107:A:MET:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	13	4.1
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	8	4.08
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	4	4.07
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	6	4.05
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	9	4.05
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	3	4.01
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	7	4.01
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	16	4.01
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	20	3.97
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	9	3.96
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	16	3.93
(1,84)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:MET:N	14	3.93
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	6	3.92
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	5	3.92
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	17	3.92
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	13	3.91
(1,1)	1:107:A:MET:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	15	3.9
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	20	3.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	20	3.88
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	3	3.88
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	18	3.86
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	18	3.85
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	9	3.85
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	16	3.85
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	12	3.84
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	3	3.83
(1,128)	1:177:A:GLY:N	1:177:A:GLY:CA	1:177:A:GLY:C	1:178:A:ASP:N	14	3.82
(1,90)	1:156:A:ARG:N	1:156:A:ARG:CA	1:156:A:ARG:C	1:157:A:ARG:N	5	3.82
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	10	3.82
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	2	3.82
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1	3.79
(1,84)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:MET:N	11	3.78
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	11	3.77
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	1	3.76
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	5	3.75
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	8	3.75
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	11	3.74
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	11	3.74
(1,94)	1:159:A:PHE:N	1:159:A:PHE:CA	1:159:A:PHE:C	1:160:A:ASP:N	5	3.69
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	18	3.67
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	15	3.66
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	14	3.65
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	19	3.64
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1	3.62
(1,12)	1:113:A:LEU:N	1:113:A:LEU:CA	1:113:A:LEU:C	1:114:A:GLU:N	10	3.62
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	1	3.6
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1	3.6
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	4	3.6
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	13	3.58
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	8	3.57
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	9	3.55
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	19	3.54
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	18	3.5
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	3	3.49
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	2	3.49
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	6	3.47
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	15	3.47
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	5	3.46
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	11	3.44
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	1	3.44
(1,165)	1:195:A:PHE:C	1:196:A:ARG:N	1:196:A:ARG:CA	1:196:A:ARG:C	9	3.42
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	12	3.4
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	1	3.37
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	13	3.36
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	3	3.36
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	8	3.36
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	8	3.34
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	10	3.32
(1,84)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:MET:N	20	3.32

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	4	3.32
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	14	3.31
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	7	3.31
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	14	3.28
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	6	3.28
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	3	3.27
(1,118)	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	1:173:A:LEU:N	20	3.26
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	15	3.26
(1,32)	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	1:125:A:VAL:N	8	3.24
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	9	3.24
(1,165)	1:195:A:PHE:C	1:196:A:ARG:N	1:196:A:ARG:CA	1:196:A:ARG:C	10	3.23
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1	3.23
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	9	3.21
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	7	3.21
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	20	3.2
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	10	3.18
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	11	3.18
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	8	3.18
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	15	3.18
(1,85)	1:153:A:GLU:C	1:154:A:MET:N	1:154:A:MET:CA	1:154:A:MET:C	12	3.16
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	4	3.15
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	10	3.12
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	14	3.08
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	19	3.08
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	12	3.06
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	1	3.02
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	7	3.0
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	16	2.97
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	2	2.96
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	8	2.94
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	9	2.94
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	13	2.94
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	15	2.94
(1,133)	1:179:A:HIS:C	1:180:A:LEU:N	1:180:A:LEU:CA	1:180:A:LEU:C	2	2.93
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	10	2.9
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	11	2.9
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	17	2.9
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	16	2.89
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	20	2.88
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	15	2.86
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	2	2.85
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	3	2.83
(1,108)	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	1:168:A:GLN:N	9	2.81
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	9	2.8
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	11	2.79
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	16	2.78
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	15	2.78
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	12	2.77
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	9	2.76
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	13	2.75
(1,126)	1:176:A:ASP:N	1:176:A:ASP:CA	1:176:A:ASP:C	1:177:A:GLY:N	5	2.73

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	9	2.71
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	18	2.71
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	10	2.69
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	14	2.68
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	11	2.66
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	20	2.66
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	8	2.66
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	4	2.66
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	17	2.65
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	12	2.64
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	2	2.63
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	13	2.62
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	4	2.6
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	2	2.59
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	20	2.59
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	5	2.59
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	20	2.57
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	9	2.57
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	7	2.52
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	13	2.51
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	10	2.51
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	6	2.5
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	6	2.48
(1,76)	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1:148:A:GLN:N	11	2.47
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	8	2.46
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	5	2.45
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	17	2.43
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	19	2.43
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	19	2.41
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	4	2.41
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	15	2.41
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	18	2.41
(1,31)	1:123:A:GLU:C	1:124:A:MET:N	1:124:A:MET:CA	1:124:A:MET:C	6	2.4
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	5	2.37
(1,1)	1:107:A:MET:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	19	2.36
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	20	2.35
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	15	2.35
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	5	2.35
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	4	2.33
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	5	2.33
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	14	2.32
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	2	2.31
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	12	2.3
(1,97)	1:160:A:ASP:C	1:161:A:PHE:N	1:161:A:PHE:CA	1:161:A:PHE:C	20	2.27
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	16	2.27
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	19	2.27
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	11	2.26
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	2	2.25
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	14	2.25
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	10	2.25
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	15	2.23

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	17	2.23
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	20	2.23
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	19	2.21
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	20	2.21
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	18	2.19
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	3	2.18
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	3	2.18
(1,103)	1:164:A:SER:C	1:165:A:LYS:N	1:165:A:LYS:CA	1:165:A:LYS:C	10	2.17
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	17	2.17
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	3	2.17
(1,8)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:ASN:N	12	2.16
(1,70)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:PHE:N	13	2.15
(1,135)	1:180:A:LEU:C	1:181:A:ALA:N	1:181:A:ALA:CA	1:181:A:ALA:C	5	2.14
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	1	2.13
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	6	2.12
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	8	2.11
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	8	2.1
(1,70)	1:144:A:GLU:N	1:144:A:GLU:CA	1:144:A:GLU:C	1:145:A:PHE:N	1	2.1
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	7	2.1
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	14	2.09
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	18	2.09
(1,165)	1:195:A:PHE:C	1:196:A:ARG:N	1:196:A:ARG:CA	1:196:A:ARG:C	7	2.08
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	8	2.08
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	3	2.08
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	19	2.08
(1,76)	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1:148:A:GLN:N	19	2.07
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	16	2.06
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	6	2.06
(1,12)	1:113:A:LEU:N	1:113:A:LEU:CA	1:113:A:LEU:C	1:114:A:GLU:N	14	2.06
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	4	2.03
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	20	2.03
(1,77)	1:149:A:ALA:C	1:150:A:ASN:N	1:150:A:ASN:CA	1:150:A:ASN:C	6	2.02
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	16	2.02
(1,144)	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	1:186:A:MET:N	4	2.0
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	16	2.0
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	9	2.0
(1,3)	1:108:A:GLY:C	1:109:A:ARG:N	1:109:A:ARG:CA	1:109:A:ARG:C	6	2.0
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	16	1.99
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	7	1.98
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	14	1.98
(1,76)	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1:148:A:GLN:N	1	1.97
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	14	1.95
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	20	1.94
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	6	1.94
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	3	1.94
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	20	1.94
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	14	1.94
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	15	1.94
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	19	1.93
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	2	1.93
(1,111)	1:168:A:GLN:C	1:169:A:VAL:N	1:169:A:VAL:CA	1:169:A:VAL:C	4	1.92

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	19	1.89
(1,56)	1:136:A:VAL:N	1:136:A:VAL:CA	1:136:A:VAL:C	1:137:A:SER:N	13	1.89
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	16	1.88
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	11	1.88
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	10	1.87
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	1	1.87
(1,133)	1:179:A:HIS:C	1:180:A:LEU:N	1:180:A:LEU:CA	1:180:A:LEU:C	9	1.86
(1,9)	1:111:A:VAL:C	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	15	1.86
(1,99)	1:162:A:PRO:C	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	7	1.84
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	13	1.84
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	12	1.84
(1,17)	1:116:A:ASP:C	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	9	1.84
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	14	1.83
(1,5)	1:109:A:ARG:C	1:110:A:MET:N	1:110:A:MET:CA	1:110:A:MET:C	14	1.82
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	19	1.81
(1,27)	1:121:A:LYS:C	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	7	1.79
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	4	1.78
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	20	1.77
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	18	1.75
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	4	1.73
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	18	1.72
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	7	1.72
(1,102)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:LYS:N	3	1.71
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	10	1.71
(1,106)	1:166:A:GLU:N	1:166:A:GLU:CA	1:166:A:GLU:C	1:167:A:GLY:N	2	1.7
(1,101)	1:163:A:ASP:C	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	5	1.7
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	15	1.7
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	14	1.69
(1,26)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:ASN:N	14	1.69
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	9	1.68
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	17	1.67
(1,144)	1:185:A:ASN:N	1:185:A:ASN:CA	1:185:A:ASN:C	1:186:A:MET:N	8	1.66
(1,103)	1:164:A:SER:C	1:165:A:LYS:N	1:165:A:LYS:CA	1:165:A:LYS:C	1	1.66
(1,161)	1:193:A:GLY:C	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	5	1.65
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	6	1.65
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	18	1.65
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	17	1.64
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	10	1.63
(1,103)	1:164:A:SER:C	1:165:A:LYS:N	1:165:A:LYS:CA	1:165:A:LYS:C	3	1.63
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	4	1.63
(1,30)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	7	1.63
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	5	1.62
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	12	1.62
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	7	1.59
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	15	1.59
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	16	1.59
(1,23)	1:119:A:ILE:C	1:120:A:SER:N	1:120:A:SER:CA	1:120:A:SER:C	7	1.59
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	17	1.58
(1,140)	1:183:A:ILE:N	1:183:A:ILE:CA	1:183:A:ILE:C	1:184:A:VAL:N	13	1.58
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	6	1.58
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	2	1.57

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	11	1.57
(1,46)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	14	1.57
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	4	1.56
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	12	1.56
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	10	1.56
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	6	1.55
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	18	1.55
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	18	1.54
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	18	1.54
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	11	1.54
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	9	1.53
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	5	1.53
(1,88)	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	1:156:A:ARG:N	5	1.53
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	13	1.52
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	16	1.51
(1,99)	1:162:A:PRO:C	1:163:A:ASP:N	1:163:A:ASP:CA	1:163:A:ASP:C	17	1.5
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	6	1.5
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	16	1.49
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	12	1.49
(1,61)	1:138:A:LYS:C	1:139:A:MET:N	1:139:A:MET:CA	1:139:A:MET:C	15	1.49
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	19	1.48
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	8	1.47
(1,17)	1:116:A:ASP:C	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	4	1.47
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	4	1.46
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	5	1.46
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	11	1.44
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	14	1.44
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	7	1.44
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	8	1.44
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	9	1.43
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	4	1.43
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	15	1.42
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	10	1.42
(1,1)	1:107:A:MET:C	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	7	1.42
(1,103)	1:164:A:SER:C	1:165:A:LYS:N	1:165:A:LYS:CA	1:165:A:LYS:C	16	1.41
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	9	1.41
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	4	1.41
(1,133)	1:179:A:HIS:C	1:180:A:LEU:N	1:180:A:LEU:CA	1:180:A:LEU:C	11	1.4
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	7	1.4
(1,71)	1:144:A:GLU:C	1:145:A:PHE:N	1:145:A:PHE:CA	1:145:A:PHE:C	14	1.4
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	14	1.4
(1,29)	1:122:A:ASN:C	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	13	1.4
(1,20)	1:118:A:THR:N	1:118:A:THR:CA	1:118:A:THR:C	1:119:A:ILE:N	5	1.39
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	16	1.38
(1,106)	1:166:A:GLU:N	1:166:A:GLU:CA	1:166:A:GLU:C	1:167:A:GLY:N	17	1.38
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	1	1.37
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1	1.37
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	18	1.37
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	2	1.37
(1,133)	1:179:A:HIS:C	1:180:A:LEU:N	1:180:A:LEU:CA	1:180:A:LEU:C	13	1.36
(1,17)	1:116:A:ASP:C	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	7	1.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,118)	1:172:A:ARG:N	1:172:A:ARG:CA	1:172:A:ARG:C	1:173:A:LEU:N	12	1.34
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	13	1.34
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	19	1.34
(1,106)	1:166:A:GLU:N	1:166:A:GLU:CA	1:166:A:GLU:C	1:167:A:GLY:N	7	1.33
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	8	1.33
(1,77)	1:149:A:ALA:C	1:150:A:ASN:N	1:150:A:ASN:CA	1:150:A:ASN:C	8	1.33
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	13	1.33
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	18	1.32
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	14	1.32
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	3	1.31
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	19	1.31
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	4	1.31
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	7	1.31
(1,33)	1:124:A:MET:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	7	1.3
(1,30)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	6	1.3
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	14	1.29
(1,102)	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	1:165:A:LYS:N	1	1.28
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	1	1.28
(1,30)	1:123:A:GLU:N	1:123:A:GLU:CA	1:123:A:GLU:C	1:124:A:MET:N	9	1.28
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	19	1.28
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	7	1.28
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	13	1.26
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	17	1.26
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	13	1.25
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	15	1.24
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	1	1.24
(1,87)	1:154:A:MET:C	1:155:A:ILE:N	1:155:A:ILE:CA	1:155:A:ILE:C	9	1.24
(1,133)	1:179:A:HIS:C	1:180:A:LEU:N	1:180:A:LEU:CA	1:180:A:LEU:C	7	1.23
(1,164)	1:195:A:PHE:N	1:195:A:PHE:CA	1:195:A:PHE:C	1:196:A:ARG:N	20	1.22
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	18	1.22
(1,76)	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1:148:A:GLN:N	2	1.18
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	19	1.18
(1,26)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:ASN:N	8	1.18
(1,46)	1:131:A:THR:N	1:131:A:THR:CA	1:131:A:THR:C	1:132:A:GLN:N	10	1.17
(1,113)	1:169:A:VAL:C	1:170:A:ARG:N	1:170:A:ARG:CA	1:170:A:ARG:C	12	1.16
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	18	1.16
(1,39)	1:127:A:LEU:C	1:128:A:LEU:N	1:128:A:LEU:CA	1:128:A:LEU:C	17	1.16
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	19	1.15
(1,28)	1:122:A:ASN:N	1:122:A:ASN:CA	1:122:A:ASN:C	1:123:A:GLU:N	17	1.15
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	5	1.15
(1,162)	1:194:A:PHE:N	1:194:A:PHE:CA	1:194:A:PHE:C	1:195:A:PHE:N	8	1.14
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	5	1.14
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	5	1.14
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	7	1.14
(1,53)	1:134:A:ARG:C	1:135:A:GLN:N	1:135:A:GLN:CA	1:135:A:GLN:C	11	1.14
(1,63)	1:139:A:MET:C	1:140:A:THR:N	1:140:A:THR:CA	1:140:A:THR:C	12	1.13
(1,77)	1:149:A:ALA:C	1:150:A:ASN:N	1:150:A:ASN:CA	1:150:A:ASN:C	3	1.12
(1,76)	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1:148:A:GLN:N	7	1.12
(1,59)	1:137:A:SER:C	1:138:A:LYS:N	1:138:A:LYS:CA	1:138:A:LYS:C	17	1.12
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	3	1.12
(1,10)	1:112:A:ASN:N	1:112:A:ASN:CA	1:112:A:ASN:C	1:113:A:LEU:N	20	1.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,33)	1:124:A:MET:C	1:125:A:VAL:N	1:125:A:VAL:CA	1:125:A:VAL:C	18	1.11
(1,150)	1:188:A:ASN:N	1:188:A:ASN:CA	1:188:A:ASN:C	1:189:A:ASN:N	6	1.09
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	11	1.09
(1,107)	1:166:A:GLU:C	1:167:A:GLY:N	1:167:A:GLY:CA	1:167:A:GLY:C	11	1.09
(1,83)	1:152:A:ILE:C	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	12	1.09
(1,2)	1:108:A:GLY:N	1:108:A:GLY:CA	1:108:A:GLY:C	1:109:A:ARG:N	15	1.09
(1,75)	1:146:A:THR:C	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	7	1.08
(1,168)	1:197:A:LEU:N	1:197:A:LEU:CA	1:197:A:LEU:C	1:198:A:ASP:N	10	1.07
(1,133)	1:179:A:HIS:C	1:180:A:LEU:N	1:180:A:LEU:CA	1:180:A:LEU:C	4	1.07
(1,96)	1:160:A:ASP:N	1:160:A:ASP:CA	1:160:A:ASP:C	1:161:A:PHE:N	2	1.07
(1,74)	1:146:A:THR:N	1:146:A:THR:CA	1:146:A:THR:C	1:147:A:VAL:N	12	1.07
(1,146)	1:186:A:MET:N	1:186:A:MET:CA	1:186:A:MET:C	1:187:A:GLU:N	13	1.06
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	16	1.05
(1,18)	1:117:A:MET:N	1:117:A:MET:CA	1:117:A:MET:C	1:118:A:THR:N	6	1.05
(1,101)	1:163:A:ASP:C	1:164:A:SER:N	1:164:A:SER:CA	1:164:A:SER:C	13	1.03
(1,76)	1:147:A:VAL:N	1:147:A:VAL:CA	1:147:A:VAL:C	1:148:A:GLN:N	15	1.03
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	5	1.03
(1,57)	1:136:A:VAL:C	1:137:A:SER:N	1:137:A:SER:CA	1:137:A:SER:C	13	1.03
(1,103)	1:164:A:SER:C	1:165:A:LYS:N	1:165:A:LYS:CA	1:165:A:LYS:C	18	1.02
(1,84)	1:153:A:GLU:N	1:153:A:GLU:CA	1:153:A:GLU:C	1:154:A:MET:N	13	1.01